[pex34] Polymer with energetically favored internal rotation angles II

Consider an ideal polymer chain with fixed valence angle $\cos_{i,i+1} = \gamma$ and an internal rotation angle $\phi_{i,i+1} \doteq \phi_i$ subject to a potential $U(\phi_i)$ with symmetry $U(-\phi_i) = U(\phi_i)$. Here we use the result from [pex33] for the angle $\theta_{i,i+k}$ between links *i* and *k* to calculate the thermal average $\langle \theta_{i,i+k} \rangle$ for use in the expression from [pex30] for the mean-square end-to-end distance $\langle R^2 \rangle$. (a) Provide a chain of reasoning that leads to the following result:

$$\langle \theta_{i,i+k} \rangle = \left[\langle \mathbf{T} \rangle^k \right]_{11}, \quad \langle \mathbf{T} \rangle = \left(\begin{array}{cc} \cos \gamma & \sin \gamma \langle \cos \phi \rangle & 0\\ \sin \gamma & -\cos \gamma \langle \cos \phi \rangle & 0\\ 0 & 0 & -\langle \cos \phi \rangle \end{array} \right).$$

(b) Provide a chain of reasoning that leads to the following expression for the mean-square endto-end distance:

$$\langle R^2 \rangle \stackrel{N \gg 1}{\leadsto} Na^2 \left[\frac{\mathbf{E} + \langle \mathbf{T} \rangle}{\mathbf{E} - \langle \mathbf{T} \rangle} \right]_{11}, \quad \mathbf{E} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

(c) Evaluate this expression via the solution of the matrix equation $\mathbf{X} \cdot (\mathbf{E} - \langle \mathbf{T} \rangle) = \mathbf{E} + \langle \mathbf{T} \rangle$.

[adapted from Grosberg and Khokhlov 1994]

Solution: