Design and Characterization of Programmable DNA Nanotubes

Correction to *Supporting Information*

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Justification: Although the equation for $p_{\mathrm{tube}}/p_{\mathrm{helix}}$ in the paper is correct, the original Supporting Information presented an incorrect derivation (invoking *mass* moment instead of *area* moment of inertia). Here we provide a correct derivation. We use the letters J and j to emphasize that *area* moments rather than *mass* moments are being calculated, the latter of which are commonly designated by the letter I.

3 Derivation of Persistence Length Estimate for Tubes

The persistence length of a double-helix is proportional to the Young's modulus, E, and the area moment of inertia for the helix, j, about an axis that bisects its cross-section: $p_{\mathrm{helix}} = Ej/kT$.[1] Assuming that the Young's modulus of a DNA nanotube is the same as that of the helices that comprise it, the persistence length of a DNA nanotube is similarly $p_{\mathrm{tube}} = EJ/kT$, where J is the area moment of inertia of the tube about an axis that bisects its cross-section. Thus $p_{\mathrm{tube}}/p_{\mathrm{helix}} = J/j$.

Assuming a tube is a circular array of $n = 2N$ (where N is the number of tiles in circumference) rigidly linked cylindrical rods of radius r, J can be calculated in terms of j, using the parallel axis theorem:

$$J = \sum_{i=1}^{n} \left(j + a d_i^2\right) .$$

Here $a = \pi r^2$ is the cross-sectional area of a rod and d_i is the distance from the center of the i^{th} rod to the neutral axis of interest. For a neutral axis that bisects the cross-section of the tube, d_i can be expressed in terms of the radius of the tube R,

$$J = \sum_{i=1}^{n} \left[j + \pi r^2 (R \sin\theta_i)^2\right]$$

where $\theta_i = 2\pi i/n + \phi$ is the angular position of the center of the i^{th} rod along the circumference of the tube and the phase ϕ relative to the axis is arbitrary.

Solving for the ratio of the area moments,

$$\begin{aligned}
\frac{J}{j} &= \sum_{i=1}^{n} \left[1 + 4\left(\frac{R}{r}\right)^2 \sin^2\theta_i\right] \\
&= n + 4\left(\frac{R}{r}\right)^2 \left[\sum_{i=1}^{n} \sin^2\left(2\pi\frac{i}{n} + \phi\right)\right] \\
&= n + 4\left(\frac{R}{r}\right)^2 \left(\frac{n}{2}\right), \quad \text{for } n > 2 \\
&= 2N\left[1 + 2\left(\frac{R}{r}\right)^2\right], \quad \text{for } n > 2.
\end{aligned}$$

(Note that for $n \le 2$, the sum depends on the phase ϕ. When $n = 1$ it equals $\sin^2\phi$ and when $n = 2$ it equals $2\sin^2\phi$. Interestingly, the equation holds for all n if one averages over ϕ because $\langle \sin^2\phi \rangle = 1/2$.)

Here we have used the well-known result[2] that $j = \pi r^4/4$, the trigonometric identity

$$\sin^2(x) = (1 - \cos(2x))/2 ,$$

and a generalization of Lagrange's trigonometric identity[3]

$$\sum_{k=0}^{n} \sin(\phi + k\alpha) = \frac{\sin\frac{(n+1)\alpha}{2}\sin(\phi + \frac{n\alpha}{2})}{\sin\frac{\alpha}{2}} .$$

References

(1) Bloomfield, V. A.; Crothers, D. M.; Tinoco, Jr., I. Nucleic Acids: Structures, Properties, and Functions; University Science Books: 2000, Page 408.

(2) Landau, L.D.; Lifshitz, E.M., Theory of Elasticity; Elsevier: 1986, Page 67.

(3) Zygmund, A., Trigonometric Series; Cambridge University Press: 2002, Page 2.

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