Interaction Energy in Helical Array of DNA strands

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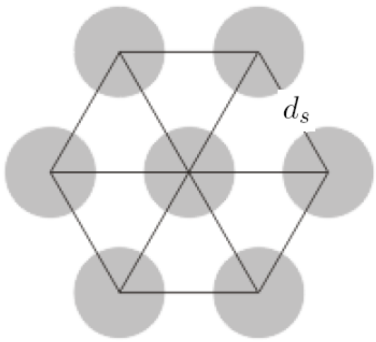
Consider a viral capsid is a DNA container with volume V and has constant temperature T and no interchange of its N particles with the surroundings. The thermodynamic relation between pressure, crystal packing, and interaction energy G_{int} is

$$\pi_{osmotic} = -(\frac{\partial G_{int}}{\partial V})_{T,N} \tag{1}$$

We further assume that the DNA is packed inside the viral capsid with hexagonal packing. In his 1984 paper, Parsegian *et. al.* has measured the osmotic pressure $\pi_{osmotic}$ as a function of DNA spacing d_s (you can download this paper in APh161 website). The spacing d_s is defined as the closest distance between two DNA centers as shown in the cross section of the DNA hexagonal array of parallel DNA strands as shown below.



The fit to their experimental result is an exponential decay function given below

$$\pi_{osmotic} = F_o e^{-d_s/c}, \tag{2}$$

where F_o and c are constants that characterize the strength and decay length, respectively.

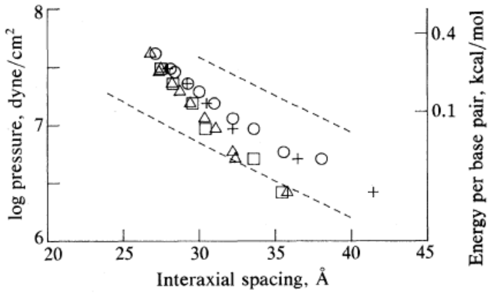


FIG. 1. Lattice pressure vs. interaxial spacing in NaCl solution. ○, 0.1 M; +, 0.25 M; △, 0.50 M; □, 1.00 M. At higher pressures and salt concentrations, the data converge to a common curve. Energy per nucleotide pair was computed by integrating the common curve for 0.50 and 1.00 M extrapolated to infinite separation. Values thus have validity only for smaller spacings. The upper and lower dashed lines are the predictions in 0.10 M solution of electrostatic double layer theory, respectively, for fully charged molecules and for molecules bearing the residual charge density predicted by Manning condensation theory.

The infinitesimal volume ∂V can be expressed as a function of interaxial spacing d_s

$$\partial V \propto \partial d_s \tag{3}$$

$$\partial V = \partial (L A_{hexagon}), \tag{4}$$

where L is the length of the DNA and $A_{hexagon}$ is the cross section area of the viral DNA.

$$A_{hexagon} = \frac{1}{\rho}, \tag{5}$$

where ρ is the density of DNA per cross section area. To make a calculation simpler, let's consider a equilateral triangle with a side length d_s and area of $A_{\triangle}$

$$A_{\triangle} = \frac{d_s}{2} . \frac{\sqrt{3} d_s}{2} = \frac{\sqrt{3}}{4} d_s^2 \tag{6}$$

There are only half of DNA in the triangle, thus

$$A_{hexagon} = \frac{1}{\rho} = \frac{\sqrt{3}}{2} d_s^2 \tag{7}$$

Then, we have

$$\partial V = \partial (L.A_{hexagon}) = L.\partial (\frac{\sqrt{3}}{2} d_s^2) = \sqrt{3} L d_s \partial d_s \tag{8}$$

Using thermodynamic relation between Helmholtz free energy and volume in equation 1, we can compute the G_{int}

$$\pi_{osmotic} = -\frac{\partial G_{int}}{\partial V} \Leftrightarrow G_{int} = -\int_{\infty}^{d_s} \pi_{osmotic} \partial V$$

We determine the interaction energy by calculating the work per unit length needed to bring the strands from infinite separation into d_s spacing.

$$\begin{aligned} G_{int} &= -\int_{\infty}^{d_s} \pi_{osmotic} \partial V \\ &= -\int_{\infty}^{d_s} F_o e^{-d_s'/c} \sqrt{3} L d_s \partial d_s' \\ &= -\sqrt{3} F_o L \int_{\infty}^{d_s} d_s' e^{-d_s'/c} \partial d_s' \\ &= \sqrt{3} F_o L (c^2 + c d_s) e^{-d_s/c} \end{aligned} \tag{9}$$

We have just derived the interaction free energy in hexagonal packing of DNA!