[pex33] Polymer with energetically favored internal rotation angles I

Consider an ideal polymer chain with fixed valence angle $\cos\theta_{i,i+1} = \gamma$ and an internal rotation angle $\phi_{i,i+1} \doteq \phi_i$ subject to a potential $U(\phi_i)$. As a first step in the calculation of the mean-square end-to end distance $\langle R^2 \rangle$ as expressed in [pex30] we must express the angle $\theta_{i,i+k}$ between links as a function of γ and $\phi_i, \ldots \phi_{i+k-1}$. For that purpose we introduce local coordinate systems $\vec{n}_i$ with (i) n_i^x parallel to the bond vector, (ii) n_i^y in the plane of $\vec{n}_i$ and $\vec{n}_{i-1}$ and orientation such that the angle between the directions of n_{i-1}^x and n_i^y is acute, and (iii) n_i^z to complete a right-handed Cartesian system. The internal rotation angles are measured from the trans-planar zigzag conformation. Express the relative orientation of adjacent local coordinate systems in the form

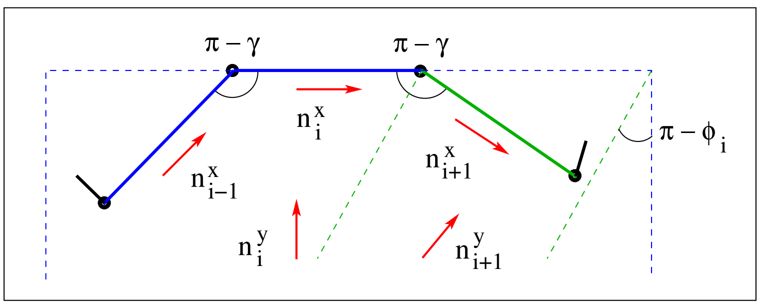
$$n_{i+1}^{\mu} = \sum_{\nu=x,y,z} T_i^{\mu\nu} n_i^{\nu}$$

(a) Find the matrix $\mathbf{T}_i(\gamma, \phi_i)$ and show that it is orthonormal.
(b) Given that the bond vector in the local coordinate system is $\vec{u}_i = (1, 0, 0)$ calculate

$$\cos\theta_{i,i+1} = \vec{u}_i \cdot \vec{u}_{i+1} = \vec{u}_i \cdot \mathbf{T}_i \cdot \vec{u}_i.$$

(c) Generalize this expression for the angle $\cos\theta_{i,i+k}$.

[adapted from Grosberg and Khokhlov 1994]



Solution: