SIF40AH/DIF4997
Nano-particle and polymer physics I
EXERCISE 4

Equilibrium probability distribution of a three-bead Kramer's chain

A Kramer's chain consists of three spherical beads with masses $m_1 = m_2 = m$ and segment lengths $a_1 = a_2 = a$. To simplify the notation we choose $m = 2$ and $a = 1$ (dimensionless). Assume no external fluid velocity (no flow).

A. The chain in two dimensions with bead 1 being fixed to origo

Assume bead 1 is fixed to origo and assume the following two generalized coordinates: The angle θ_1 between segment vector 1 and the y-axis and the angle θ_2 between segment vector 2 and the y-axis. These may be denoted polar angles. Show that at thermodynamic equilibrium the probability distribution function Ψ for the included angle can be expressed

$$\Psi(\theta_1, \theta_2) = \Psi(\xi) = C\sqrt{1 - \frac{1}{2}\cos^2\xi}$$

where C is a constant and $\xi = \theta_2 - \theta_1$ is the included angle.

Hint: Find an expression for $\mathcal{K}(\theta_1, \theta_2, p_1, p_2)$ where $p_i = \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}\theta_i}$ are the generalized momenta. Integrate $\exp\{-\mathcal{H}/k_\mathrm{B}T\}$ over p_1 and p_2.

B. The chain in two dimensions with no fixed point

When the three-bead Kramer's chain is free to move in all directions, we can still use the generalized coordinates θ_1 and θ_2 as defined as above. Apply the expression of kinetic energy in the example of Ch. 3.2.3 (Eq. (3.40)), follow the procedure above and show that at thermodynamic equilibrium the probability distribution function Ψ for the included angle can be expressed

$$\Psi(\theta_1, \theta_2) = \Psi(\xi) = C\sqrt{1 - \frac{1}{4}\cos^2\xi}$$

C. The chain in three dimensions with no fixed point

There are four internal generalized coordinates: The orientational polar angles (θ_1, ϕ_1) and (θ_2, ϕ_2) of segment vector 1 and 2, respectively. Show that at thermodynamic equilibrium the probability distribution function $\Psi(\theta_1, \theta_2, \phi_1, \phi_2)$ can be expressed

$$\Psi(\theta_1, \theta_2, \xi) = C\sin\theta_1\sin\theta_2\sqrt{1 - \frac{1}{4}\cos^2\xi}$$

where C is a constant and ξ is the included angle defined by

$$\cos\xi = \sin\theta_1\sin\theta_2\cos(\phi_1 - \phi_2) + \cos\theta_1\cos\theta_2.$$

Finally find the normalization constant C.