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Erratum on the Paper "Mathematical Properties of DNA Structure in 3-Dimensional Space"

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Abstract

In this paper, we correct some mathematical mistakes of the paper titled "Mathematical properties of DNA structure in 3-dimensional space" Int. J. Open Problems Compt. Math., Vol. 1, No. 3, December 2008. In addition, we calculate the circle of curvature or osculating circle and the axis curvature.

Keywords: *DNA structure, the circle of curvature, osculating circle, the axis curvature, Double-Helix, Super-Coils, Balanced Ply*

We have the vector position (path) of strand - helix is given by [Stump et al., 2000]:

$$R(t) = (r\cos t)i + (r\sin t)\,j + (\cos\beta)t\,k = (r\cos t,\, r\sin t,\, (\cos\beta)t).$$

where $x = r\cos t$ *and* $y = r\sin t$ describe a circle of radius r, but $z = (\cot\beta)t$ increases (or decreases) indirect to t.

Therefore, the tangent vector field of the strand – helix is

$$R'(t) = (-r\sin t, r\cos t, \cot\beta).$$

Hence, the length of tangent vector field is

$$\begin{aligned}\|R'(t)\| &= \sqrt{r^2\sin^2 t + r^2\cos^2 t + \cot^2\beta}\\ &= \sqrt{r^2\left(\sin^2 t + \cos^2 t\right) + \cot^2\beta}\\ &= \sqrt{r^2 + \cot^2\beta}.\end{aligned}$$

(i) Then the arc-length function is

$$s(t)=\int_a^t \left\|R'(u)\right\| du$$

$$s(t)=\int_0^t \sqrt{r^2+\cot^2\beta}\, du$$
$$=t\sqrt{r^2+\cot^2\beta}\,.$$

(ii) The reparametrization of the strand in terms of s is given by:

$$R(s)=\left(r\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right), r\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right), \cot\beta\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\right).$$

(iii) The curvature of the strand is a constant (not depend on t or s) and given by:

$$\kappa=\frac{\left\|R'(t)\times R''(t)\right\|}{\left\|R'(t)\right\|^3}=\left\|R''(s)\right\|=\frac{r}{r^2+\cot^2\beta}.$$

Now, the proof of κ will be done clearly. From

$$R(t)=(r\cos t, r\sin t, (\cot\beta)t)$$
$$R'(t)=(-r\sin t, r\cos t, \cot\beta)$$
$$R''(t)=(-r\cos t, -r\sin t, 0)$$

we have

$$R'(t)\times R''(t)=\det\begin{bmatrix} i & j & k \\ -r\sin t & r\cos t & \cos\beta \\ -r\cos t & -r\sin t & 0 \end{bmatrix}$$
$$=\left(r\sin t\cot\beta\right)i-\left(r\cos t\cot\beta\right)j+\left(r^2\sin^2 t+r^2\cos^2 t\right)k.$$

Hence, we get

$$\kappa=\frac{\left\|R'(t)\times R''(t)\right\|}{\left\|R'(t)\right\|^3}=\frac{\sqrt{r^2\sin^2 t\cot^2\beta+r^2\cos^2 t\cot^2\beta+r^4}}{(r^2\sin^2 t+r^2\cos^2 t+\cot^2\beta)^{\frac{3}{2}}}$$
$$=\frac{\sqrt{r^2\cot^2\beta+r^4}}{(r^2+\cot^2\beta)^{\frac{3}{2}}}$$
$$=\frac{r(\cot^2\beta+r^2)^{\frac{1}{2}}}{(r^2+\cot^2\beta)^{\frac{3}{2}}}=\frac{r}{r^2+\cot^2\beta}.$$

The proof of κ will be done clearly with respect to the arc-length parametrization of the strand.

$$R'(s)=\left(-r\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{\sqrt{r^2+\cot^2\beta}}, r\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{\sqrt{r^2+\cot^2\beta}}, \cot\beta\left(\frac{1}{\sqrt{r^2+\cot^2\beta}}\right)\right)$$

$$R''(s)=\left(-r\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{r^2+\cot^2\beta}, -r\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{r^2+\cot^2\beta}, 0\right)$$

$$\kappa=\|R''(s)\|=\sqrt{r^2\cos^2\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{(r^2+\cot^2\beta)^2}+r^2\sin^2\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{(r^2+\cot^2\beta)^2}+0^2)}$$

$$=\sqrt{\frac{r^2}{(r^2+\cot^2\beta)^2}}$$

$$=\frac{r}{r^2+\cot^2\beta}.$$

The radius of curvature is given by:

$$\rho=\frac{1}{\kappa}=\frac{r^2+\cot^2\beta}{r}.$$

(iv) The unit tangent vector to the curve of strand is given by:

$$T=\frac{R'(t)}{\|R'(t)\|}=\frac{1}{\sqrt{r^2+\cot^2\beta}}\{(-r\sin t)i+(r\cos t)j+(\cot\beta)k\}$$

$$=\frac{R'(s)}{\|R'(s)\|}=\frac{1}{\sqrt{r^2+\cot^2\beta}}\left(-r\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right), r\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right), \cot\beta\right).$$

The proof of the unit tangent vector T will be done clearly. From

$$R'(t)=(-r\sin t, r\cos t, \cot\beta)$$

we have

$$\|R'(t)\|=\sqrt{r^2\sin^2 t+r^2\cos^2 t+\cot^2\beta}$$
$$=\sqrt{r^2+\cot^2\beta}.$$

Hence, we get

$$T=\frac{R'(t)}{\|R'(t)\|}=\frac{1}{\sqrt{r^2+\cot^2\beta}}\left(-r\sin t, r\cos t, \cot\beta\right).$$

The proof of the unit tangent vector T will be done with respect to the arc-length parametrization of the strand s. From

$$R'(s)=\left(-r\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{\sqrt{r^2+\cot^2\beta}},r\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{\sqrt{r^2+\cot^2\beta}},\cot\beta\left(\frac{1}{\sqrt{r^2+\cot^2\beta}}\right)\right)$$

$$\|R'(s)\|=\sqrt{r^2\sin^2\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{r^2+\cot^2\beta}+r^2\cos^2\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{r^2+\cot^2\beta}+\cot^2\beta\frac{1}{r^2+\cot^2\beta}}$$
$$=1.$$

we get

$$T=\frac{R'(s)}{\|R'(s)\|}=\frac{\left(-r\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{\sqrt{r^2+\cot^2\beta}},r\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{\sqrt{r^2+\cot^2\beta}},\cot\beta\left(\frac{1}{\sqrt{r^2+\cot^2\beta}}\right)\right)}{1}$$
$$=\frac{1}{\sqrt{r^2+\cot^2\beta}}\left(-r\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right),r\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right),\cot\beta\right).$$

(v) The unit normal vector to the curve of strand is given by:

$$N=\frac{T'(t)}{\|T'(t)\|}=(-\cos t)i+(-\sin t)j+(0)k$$
$$N=\frac{T'(s)}{\|T'(s)\|}=\left(-\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right),-\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right),0\right).$$

In fact;

$$T'(t)=\frac{1}{\sqrt{r^2+\cot^2\beta}}(-r\cos t,-r\sin t,0)$$
$$\|T'(t)\|=\sqrt{\frac{1}{r^2+\cot^2\beta}\left(r^2\cos^2 t+r^2\sin^2 t+0\right)}$$
$$=\frac{r}{\sqrt{r^2+\cot^2\beta}}$$
$$N=\frac{T'(t)}{\|T'(t)\|}=\frac{\frac{1}{\sqrt{r^2+\cot^2\beta}}(-r\cos t,-r\sin t,0)}{\frac{r}{\sqrt{r^2+\cot^2\beta}}}$$
$$=(-\cos t,-\sin t,0).$$

The calculation of the unit normal vector with respect to s as follows.

$$T(s)=\frac{1}{\sqrt{r^2+\cot^2\beta}}\left(-r\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right), r\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right), \cot\beta\right)$$

$$T'(s)=\left(-\frac{r}{r^2+\cot^2\beta}\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right), -\frac{r}{r^2+\cot^2\beta}\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right), 0\right)$$

$$\|T'(s)\|=\sqrt{\left(\frac{r}{r^2+\cot^2\beta}\right)^2\cos^2\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)+\left(\frac{r}{r^2+\cot^2\beta}\right)^2\sin^2\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)+0}$$

$$=\left(\frac{r}{r^2+\cot^2\beta}\right)$$

$$N=\frac{T'(s)}{\|T'(s)\|}=\frac{\frac{r}{r^2+\cot^2\beta}\left(-\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right), -\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right), 0\right)}{\frac{r}{r^2+\cot^2\beta}}$$

$$=\left(-\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right), -\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right), 0\right).$$

(vi) The binormal vector to the curve of strand is given by:

$$B(t)=T(t)\times N(t)=\det\begin{bmatrix} i & j & k \\ \frac{-r\sin t}{\sqrt{r^2+\cot^2\beta}} & \frac{r\cos t}{\sqrt{r^2+\cot^2\beta}} & \frac{\cot\beta}{\sqrt{r^2+\cot^2\beta}} \\ -\cos t & -\sin t & 0 \end{bmatrix}$$

$$=\left(\sin t\frac{\cot\beta}{\sqrt{r^2+\cot^2\beta}}\right)i-\left(\cos t\frac{\cot\beta}{\sqrt{r^2+\cot^2\beta}}\right)j+\left(r\frac{\sin^2 t}{\sqrt{r^2+\cot^2\beta}}+r\frac{\cos^2 t}{\sqrt{r^2+\cot^2\beta}}\right)k$$

$$=\left(\frac{\cot\beta\sin t}{\sqrt{r^2+\cot^2\beta}}\right)i+\left(\frac{-\cot\beta\cos t}{\sqrt{r^2+\cot^2\beta}}\right)j+\left(\frac{r}{\sqrt{r^2+\cot^2\beta}}\right)k.$$

The calculation of the unit binormal vector with respect to s as follows.

$$B(s)=T(s)\times N(s)=\frac{1}{\sqrt{r^2+\cot^2\beta}}\det\begin{bmatrix} i & j & k \\ -r\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right) & r\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right) & \cot\beta \\ -\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right) & -\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right) & 0 \end{bmatrix}$$

$$B(s)=\frac{1}{\sqrt{r^2+\cot^2\beta}}\left(\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\cot\beta,\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\cot\beta, r\left(\sin^2\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)+\cos^2\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\right)\right)$$

$$=\left(\frac{\cot\beta\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)}{\sqrt{r^2+\cot^2\beta}}\right)i+\left(\frac{-\cot\beta\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)}{\sqrt{r^2+\cot^2\beta}}\right)j+\left(\frac{r}{\sqrt{r^2+\cot^2\beta}}\right)k.$$

(vii) The torsion (twisting) of the strand will affect a rotation of the crosssectional pattern. In fact the unit normal vector *N* turns toward the binormal vector *B* at the rate *Tw* , and the fact that *N* and B are rigidly fixed at right angles, imply that *B* turns towaed – *N* at the same rate. If this happened, the unit tangent vector *T* would be forced by rigidity into turning in the direction –*B*, but *T* turns only in the direction *N*. Thus, the torsion of the strand is given by (using dot product):

$$T\omega=-N\frac{dB}{ds}=\pm\left\|\frac{dB}{ds}\right\|=\pm\frac{\cot\beta}{r^2+\cot^2\beta}.$$

The proof of Tw will be done.We know that

$$B(s)=\left(\frac{\cot\beta\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)}{\sqrt{r^2+\cot^2\beta}},\frac{-\cot\beta\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)}{\sqrt{r^2+\cot^2\beta}},\frac{r}{\sqrt{r^2+\cot^2\beta}}\right)$$

Therefore, we get

$$\frac{dB}{ds}=\left(\frac{\cot\beta\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{\sqrt{r^2+\cot^2\beta}}}{\sqrt{r^2+\cot^2\beta}},\frac{\cot\beta\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)\frac{1}{\sqrt{r^2+\cot^2\beta}}}{\sqrt{r^2+\cot^2\beta}},0\right)$$

$$=\left(\frac{\cot\beta\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)}{r^2+\cot^2\beta},\frac{\cot\beta\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)}{r^2+\cot^2\beta},0\right).$$

Since the normal vector field is

$$N=\left(-\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right),-\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right),0\right)$$

we have

$$-N=\left(\cos\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right),\sin\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right),0\right).$$

Therefore, we obtain

$$T\omega=-N.\frac{dB}{ds}=\frac{\cot\beta\cos^2\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)}{r^2+\cot^2\beta}+\frac{\cot\beta\sin^2\left(\frac{s}{\sqrt{r^2+\cot^2\beta}}\right)}{r^2+\cot^2\beta}$$

$$=\frac{\cot\beta}{r^2+\cot^2\beta}.$$

Furthermore, we calculate the circle of curvature (osculating circle) and the axis curvature as follows.

(viii) Let m be the center of osculating circle of the strand [2]. We obtain

$$m=R(t)+\rho(t)N(t)$$

$$=\left(r\cos t,r\sin t,(\cot\beta)t\right)+\frac{r^2+\cot^2\beta}{r}(-\cos t,-\sin t,0)$$

$$=\left(\left(r-\frac{r^2+\cot^2\beta}{r}\right)\cos t,\left(r-\frac{r^2+\cot^2\beta}{r}\right)\sin t,\cot\beta t\right)$$

$$=\left(\left(\frac{-\cot^2\beta}{r}\right)\cos t,\left(\frac{-\cot^2\beta}{r}\right)\sin t,(\cot\beta)t\right).$$

(ix) Let d_t be the axis curvature of osculating circle of the strand. We obtain

$$d_t(\mu)=m+\mu B(t)\quad,\qquad \mu\in\mathbb{R}$$

$$=\left(-\frac{\cot^2\beta}{r}\cos t,-\frac{\cot^2\beta}{r}\sin t,(\cot\beta)t\right)+\mu\left(\frac{\cot\beta\sin t}{\sqrt{r^2+\cot^2\beta}},\frac{-\cot\beta\cos t}{\sqrt{r^2+\cot^2\beta}},\frac{r}{\sqrt{r^2+\cot^2\beta}}\right)$$

$$=\left(-\frac{\cot^2\beta}{r}\cos t+\mu\frac{\cot\beta\sin t}{\sqrt{r^2+\cot^2\beta}},-\frac{\cot^2\beta}{r}\sin t-\mu\frac{\cot\beta\cos t}{\sqrt{r^2+\cot^2\beta}},(\cot\beta)t+\mu\frac{r}{\sqrt{r^2+\cot^2\beta}}\right).$$

(x) Let $\gamma(\theta)$ be the equation of osculating circle of the strand. We obtain

$$\gamma(\theta)=R(t)+\rho(t)N(t)+\rho(t)\cos\frac{\theta}{\rho(t)}\left(-N(t)\right)+\rho(t)\sin\frac{\theta}{\rho(t)}T(t)$$

$$\gamma(\theta)=\left(r\cos t,r\sin t,(\cot\beta)t\right)+\left(\frac{r^2+\cot^2\beta}{r}\right)\left(-\cos t,-\sin t,0\right)$$
$$+\left(\frac{r^2+\cot^2\beta}{r}\right)\cos\left(\frac{\theta r}{r^2+\cot^2\beta}\right)\left(\cos t,\sin t,0\right)$$
$$+\left(\frac{r^2+\cot^2\beta}{r}\right)\sin\left(\frac{\theta r}{r^2+\cot^2\beta}\right)\frac{1}{\sqrt{r^2+\cot^2\beta}}\left(-r\sin t,r\cos t,\cot\beta\right)$$

$$=\begin{pmatrix}\left(-\frac{\cot^2\beta}{r}+\left(\frac{r^2+\cot^2\beta}{r}\right)\cos\left(\frac{\theta r}{r^2+\cot^2\beta}\right)\right)\cos t-\sqrt{r^2+\cot^2\beta}\sin\left(\frac{\theta r}{r^2+\cot^2\beta}\right)\sin t,\\ \left(-\frac{\cot^2\beta}{r}+\left(\frac{r^2+\cot^2\beta}{r}\right)\cos\left(\frac{\theta r}{r^2+\cot^2\beta}\right)\right)\sin t+\sqrt{r^2+\cot^2\beta}\sin\left(\frac{\theta r}{r^2+\cot^2\beta}\right)\cos t,\\ \cot\beta\left(t+\frac{\sqrt{r^2+\cot^2\beta}}{r}\right)\sin\left(\frac{\theta r}{r^2+\cot^2\beta}\right)\end{pmatrix}.$$

That is

$$\gamma(\theta)=\left(\left(-\frac{\cot^2\beta}{r}+\left(\frac{r^2+\cot^2\beta}{r}\right)\cos\left(\frac{\theta r}{r^2+\cot^2\beta}\right)\right)\cos t-\sqrt{r^2+\cot^2\beta}\sin\left(\frac{\theta r}{r^2+\cot^2\beta}\right)\sin t\right)i$$
$$+\left(\left(-\frac{\cot^2\beta}{r}+\left(\frac{r^2+\cot^2\beta}{r}\right)\cos\left(\frac{\theta r}{r^2+\cot^2\beta}\right)\right)\sin t+\sqrt{r^2+\cot^2\beta}\sin\left(\frac{\theta r}{r^2+\cot^2\beta}\right)\cos t\right)j$$
$$+\left(\cot\beta\left(t+\frac{\sqrt{r^2+\cot^2\beta}}{r}\right)\sin\left(\frac{\theta r}{r^2+\cot^2\beta}\right)\right)k.$$

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