Norges teknisk-naturvitenskapelige universitet
Institutt for fysikk

EKSAMENSOPPGAVE I DIF4997 - POLYMERFYSIKK 1
EKSAMENSOPPGAVE I SIF40AH - POLYMERFYSIKK

Eksamensdato: Torsdag 12. desember 2002
Eksamenstid: 09:00 - 14:00
Språkform: Engelsk

Faglig kontakt under eksamen: Arne Mikkelsen, tlf. 7359 3433
Vekttall: 2,5
Tillatte hjelpemidler (kode C):
Enkel kalkulator (HP 30S)
Rottmann: Matematische Formelsammlung (norsk eller tysk utgave).

Sensurdato: 2. januar 2003.

Exercise 1

A. Describe the following polymer models in the three-dimensional Cartesian space: Bead-spring chain, Kramers chain, Kirkwood-Riseman freely rotating chain and a nugget-spring chain. Assume each chain has N beads or nuggets. For each model, give the number of freedoms. Also define a suitable set of generalized coordinates.

B. A Kramers chain can be defined by the position $\vec{\boldsymbol{R}}_\nu$ of bead ν relative to the center of mass of the chain. Show that the segment connector vector $\vec{\boldsymbol{Q}}_k$ for segment k can be expressed

$$\vec{\boldsymbol{Q}}_k = \sum_\nu \overline{B}_{k\nu}\, \vec{\boldsymbol{R}}_\nu, \quad \text{alternatively, on matrix form:} \quad \vec{\boldsymbol{Q}} = \overline{\overline{\boldsymbol{B}}} \cdot \vec{\boldsymbol{R}},$$

and find the components of tensor $\overline{\overline{\boldsymbol{B}}}$. What is the dimension of tensor $\overline{\overline{\boldsymbol{B}}}$ when the chain has N beads?

C. A polymer in two dimensions is modelled as a Kramers chain consisting of three beads and two rods. Each bead has mass m and each rod length a. Assume that the internal potential energy of the polymer is independent of the included angle, ξ. The kinetic energy og the chain can be expressed

$$\mathcal{K} = \frac{1}{2} m_p \dot{\vec{\boldsymbol{r}}}_c^{\,2} + \frac{1}{6} a^2 m \begin{pmatrix} \dot{\theta}_1 \\ \dot{\theta}_2 \end{pmatrix}^T \cdot \begin{pmatrix} 2 & \cos\xi \\ \cos\xi & 2 \end{pmatrix} \cdot \begin{pmatrix} \dot{\theta}_1 \\ \dot{\theta}_2 \end{pmatrix}.$$

Explain how the generalized coordinates θ_1 and θ_2 are defined, then deduce an analytical expression for the conjugated generalized momenta $p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$. Use these expressions to find an analytical expression for the probability distribution function for the included angle ξ for the Kramers chain when the system is in thermodynamic equilibrium.

Exercise 2

A. Consider a Rouse chain where alle springs have spring constant H and all beads mass m. The potential energy is

$$\Phi \; = \; \frac{1}{2}\vec{\boldsymbol{r}} \cdot \vec{\vec{\boldsymbol{H}}} \cdot \vec{\boldsymbol{r}},$$

and the kinetic energy is

$$\mathcal{K} = \frac{1}{2}\dot{\vec{\boldsymbol{r}}} \cdot \vec{\vec{\boldsymbol{m}}} \cdot \dot{\vec{\boldsymbol{r}}}.$$

Express $\vec{\vec{\boldsymbol{H}}}$ and $\vec{\vec{\boldsymbol{m}}}$ on matrix form.

B. Normal mode analysis can be applied to many different physical systems. What do we mean with normal mode analysis? Give one or two examples of system which can by analysed by normal modes.

C. Show how introduction of the new variable $\vec{\boldsymbol{X}} := \vec{\vec{\boldsymbol{\Omega}}}^{-1} \cdot \vec{\boldsymbol{r}}$ makes it possible to introduce the normal modes $\vec{\boldsymbol{X}}_p$ of the Rouse chain.
Hint: All elements of matrix $(\vec{\vec{\boldsymbol{\Omega}}})^{-1}$ are constants and are chosen so that

$$\vec{\vec{\boldsymbol{\Omega}}}^{-1} \cdot \vec{\vec{\boldsymbol{H}}} \cdot \vec{\vec{\boldsymbol{\Omega}}} = \vec{\vec{\boldsymbol{\lambda}}},$$

where matrix $\vec{\vec{\boldsymbol{\lambda}}}$ is diagonal.

D. What is the equilibrium probability distribution of the Rouse chain expressed in normal modes? Given the Boltzmann distribution function

$$p^{(\mathrm{eq,q})}\left(\vec{\boldsymbol{q}}\right) = \frac{\exp\left\{-\Phi(\vec{\boldsymbol{q}})/(k_{\mathrm{B}}T)\right\} \left|\vec{\vec{\boldsymbol{m}}}^{(\mathrm{q})}\right|^{1/2}}{\int \exp\left\{-\Phi(\vec{\boldsymbol{q}})/(k_{\mathrm{B}}T)\right\} \left|\vec{\vec{\boldsymbol{m}}}^{(\mathrm{q})}\right|^{1/2} \, \mathrm{d}\,\vec{\boldsymbol{q}}} \quad .$$

Exercise 3

The Fokker-Planck equation for segmented polymer chains in vector space $V^{(q)}$ generally reads

$$\frac{\partial p(\vec{\boldsymbol{q}},t)}{\partial t} = -\sum_{s=1}^{d} \frac{\partial}{\partial q_s} \left\{A_s(\vec{\boldsymbol{q}})\, p(\vec{\boldsymbol{q}},t)\right\} + k_{\mathrm{B}}T \sum_{s,t=1}^{d} \frac{\partial}{\partial q_s}\frac{\partial}{\partial q_t} \left\{\mu_{st}^{(\mathrm{q})}(\vec{\boldsymbol{q}})\, p(\vec{\boldsymbol{q}},t)\right\}.$$

Given the following stochastic differential equation (SDE) or generalized Langevin equation:

$$\mathrm{d}\,\vec{\boldsymbol{q}} = \vec{\boldsymbol{A}}\,(\vec{\boldsymbol{q}})\;\mathrm{d}t \; + \; \sqrt{2\,k_{\mathrm{B}}T}\;\vec{\vec{\boldsymbol{B}}}(\vec{\boldsymbol{q}}) \cdot \mathrm{d}\,\vec{\boldsymbol{W}} \quad .$$

The Fokker-Planck equation and the SDE will offer alternative descriptions of the same physical system provided the coefficients in the two equation are selected in such a manner that the processes represented are identical.

Explain the symbols used in these two equations and which physical processes the different terms represent. What is the required relation between $\mu_{st}^{(\mathrm{q})}$ and $\vec{\vec{\boldsymbol{B}}}(\vec{\boldsymbol{q}})$?

Is the choice of the SDE unique to represent the Fokker-Planck equation? If not, what is the reason for this and what do we call this sort of equivalence?