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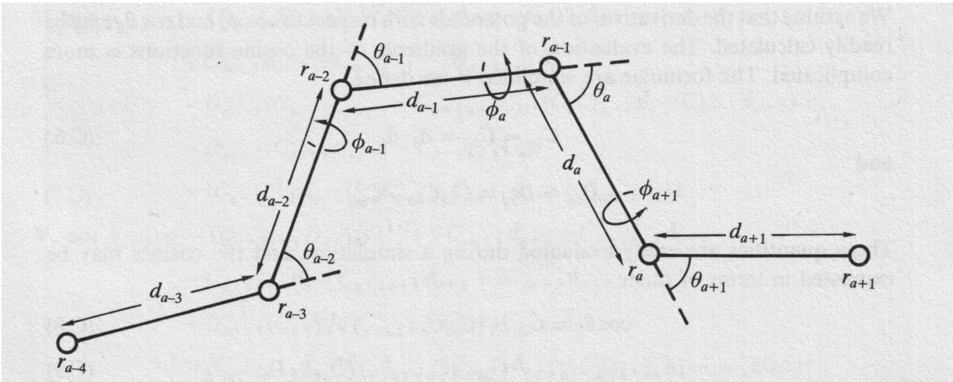
Molekulardynamik (SS09)
Übungsblatt 3

The Polymer Chain

1 Cartesian forces



We consider the depicted model for a polymer chain of identical beads. We neglect the non-bonding part of the interaction potential. The resulting potential consists of contributions due to bond elongations (1-2 interactions), angle bendings (1-2-3 interactions), and torsional motion (1-2-3-4 interactions):

$$V_{\text{chain}} = \sum_{\text{a}} v_d(d_{\text{a}}) + \sum_{\text{a}'} v_\theta(\theta_{\text{a}'}) + \sum_{\text{a}''} v_\phi(\phi_{\text{a}''}),$$

The bonds and angles are described by harmonic terms,

$$v_d(d_{\text{a}}) = \frac{1}{2} k_d (d_{\text{a}} - d_0)^2,$$

$$v_\theta(\theta_{\text{a}}) = \frac{1}{2} k_\theta (\theta_{\text{a}} - \theta_0)^2,$$

and the torsional potential is given by

$$v_\phi(\phi_{\text{a}}) = \sum_k c_k \cos^k(\phi_{\text{a}}).$$

We calculate the forces acting on one bead of the polymer model due to the bonded interactions.

a) Express the bond potential $v_d(d_{\text{a}})$, the bending potential $v_\theta(\theta_{\text{a}})$, and the dihedral potential

$v_\phi(\phi_\mathrm{a})$ in terms of the bead coordinates $\vec{r}_\mathrm{a}$.

b) Determine the cartesian forces acting on one bead by taking the gradient of the interaction potential with respect to its coordinates $\vec{r}_\mathrm{a}$. Which terms of the potential depend on the coordinates $\vec{r}_\mathrm{a}$?

Hint:
Lagrange's Identity: $(\vec{a} \times \vec{b}) \cdot (\vec{c} \times \vec{d}) = (\vec{a} \cdot \vec{c})(\vec{b} \cdot \vec{d}) - (\vec{b} \cdot \vec{c})(\vec{a} \cdot \vec{d})$

2 End-to-end distance of polymer models

An important observable in polymer physics is the mean end-to-end distance R of a polymer chain. We determine the average end-to-end distance of different polymer models in simulations:

- a polymer where we only consider the bond elongations

$$V_\mathrm{chain} = \sum_\mathrm{a} \frac{1}{2} k_d (d_\mathrm{a} - d_0)^2,$$

- a polymer where we only consider bond elongations and angle bends

$$V_\mathrm{chain} = \sum_\mathrm{a} \frac{1}{2} k_d (d_\mathrm{a} - d_0)^2 + \sum_{\mathrm{a}'} \frac{1}{2} k_\theta (\theta_{\mathrm{a}'} - \theta_0)^2,$$

- a polymer where we only consider all bonding interactions

$$V_\mathrm{chain} = \sum_\mathrm{a} \frac{1}{2} k_d (d_\mathrm{a} - d_0)^2 + \sum_{\mathrm{a}'} \frac{1}{2} k_\theta (\theta_{\mathrm{a}'} - \theta_0)^2 + \sum_{\mathrm{a}''} \sum_k c_k \cos^k(\phi_{\mathrm{a}''}).$$

Compare your results with theoretical predictions for a freely jointed chain (FJC) and a freely rotating chain (FRC)

$$R_\mathrm{FJC} = N d^2,$$

and

$$R_\mathrm{FRC} = N d^2 \frac{1 + \cos\theta}{1 - \cos\theta}.$$

For what force constants k_d and k_θ do we get good agreement?