

$$R_g^2 = \left\langle \frac{1}{N} \sum_{i=1}^N (\mathbf{r}_i - \mathbf{r}_{CM})^2 \right\rangle \quad (1)$$

$$Q_{xy} = \frac{1}{N} \sum_{i=1}^N \mathbf{r}_x^i \mathbf{r}_y^i \quad (2)$$

$$Q = \begin{bmatrix} Q_{xx} & Q_{xy} & Q_{xz} \\ Q_{yx} & Q_{yy} & Q_{yz} \\ Q_{zx} & Q_{zy} & Q_{zz} \end{bmatrix} = \begin{bmatrix} \lambda_x^2 & 0 & 0 \\ 0 & \lambda_y^2 & 0 \\ 0 & 0 & \lambda_z^2 \end{bmatrix} \quad (3)$$

$$\lambda_x^2 \leq \lambda_y^2 \leq \lambda_z^2 \quad (4)$$

$$b = \lambda_z^2 - \frac{1}{2}(\lambda_x^2 + \lambda_y^2) \quad (5)$$

$$c = \lambda_y^2 - \lambda_x^2 \quad (6)$$

$$\kappa = \frac{3}{2} \frac{Tr \hat{Q}^2}{(Tr Q)^2} \quad (7)$$

$$\hat{Q}_{ij} = Q_{ij} - \delta_{ij} Tr Q / 3 \quad (8)$$

$$\kappa^2 = \frac{3}{2} \frac{\lambda_x^4 + \lambda_y^4 + \lambda_z^4}{(\lambda_x^2 + \lambda_y^2 + \lambda_z^2)^2} - \frac{1}{2} \quad (9)$$

$$0 \leq \kappa \leq 1 \quad (10)$$