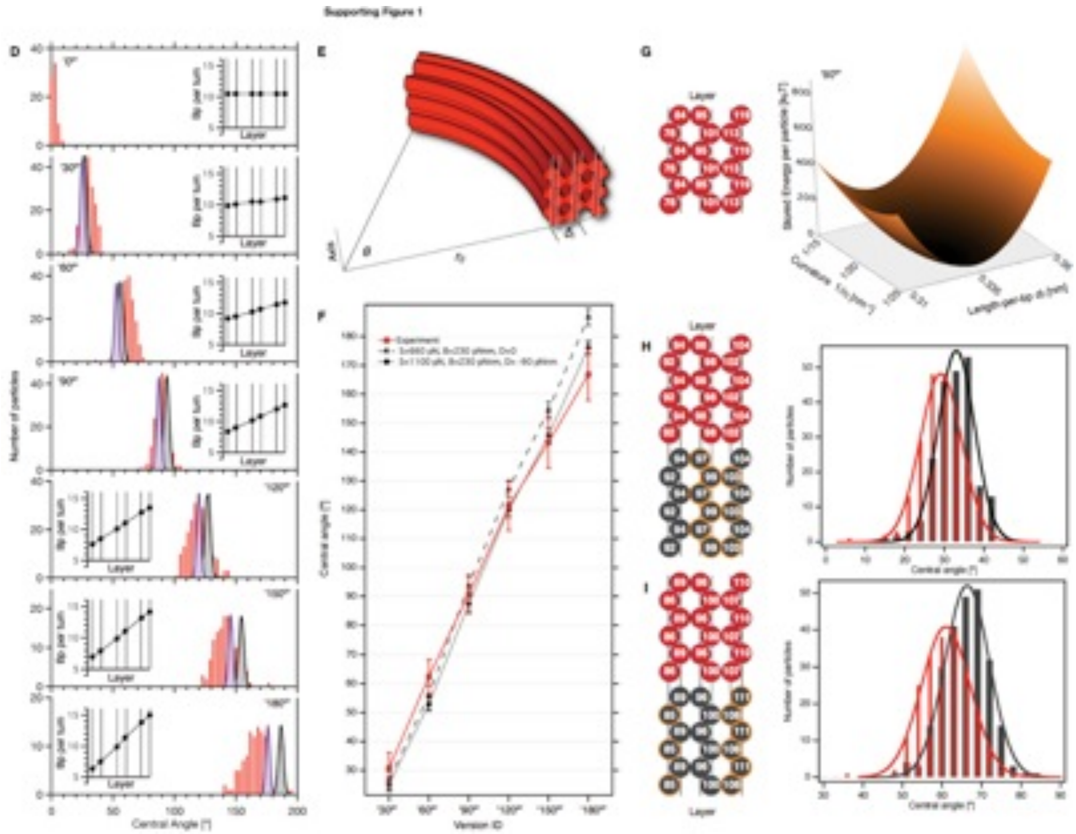

Approximation of Energy for bending DNA bundle

(stretch-compression and bend terms only)
(no twist, twist-stretch coupling yet)

$$E_{total} = E_{stretch/compression} + E_{bend}$$

$$E_{stretch/compression} = \frac{1}{2}\frac{S}{d_{eq}}\sum_i n_i\left(d_i - d_{eq}\right)^2$$

$$E_{bend} = \frac{1}{2}Bd_{eq}\sum_i \frac{n_i}{r_i^2}$$

$$where\ r_i = r_{ref}\left(\frac{delta_i}{r_{ref}} + 1\right)$$

$$\theta_i = \frac{n_i d_{eq}}{r_i}$$

$$E_{bend} = \frac{1}{2}\frac{B}{d_{eq}}\sum_i \theta_i^2 \frac{1}{n_i}$$

$$but\ \sum_i \theta_i^2 \frac{1}{n_i} \approx \theta^2 \sum_i \frac{1}{n_i}$$

$$\therefore E_{bend} \approx \frac{1}{2}\frac{B}{d_{eq}}\theta^2 \sum_i \frac{1}{n_i}$$

The rationale for the above approximation is based on the idea that the underestimate in bending energy for the convex-face helices will be mostly offset by the overestimate in bending energy for the concave-face helices.

$$E_{total} = \frac{1}{2}\frac{S}{d_{eq}}\sum_i n_i\left(d_i - d_{eq}\right)^2 + \frac{1}{2}\frac{B}{d_{eq}}\theta^2\sum_i \frac{1}{n_i}$$

Please note that for this approximation of energy, the following relations hold:

At fixed values of d_i

$$\frac{\partial E_{stretch/compression}}{\partial \theta} = 0$$

At fixed values of q

$$\frac{\partial E_{bend}}{\partial d_i} = 0$$

Step 0: Obtain an expression for the length $n_{ref}d_{ref}$ of a reference double helix in the curved bundle as a function of angle, assuming the bundle is at the equilibrium length for that angle. Do this by letting $\partial E_{stretch/compression}/\partial n_{ref}d_{ref} = 0$ and solving for $n_{ref}d_{ref}$ (recall from the previous page that $\partial E_{bend}/\partial d_{ref} = 0$). The position in the bundle of the reference double helix is encoded in the $delta_i$ offset values. The reference helix could be imaginary, the position within the bundle is arbitrary, and the value of n_{ref} never has to be specified (it cancels out during Step 1).

$$E_{stretch/compression} = \frac{1}{2}\frac{S}{d_{eq}}\sum_i n_i\left(d_i - d_{eq}\right)^2$$

$$d_i = \frac{n_{ref}d_{ref}}{n_i}\left(\frac{delta_i}{r_{ref}} + 1\right)$$

$$r_{ref} = n_{ref}d_{ref}/\theta$$

$$E_{stretch/compression} = \frac{1}{2}\frac{S}{d_{eq}}\sum_i n_i\left(\frac{n_{ref}d_{ref}}{n_i}\left(\frac{delta_i}{n_{ref}d_{ref}/\theta} + 1\right) - d_{eq}\right)^2$$

$$E_{stretch/compression} = \frac{1}{2}\frac{S}{d_{eq}}\sum_i n_i\left(\frac{1}{n_i}\left(n_{ref}d_{ref} + \theta\cdot delta_i\right) - d_{eq}\right)^2$$

$$\frac{\partial E_{stretch/compression}}{\partial(n_{ref}d_{ref})} = \frac{S}{d_{eq}}\sum_i n_i\left(\frac{1}{n_i}\left(n_{ref}d_{ref} + \theta\cdot delta_i\right) - d_{eq}\right)\frac{1}{n_i}$$

$$= \frac{S}{d_{eq}}\sum_i\left(\frac{1}{n_i}\left(n_{ref}d_{ref} + \theta\cdot delta_i\right) - d_{eq}\right)$$

$$0 = \frac{S}{d_{eq}}\sum_i\left(\frac{1}{n_i}\left(n_{ref}d_{ref} + \theta\cdot delta_i\right) - d_{eq}\right)$$

$$= n_{ref}d_{ref}\sum_i\frac{1}{n_i} + \theta\sum_i\frac{delta_i}{n_i} - d_{eq}\sum_i 1$$

$$n_{ref}d_{ref} = \frac{1}{\sum_i \frac{1}{n_i}}\left(d_{eq}\sum_i 1 - \theta\sum_i\frac{delta_i}{n_i}\right)$$

Step 1: Use the expression for the length $n_{ref}d_{ref}$ from Step 0 to obtain an expression for the length d_i of double helix$_i$ in the curved bundle as a function of angle, assuming the bundle is at its equilibrium length for that angle.

$$n_{ref}d_{ref} = \frac{1}{\sum_i \frac{1}{n_i}}\left(d_{eq}\sum_i 1 - \theta\sum_i \frac{delta_i}{n_i}\right)$$

$$d_i = \frac{n_{ref}d_{ref}}{n_i}\left(\frac{delta_i}{r_{ref}} + 1\right)$$

$$\theta = \frac{n_{ref}d_{ref}}{r_{ref}}$$

$$d_i = \frac{1}{n_i}\left(\theta \cdot delta_i + n_{ref}d_{ref}\right)$$

$$= \frac{1}{n_i\sum_i \frac{1}{n_i}}\left(\theta \cdot delta_i\sum_i \frac{1}{n_i} + d_{eq}\sum_i 1 - \theta\sum_i \frac{delta_i}{n_i}\right)$$

$$d_i = \frac{1}{n_i\sum_i \frac{1}{n_i}}\left(\theta\left(delta_i\sum_i \frac{1}{n_i} - \sum_i \frac{delta_i}{n_i}\right) + d_{eq}\sum_i 1\right)$$

Step 2: Use the expression for the length d_i from Step 1 to obtain an expression for the total (= stretch/compression + bending) of the bundle as a function of angle. Since we are concerning ourselves here with only the equilibrium length of the bundle at every angle, therefore length is a dependent variable, and angle is the only independent variable.

$$d_i = \frac{1}{n_i\sum_i \frac{1}{n_i}}\left(\theta\left(delta_i\sum_i \frac{1}{n_i} - \sum_i \frac{delta_i}{n_i}\right) + d_{eq}\sum_i 1\right)$$

$$E_{total} = \frac{1}{2}\frac{S}{d_{eq}}\sum_i n_i\left(d_i - d_{eq}\right)^2 + \frac{1}{2}\frac{B}{d_{eq}}\theta^2\sum_i \frac{1}{n_i}$$

$$E_{total} = \frac{1}{2}\frac{S}{d_{eq}}\sum_i n_i\left(\frac{1}{n_i\sum_i \frac{1}{n_i}}\left(\theta\left(delta_i\sum_i \frac{1}{n_i} - \sum_i \frac{delta_i}{n_i}\right) + d_{eq}\sum_i 1\right) - d_{eq}\right)^2 + \frac{1}{2}\frac{B}{d_{eq}}\theta^2\sum_i \frac{1}{n_i}$$

Step 3: Use the expression for total energy from Step 2 to obtain an expression for the angle of curvature that gives the minimum stretch-compression plus bending energy for the bundle. Do this by setting to zero the derivative of the combined energy with respect to angle, and solving for angle.

$$E_{total} = \frac{1}{2}\frac{S}{d_{eq}}\sum_i n_i\left(\frac{1}{n_i\sum_i \frac{1}{n_i}}\left(\theta\left(delta_i\sum_i \frac{1}{n_i} - \sum_i \frac{delta_i}{n_i}\right) + d_{eq}\sum_i 1\right) - d_{eq}\right)^2 + \frac{1}{2}\frac{B}{d_{eq}}\theta^2\sum_i \frac{1}{n_i}$$

$$\frac{\partial E_{total}}{\partial\theta} = \frac{S}{d_{eq}}\sum_i n_i\left(\frac{1}{n_i\sum_i \frac{1}{n_i}}\left(\theta\left(delta_i\sum_i \frac{1}{n_i} - \sum_i \frac{delta_i}{n_i}\right) + d_{eq}\sum_i 1\right) - d_{eq}\right)\left(\frac{1}{n_i\sum_i \frac{1}{n_i}}\left(delta_i\sum_i \frac{1}{n_i} - \sum_i \frac{delta_i}{n_i}\right)\right)$$
$$+\theta\frac{B}{d_{eq}}\sum_i \frac{1}{n_i}$$

$$for\ convenience, let \quad \beta_i = \frac{1}{n_i \sum_j \frac{1}{n_j}} \left(delta_i \sum_j \frac{1}{n_j} - \sum_j \frac{delta_j}{n_j} \right)$$

$$0 = \frac{S}{d_{eq}} \sum_i \beta_i n_i \left(\frac{1}{n_i \sum_i \frac{1}{n_i}} \left(\theta \left(delta_i \sum_i \frac{1}{n_i} - \sum_i \frac{delta_i}{n_i} \right) + d_{eq} \sum_i 1 \right) - d_{eq} \right) + \theta \frac{B}{d_{eq}} \sum_i \frac{1}{n_i}$$

$$= \theta \left(\sum_i \beta_i delta_i \sum_i \frac{1}{n_i} - \sum_i \beta_i \sum_i \frac{delta_i}{n_i} + \frac{B}{S} \left(\sum_i \frac{1}{n_i} \right)^2 \right) + d_{eq} \left(\sum_i \beta_i \sum_i 1 - \sum_i \beta_i n_i \sum_i \frac{1}{n_i} \right)$$

$$\theta = d_{eq} \frac{\sum_i \beta_i n_i \sum_i \frac{1}{n_i} - \sum_i \beta_i \sum_i 1}{\sum_i \beta_i delta_i \sum_i \frac{1}{n_i} - \sum_i \beta_i \sum_i \frac{delta_i}{n_i} + \frac{B}{S} \left(\sum_i \frac{1}{n_i} \right)^2}$$

$$where\ \beta_i = \frac{1}{n_i \sum_j \frac{1}{n_j}} \left(delta_i \sum_j \frac{1}{n_j} - \sum_j \frac{delta_j}{n_j} \right)$$

Note that $\sum_i \beta_i = 0$

Therefore

$$\theta = \frac{d_{eq} \sum_i \beta_i n_i}{\sum_i \beta_i delta_i + \frac{B}{S} \sum_i \frac{1}{n_i}}$$

$$where\ \beta_i = \frac{1}{n_i \sum_j \frac{1}{n_j}} \left(delta_i \sum_j \frac{1}{n_j} - \sum_j \frac{delta_j}{n_j} \right)$$

and from before

$$d_i = \frac{1}{n_i \sum_i \frac{1}{n_i}} \left(\theta \left(delta_i \sum_i \frac{1}{n_i} - \sum_i \frac{delta_i}{n_i} \right) + d_{eq} \sum_i 1 \right)$$