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EXAM I COURSE
TFY4310 MOLECULAR BIOPHYSICS

Suggested solutions

Friday, 15 December 2017
Time: kl. 09.00 - 13.00

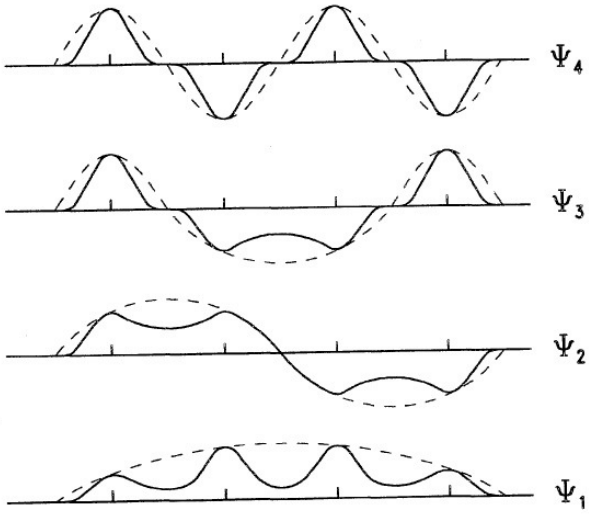
All questions have the same weight. None of the questions require lengthy answers so answer as precisely and concisely as possible. Good luck!

Exercise 1.

Justify **six** (6) of the following (correct) sentences:

1. Contrarily to the molecular orbital theory, the valence bond theory fails to describe the delocalization of electrons in conjugated molecules.

   Answer: One of the main differences between the valence bond theory and the molecular orbital (MO) theory is that the first describes a covalent bond as the overlap of atomic bonds, and fundamentally restricting the spatial location of the electrons in these overlap regions of the molecule. For the MO theory, on the other hand, a molecule us viewed as a collection of nucleic surrounded by delocalized MOs that are calculated has linear combination of the atomic orbitals.



If we take the example of a conjugated molecule with 4 carbons, H_2C=CH–CH=CH_2, and combining the 4 p atomic orbitals that form the π molecular orbitals, it can be seen that from the scheme above that the wavefunction with the lowest energy does not posses a node, meaning that the electrons in that orbital are delocalized throughout the entire molecule.

2. Water has a tetrahedrical structure.

   Answer: The oxygen in water is sp^3 hybridized, thus, it possessed 4 bonding orbitals with about 109° between them, giving the tetrahedrical shape. Two of the binding orbitals get linearly combined with 1s orbital of the hydrogens to form sigma bonds, the other two binding orbitals are filled with the 4 left valency electrons of the oxygen and form non-binding orbitals.

3. The critical micellar concentration of a cationic surfactant decreases when the hydrocarbon tail is increased.

   Answer: The critical micellar concentration is defined as the surfactant concentration at which the surfactant aggregates into micelles in solution. The formation of micelles occur to minimize the contact between the hydrocarbon tails of the surfactants, which are apolar and form no H-bonds, and water. The hydrocarbon tails are then said to be hydrophobic. Above a certain concentration the surfactant molecules are pushed towards each other to decrease the hydrophobic area exposed to water, and releasing thus some of the water molecules that were organized around the individual surfactant tails. The larger the hydrophobic hydrocarbon groups the stronger this effect will be and thus, surfactants with longer chains lengths have a lower critical micellar concentration.

4. If a polymer is moved from an ideal solvent to a good solvent, the overlap concentration decreases and scales with $n^{-4/5}$.

   Answer: In an ideal solvent the interactions between the polymer segments and the solvent is equivalent to the interactions between the polymer segments. In a good solvent, the interactions between the polymer and the solvents is preferred and so the polymer chain will expand, in other to increase the contact with the solvent. If the polymer adopts a more stretched conformation the $c^\star$ will decrease, as lower concentrations are required for the polymers to start overlapping.

   Regarding the scaling, in a good solvent the root-mean-square (rms) of the end-to-end distance scales 3/5, as so does the rms of the radius of gyration, as given by the equation in the end of the exam:

$$\left\langle R_{\mathrm{ee}}^2 \right\rangle^{1/2} \sim Q n^{3/5}$$
$$\left\langle R_{\mathrm{G}}^2 \right\rangle^{1/2} \sim Q n^{3/5}$$

   Knowing that

$$C^\star = \frac{3N_p}{4\pi N_{\mathrm{Av}}} \frac{10^{-3}}{R_G^3} \sim \frac{n}{R_G^3} \ ,$$

   assuming that $N_p \approx n$, for long chains. We get them,

$$C^\star \sim \frac{n}{n^{9/5}} \sim n^{-4/5} \ .$$

5. In transient electric birefringence, an important part of the experimental set-up consists in the application of a square electric pulse.

Answer: With transient electric birefringence one can measure the rotational diffusion coefficient, D_R, of long (and somewhat stiff) macromolecules. Macromolecules in solution have a random orientation which makes it very challenging to measure their D_R. In order to measure it, it becomes necessary to align the molecules in solution. This can be done using electric field, since all biological macromolecules have dipolar moments, and providing that the macromolecules are sufficiently rigid. The applied electric field should be sufficiently strong and long to align the molecules in solution, but not enough to induce their translational diffusion. When the electric field is switched off, the molecules relax to a random orientation in the sample, which is measured in terms of changes in birefringence, and used to calculated D_R. A square electric field is thus the best for this application.

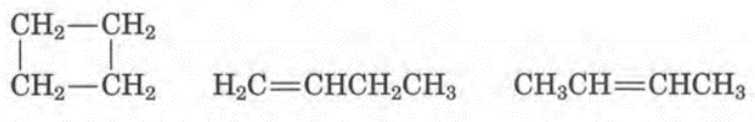
6. In Raman IR spectroscopy, bands corresponding to C=O stretching vibrations appear at larger wavenumbers (shorter wavelengths) than those of C–O.

   Answer: The strength of the covalent bond is larger in the C=O group than in the C–O group, and so a larger energy is required to excite the vibrational mode of the C=O bond. Since the energy is inversely proportional to the wavelength, the band corresponding to C=O stretching vibration will appear at shorter wavelengths or at larger wavenumbers.

7. Parts per million (ppm) in relation to a widely used reference sample (chemical shift), is a convenient way of expressing the frequency in nuclear magnetic resonance (NMR) spectra.

   Answer: In NMR spectroscopy, one excites the nuclear magnetic spins of nuclei that have an angular momentum different than zero. The excitation occurs upon the absorption of an irradiated radio-frequency signal that matches the energy difference between the spin levels, the Larmor frequency. This is detected and the resulting information is plotted as intensities (of adsorbed radiation) versus the frequency of the transitions. Now, the Larmor frequency depends on the strength of the magnetic flux density, B_0, that is initially applied to orient the spins, and so using instruments with different B_0 will result in peaks at different Larmor frequencies, even if the studied molecule is the same. In order to normalize the results, and be able to compare spectra of the same molecules taken in instruments with different magnets, it is common to express the frequencies using the chemical shift instead. In this case, the peaks are collected and presented as a shift or deviation (expressed in ppm) from a known and used reference molecule, such as TMS.

8. ^{1}H-NMR is a convenient method to identify and distinguish the structure of the following (isomeric) compounds of formula C_4H_8:



   Answer: Although these compounds have the same number of protons, it is possible to use ^{1}H-NMR to distinguish them. All protons is the cyclic molecule are said to be equivalent, that is, they all experience the same chemical environment. As such, the NMR spectra of the molecule will only show one peak with an intensity corresponding

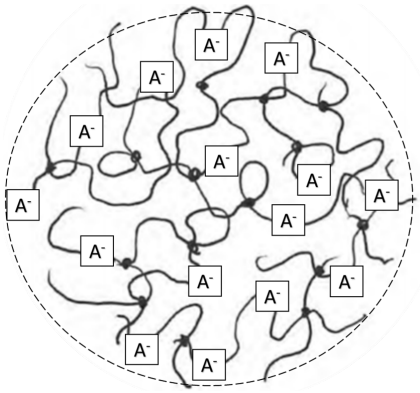
to all 8 protons. The second compound has 5 different types of protons (the two protons of the CH_2 group feel different chemical environments because of the double bond), and so will show 5 peaks in the NMR spectrum. The third compound is symmetry and has two different types of protons, thus the NMR spectrum of this compound will show two peaks, one with relative intensity 3 (a doublet) and the other with a relative intensity of 1 (a quadruplet).

9. Small angle neutron scattering (SANS) is a powerful tool to study the structure of DNA-lipid complexes, lipoplexes, currently studied for the purpose of gene delivery to cells.

   Answer: We can only observe scattering if there is a source of "contrast" in the sample. In SANS the contrast is given by the scattering length density which varies with the nuclei composition. As seen in the table in the end of the exam, the scattering density of water and deuterated water are quite different, and the scattering density of the major classes of biological molecules are also different and conveniently placed between the two solvent. This means that by choosing different H_2O to D_2O compositions one can selectively match the contrast of, say, the lipids to the solvent and make them "transparent". In this case one would be able to obtain the form and or structure factors of the nucleic acid only, and vice-versa.

Exercise 2.

1. The figure below shows a scheme of an anionic hydrogel immersed in aqueous solution. Is the scheme complete? If not, identify the missing item(s). Describe qualitatively



   the molecular aspects of the process leading to an increase in the hydrogel swelling volume due to the anionic character of the network.

   Answer: The counterions of the network are missing from the representation.

   Since the network is negatively charged, the oppositely charged counterions will be attracted into the network. This leads to a swelling of the gel as the water rushes into the gel particle to equalize the concentration of ions inside and outside of the gel.

2. Does the swelling volume of the hydrogel change when the salt concentration of the aqueous solution is increased? Justify.

   Answer: If the salt concentration outside the gel is increased, the difference between the small ions inside of the gel (due to the charged polymer network) and the small

ions outside the gel (due to the addition of salt), is reduced. The gel will de-swell in this case.

3. The equation

$$\Delta G = k_{\mathrm{B}}T\left[(n_1 \ln v_1 + \chi n_1 v_2) + \frac{3}{2}n\left(v_2^{-2/3} - 1 + \frac{1}{3}\ln v_2\right)\right].$$

can be used in conjunction with the mathematical description of the swelling of hydrogels. Describe the underlying molecular mechanisms that give rise to the two terms of the equation. Can this equation be used to describe the swelling of the represented hydrogel? Justify.

Answer: The first term is due to the mixing of the polymer and the solvent. It includes the enthalpic part, where χ is the Flory parameter that described the quality of the solvent, that is, if the polymer will mix well with the solvent or not, and the mixing entropy of the system, which is always favorable. n_1 refers to the number of solvent molecules and, v_1 and v_2 refer to the volume fraction of the solvent and polymer, respectively. The second term refers to the elastic contribution which accounts for the fact that since the polymers are crosslinked, there is a limit in how much the network can swell. Here n refers to the number of polymer chain segments in the gel, that is, it is a measure of the crosslinking.

In order to describe the anionic network represented in the figure, one would have to add the ionic term, which is simply described by the difference in the concentration of ions in the inside and outside of the network.

Exercise 3.

1. You are given a protein solution with a known extinction coefficient (ε). While measuring the absorption of the sample, to calculate the concentration of the protein solution, you realize that the obtained value is too high and out of the so-called linear regime of the instrument.

   What is it meant with the linear regime and why is this a problem?

   Answer: A common procedure to measure the concentration of a protein solution is to apply the Beer-Lambert law: $A(\lambda) = \varepsilon(\lambda)cl$, where A is the absorption, ε is the extinction coefficient of the protein, c the protein concentration, and l, the sample optical path. This, of course, assumes that the absorption of the sample is directly proportional to the number of proteins in solution and hence the protein concentration. If the measured absorbance is too high, there may be deviations from linearity due to instrumental limitations. In this case, the Beer-Lambert law is no longer applicable.

2. Describe two procedures to reduce the value of the measured absorption by 5?

   Answer: Looking again the Beer-Lambert law,

$$A(\lambda) = \varepsilon(\lambda)cl\ ,$$

   we can conclude that it is possible to reduce the value of the absorption by 5 by, (i) diluting the sample 5 times or (ii) reducing the optical path length (thickness of the cuvette) by 5.

   Note: A large protein concentration can also lead to changes in the way the protein absorb light due to intermolecular interactions and, for example, conformational

changes. In these cases, the decrease in the optical path length would not help, as the high concentration effect would still be present. One would have to dilute the protein sample.

3. The radius of gyration can be easily calculated using molecular simulations but it is also possible to determine it experimentally. Describe an experimental procedure to measure the radius of gyration of the protein. Mention the used technique and any approximation that may be needed.

   Answer: There are a few different ways to experimentally measure the radius of gyration of a protein. One can use a small angle scattering technique, and providing that one can measure small angles ($q \to 0$) with some accuracy, one can use the Guinier approximation:

$$\ln\left(\frac{I_{\rm s}(q)}{I_0}\right) = -\frac{1}{3}q^2 R_G^2 \ .$$

   which is valid for small q values. Here we could measure the intensity of the scattered radiation for different (and sufficiently small) values of q and plot the $\ln\left(\frac{I_{\rm s}(q)}{I_0}\right)$ as a function of q^2. The data should give a straight line with a slope equal to $-1/3R_G^2$.

   One can also use static light scattering and construct a Zimm plot, based on

$$\frac{\kappa c}{R_\theta} \ = \ \frac{1}{M}\left[1 + \frac{16\pi^2}{3\lambda^2}R_{\rm G}^2 \sin^2\frac{\theta}{2}\right] \ \cdot [1 + 2B_2 c]$$

   Here, one prepares samples with different protein concentration and measures the intensity of the scattered light at different angles. Knowing the geometry of the light scattering setup, the value of c and κ, one can plot all data as $\frac{\kappa c}{R_\theta}$ versus $\sin^2\frac{\theta}{2} + c$. Extrapolating the data to $c = 0$ one gets:

$$\lim_{c\to 0}\frac{\kappa c}{R_\theta} \ = \ \frac{1}{M}\left[1 + \frac{16\pi^2}{3\lambda^2}R_{\rm G}^2 \sin^2\frac{\theta}{2}\right] \ ,$$

   that is, the slope of the straight line is equal to $\frac{16\pi^2 M}{3\lambda^2}R_{\rm G}^2$.

   M can be determined by extrapolating to both $\theta \to 0$ and $c \to 0$.

4. Describe the Metropolis algorithm, very commonly used in Monte Carlo simulations.

   Answer: The Metropolis algorithm is commonly used in Monte Carlo simulations to decrease the simulation time by probing the configurational space more efficiently. Instead of generating N completely random configurations and hope that those N configurations are enough to give a good description of the system, the Metropolis algorithm is based on going from one configuration to the next by randomly moving one particle. When a particle is moved the difference in energy between the new configuration and the old configuration is calculated according to: $\Delta E = E_{\rm new} - E_{\rm old}$. If $\Delta E < 0$ the move is accepted and the new configuration is saved and taken as the basis for a new move. If $\Delta E > 0$, that is, the move leads to an increase in the energy, this move still has some probability of being accepted. A random number between 0 and 1 is generated and compared with the Boltzmann weight. If $i_{\rm random} < \exp(-\Delta E/k_{\rm B}T)$, the move is accepted, otherwise it is rejected and the system returns to the old configuration, while counting it to the ensemble averages. Each particle is attempted to move as many times as desired.

Exercise 4.

T4 is a large virus with an approximately spherical capsid which contains DNA. These spherical particles have the following characteristics: $s = 1025$ S ($1\ \text{S} = 10^{-13}$ s), and partial specific volume $\overline{V}_1^{(S)} = 0.605\ \text{cm}^3/\text{g}$. Dynamic light scattering experiments were performed of the virus in water at 20 °C, using light with a wavelength of 500 nm and a scattering angle of 40°. Plotting the results as $\ln[g^{(2)}(q,\tau) - 1]$ as a function of τ gives a straight line with a slope equal to $-532.00\ \text{s}^{-1}$.

1. Calculate the translational diffusion coefficient of the capsid.

   Answer: From the equations

   $$g^{(2)}(q,\tau) = 1 + [g^{(1)}(q,\tau)]^2 \qquad \text{and} \qquad g^{(1)}(q,\tau) = \exp(-q^2 D_T \tau)$$

   One can deduce the equation

   $$\ln\left[g^{(2)}(\tau) - 1\right] = -2q^2 D_T \tau.$$

   Since we are given the slope of the graph of $\ln[g^{(2)}(q,\tau) - 1]$ as a function of τ, we can calculate the translational diffusion from the relation:

   $$\text{slope} = -2q^2 D_T\ .$$

   We need to calculate the scattering vector using $q = \frac{4\pi}{\lambda}\sin(\frac{\theta}{2})$, where λ is the wavelength of light in the solution and θ is the angle between the incident light and the measured scattered light (detector):

   $$q^2 = \left(\frac{4\pi}{\lambda}\sin\left(\frac{\theta}{2}\right)\right)^2 = \left(\frac{4\pi}{500\times 10^{-9}[\text{m}]}\sin\left(\frac{40}{2}\right)\right)^2 = 7.389\times 10^{13}\ \text{m}^{-2}\ .$$

   Finally, we can write

   $$D_T = -\frac{\text{slope}}{2q^2} = -\frac{-532.00\ [\text{s}^{-1}]}{2\cdot 7.389\times 10^{13}\ [\text{m}^{-2}]} = 3.60\times 10^{-12}\ \text{m}^2/\text{s}\ .$$

2. Calculate the frictional coefficient of the capsid.

   Answer: To calculate the friction coefficient we use simply,

   $$f = \frac{k_B T}{D_T} = 1.123\times 10^{-9}\,\text{Kg/s}.$$

3. What is the molecular weight of the capsid?

   Answer: To calculate the molecular weight of the capsid we use the Svedberg equation:

   $$s = \frac{M_1\,(1 - \overline{V}_1^{(S)}\rho)}{N_{\text{Av}} f} \quad \Rightarrow \quad M_1 = \frac{s N_{\text{Av}} f}{(1 - \overline{V}_1^{(S)}\rho)} = 181,030\,\text{Kg/mol}.$$

   Note: This is a very large particle, as can be deduced from the large sedimentation coefficient. By curiosity, the DNA inside the protein capsid of the virus has around 166,000 base pairs. A base pair has an average molecular weight of 660 g/mol, which gives a DNA molecular weight inside the capsid of 109,560 Kg/mol.

4. Calculate the volume of the non-hydrated capsid.

   Answer: To calculate the volume of the non-hydrated virus we take the definition of specific volume given in the end of the exam and assume that $V_1^{(S)} = \overline{V}_1^{(S)}$, that is, we assume that the volume of the water plus the virus is the same as the sum of the two volume, which is a good assumption in diluted solutions of viruses. Rearranging:

   $$v = \frac{M_1 \overline{V}_1^{(S)}}{N_A} = 1.819\times 10^{-16}\text{cm}^3$$

5. Calculate the hydrodynamic volume of the capsid.

   Answer: To calculate the hydrodynamic volume of the virus capsid, we can take the Stokes formula for the translational friction coefficient:

$$f = 6\pi\eta R_H \quad \Rightarrow \quad R_H = \frac{f}{6\pi\eta} = 5.958 \times 10^{-6}\,\text{cm}.$$

   Therefore, the hydrated volume is equal to:

$$V_H = \frac{4}{3}\pi R_H^3 = 8.859 \times 10^{-16}\,\text{cm}^3.$$

   The hydrodynamic volume is larger than the non-hydrated volume as would be expected.

6. What is the hydration fraction of the virus capsid (g of water per g of virus)?

   Answer: The volume of water per virus is $(8.859 - 1.819) \times 10^{-16} = 7.040 \times 10^{-16}\,\text{cm}^3$. Because the density of water is 1.02 g/cm^3, we have 7.181×10^{-16} g of water hydrating a virus capsid. We can convert this to grams of water hydrating each gram of virus by considering the density of the virus capsid: 1/0.605 g/cm^3. That is, 1 virus with a "dry" volume of 1.819 $\times 10^{-16}$ cm^3 has 1.819 $\times 10^{-16}$ /0.605 = 3.007 $\times 10^{-16}$ g/virus.

   The hydration fraction is thus:

$$\frac{7.181 \times 10^{-16}}{3.007 \times 10^{-16}} = 2.39\,\text{g water/g virus}.$$

7. The shell of the virus (capsid) is composed of proteins that possess positively charged aminoacids towards the interior of the virus, and non-polar aminoacids on the edges of the proteins that face the other proteins in the capsid. Knowing that the proteins of the capsid do not assemble in the absence of the DNA, discuss the main intermolecular interactions that contribute to the assembly of the virus.

Answer: Coulomb interactions between the negatively charged DNA and the positively charged aminoacids inside the capsid are fundamental for the assembly of the virus capsid. In addition, the non-polar aminoacids in the edges of the protein capsid assure the correct self-assembly of the proteins into the capsid.

The following formulas and data may or may not be of use in answering the preceding questions. You do not need to derive any of the formulas but all parameters must be defined, if used.

Electron charge: $e = 1.602 \times 10^{-19}$ C

Avogadro constant: $N_{\text{Av}} = 6.022 \times 10^{23}$ mol^{-1}

Boltzmann constant: $k_{\text{B}} = 1.380 \times 10^{-23}$ m^2 kg s^{-2} K^{-1}, J K^{-1}

Permittivity in vacuum: $\varepsilon_0 = 8.854 \times 10^{-12}$ C^2 J^{-1} m^{-1}

Properties of water at 20 °C:

$\varepsilon = 78.4; \quad \eta = 0.01$ g cm^{-1}s^{-1}; $\quad \rho = 1.02$ g/cm^3

Temperature: $[\mathrm{K}] = [^\circ\mathrm{C}] + 273.15$

Atomic orbitals: H: $1s^1$; C: [He]$2s^2 2p_x^1 2p_y^1$; N: [He]$2s^2 2p_x^1 2p_y^1 2p_z^1$; O: [He]$2s^2 2p_x^2 2p_y^1 2p_z^1$

Atomic weights: $\mathrm{A}_r(\mathrm{H}) = 1.0$; $\mathrm{A}_r(\mathrm{C}) = 12.0$

Thermodynamics $G = H - TS \qquad A = U - TS \qquad \vec{F} = -\vec{\nabla} A$

$S = k_\mathrm{B} \ln W$

Coulomb potential $V(r) = \dfrac{z_1 z_2\, e^2}{4\pi\epsilon_0 \epsilon r}$

Screened Coulomb potential

$$V(r) = \frac{z_1 z_2\, e^2}{4\pi\epsilon_0 \epsilon r} \exp\left(-\frac{r}{\lambda_\mathrm{D}}\right)$$

Debye screening length $\lambda_\mathrm{D}^2 = \dfrac{\epsilon k_\mathrm{B} T}{\sum_i (eZ_i)^2\, n_{i\infty}}$

Density of ions at a charged surface $\rho_\mathrm{s} = \rho_0 + \dfrac{\sigma^2}{2\epsilon\epsilon_0 k_\mathrm{B} T}$

Statistical chain molecules $\left\langle R_\mathrm{ee}^2 \right\rangle = C_n Q^2 n$

$$C_n = 1 \; ; \; C_n = \frac{1-\cos\theta}{1+\cos\theta} \; ; \; C_n = \frac{1-\cos\theta}{1+\cos\theta}\frac{1+\langle\cos\phi\rangle}{1-\langle\cos\phi\rangle}$$

Scaling $\left\langle R_\mathrm{ee}^2 \right\rangle^{1/2} \sim Q n^\alpha \,; \; \alpha = 1/2 \; ; \; \alpha = 3/5$

For ideal chains $\left\langle R_\mathrm{ee}^2 \right\rangle = 6 \left\langle R_G^2 \right\rangle$

Radius of gyration of a sphere $R_{G,\mathrm{sph}} = \sqrt{3/5} R_{sph}$

Critical packing parameter

$$\mathrm{CPP} = v/a_0 l_c$$

Overlap concentration (in molar concentration of monomers)

$$C^\star = \frac{3N_p}{4\pi N_\mathrm{Av}} \frac{10^{-3}}{R_G^3}$$

Friction coefficients $\vec{F} = -f\vec{v}, \qquad \vec{M} = -\xi\vec{\omega}$

Stokes formula $f = 6\pi\eta R_h, \qquad \xi = 8\pi\eta R_h^3$

Hydrodynamic volume $v_{\mathrm{h},1} = \left(\overline{V}_1^{(S)} + \delta\overline{V}_0^{(S)}\right)\frac{M_1}{N_{\mathrm{Av}}}$

Specific volume (per mass) $\overline{V}_1^{(S)} = v_1\left(\frac{N_{\mathrm{Av}}}{M_1}\right)$

Fick's laws $\frac{\partial c}{\partial t} = -\vec{\nabla}\cdot\vec{J}, \qquad \vec{J} = -D_{\mathrm{T}}\vec{\nabla}c, \qquad \frac{\partial c}{\partial t} = D_{\mathrm{T}}\frac{\partial^2 c}{\partial x^2}$

Nernst-Einstein relations $fD_{\mathrm{T}} = k_{\mathrm{B}}T, \qquad \xi D_{\mathrm{R}} = k_{\mathrm{B}}T$

Lamm-equation $\frac{\partial c(r,t)}{\partial t} = D_{\mathrm{T}}\left(\frac{\partial^2 c(r,t)}{\partial r^2} + \frac{1}{r}\frac{\partial c(r,t)}{\partial r}\right) - s\omega^2\left(r\frac{\partial c(r,t)}{\partial r} + 2c(r,t)\right)$

Svedberg equation $s = \left(1 - \overline{V}_1^{(S)}\rho\right)\frac{M_1}{N_{\mathrm{Av}}f}$

Equilibrium centrifugation: $m_1(r) = m_1(r_{\mathrm{m}})\exp\left\{\frac{M_1(1-\overline{V}_1^{(\mathrm{S})}\rho)\omega^2(r^2 - r_{\mathrm{m}}^2)}{2RT}\right\}$

Planck's law $E = h\nu = \frac{hc}{\lambda} = hc\tilde{\nu}$

Beer-Lambert law $A(\lambda) = \varepsilon(\lambda)cl$

Electrically-induce birefringence

$$I(t) = \frac{I_0}{4}\delta_0^2\exp(-12D_R t)$$

Raman spectroscopy

$$P = \alpha_0 E_0\cos 2\pi\nu_0 t + \frac{1}{2}\left(\frac{\partial\alpha}{\partial q_i}\right)_0 q_{i0}\left[\cos(2\pi(\nu_0+\nu_m)t) + \cos(2\pi(\nu_0-\nu_m)t)\right]$$

Nuclear spin $\vec{m} = \gamma\vec{L}, \qquad (\vec{m})^2 = \gamma^2\hbar^2\ell(\ell+1), \qquad m_{\mathrm{z}} = m_\ell\,\gamma\,\hbar$

Gyromagnetic ratio

Nucleus	^{1}H	^{2}H	^{13}C	^{14}N	^{19}F	^{31}P
$\gamma\left(10^7\frac{\mathrm{rad/s}}{\mathrm{T}}\right)$	26.753	4.107	6.728	1.934	25.179	10.840

Larmor frequency $\nu = \frac{\gamma}{2\pi}B_0$

Small-angle scattering

$$q = \frac{4\pi}{\lambda}\sin\left(\frac{\theta}{2}\right)$$

Guinier approximation $I_s(q) = I_0\exp\left(-\frac{1}{3}q^2R_G^2\right)$

Discrete identical homogeneous particles

$$\langle I_s(q)\rangle = Nb^2(0)P(q)S(q)$$

Static light scattering
Rayleigh regime

$$\frac{\langle I_{\mathrm{S}}(q)\rangle}{I_0}R^2 = cM\kappa,$$

Large systems

$$\frac{\kappa c}{R_\theta} \;=\; \frac{1}{M}\left[1+\frac{16\pi^2}{3\lambda^2}R_{\mathrm{G}}^2\sin^2\frac{\theta}{2}\right]\cdot[1+2B_2c],$$

For y-polarized light

$$\kappa = \frac{1}{N_{\mathrm{Av}}}\frac{4\pi^2 n_0^2}{\lambda_0^4}\left(\frac{\mathrm{dn}_0}{\mathrm{dc}}\right)^2,$$

$$R_\theta \;=\; \frac{\langle I_{\mathrm{S}}(q)\rangle}{I_0}R^2,$$

Dynamic light scattering
Siegert relation

$$g^{(2)}(q,\tau) = 1 + [g^{(1)}(q,\tau)]^2$$

$$g^{(1)}(q,\tau) = \exp(-q^2 D_T \tau)$$

Scattering length density

Substance	H_2O	D_2O	proteins	nucleic acids	lipids
ρ (10^{-4} nm^{-2})	-0.55	6.36	3.11	4.44	-0.01