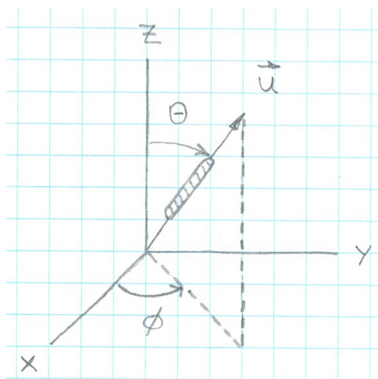
Nematic Order Parameter [pln80]

Orientation of mesogen described by unit vector,

$$\mathbf{u}^{(i)} = \left(u_x^{(i)}, u_y^{(i)}, u_z^{(i)}\right) = \left(\sin\theta_i \cos\phi_i, \sin\theta_i \sin\phi_i, \cos\theta_i\right).$$



The tensor construction of the nematic order parameter must take into account that $\langle \mathbf{u}^{(i)} \rangle = 0$ in both the isotropic phase and the nematic phase. It follows that the tensor must be of second rank or higher.

Desired attributes of the 2$^{\text{nd}}$-rank order-parameter tensor $\mathcal{N}_{\alpha\beta}$, $\alpha, \beta = x, y, z$:

- tensor is symmetric: $\mathcal{N}_{\alpha\beta} = \mathcal{N}_{\beta\alpha}$,
- tensor has zero trace: $\sum_\alpha \mathcal{N}_{\alpha\alpha} = 0$,
- $\mathcal{N}_{\alpha\beta} \equiv 0$ in isotropic phase,
- $\mathcal{N}_{\alpha\alpha} = 1$ if $\mathbf{u}^{(i)} = \hat{\mathbf{e}}_\alpha$ (perfect alignment).

These attributes are satisfied by the following construction [pex1]:[1]

$$\mathcal{N}_{\alpha\beta} = \frac{1}{2}\langle 3\cos^2\theta - 1\rangle = \frac{1}{2}\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta\, g(\theta,\phi)\big(3u_\alpha u_\beta - \delta_{\alpha\beta}\big),$$

where $g(\theta,\phi)$ is the orientation function characterizing the macrostate and

$$u_x = \sin\theta\cos\phi, \quad u_y = \sin\theta\sin\phi, \quad u_z = \cos\theta.$$

The order parameter $\mathcal{N}_{\alpha\beta}$ is being used in the Maier-Saupe theory [pln74] and in the Onsager theory [pln75].

[1] Note the relation to Legendre polynomials: $P_0(x) = 1,\ P_1(x) = x,\ P_2(x) = \frac{1}{2}(3x^2 - 1), \ldots$ In the case of a ferromagnet, the order parameter (magnetization) is constructed from a first-rank tensor (vector), corresponding to the first-order Legendre polynomial.