Fachbereich C – Mathematik und Naturwissenschaften
– Physik –

Prof. Dr. A. Klümper
M. Brockmann
(G-16.04, 439-2541, michael.brockmann@physik.uni-wuppertal.de)

Theoretical Solid State Physics, WS 08/09

8th practice sheet

Closing date: 11.12.2008, at 1:00 pm into the PO Box

18. **Periodically closed harmonic chain (10 points)**

Consider N atoms of masses $m_1, \ldots, m_N$ which are coupled by N identical springs with spring constant $k > 0$. Asuming periodic boundary conditions the equations of motion can be written in matrix form as follows:

$$M\ddot{\vec{x}} = -kT\vec{x} \tag{1}$$

where $M = \mathrm{diag}(m_1, \ldots, m_N)$ and $\vec{x} = (x_1, \ldots, x_N)^T$. The $N \times N$ matrix T is symmetric:

$$T = \begin{pmatrix} 2 & -1 & & 0 & -1 \\ -1 & 2 & -1 & & 0 \\ & & \ddots & & \\ 0 & & -1 & 2 & -1 \\ -1 & 0 & & -1 & 2 \end{pmatrix}, \qquad U = \begin{pmatrix} 0 & 1 & & & 0 \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ 0 & & & 0 & 1 \\ 1 & 0 & & & 0 \end{pmatrix} \tag{2}$$

U is the translation matrix.

(a) Verify the following relations:

$$T = 2I - U - U^T, \qquad T = (I - U)(I - U^T). \tag{3}$$

(b) Show that the equations of motion transform with $\vec{y} := \sqrt{M}\vec{x}$, $\sqrt{M} := \mathrm{diag}(\sqrt{m_1}, \ldots, \sqrt{m_N})$ into

$$\ddot{\vec{y}} = -k\tilde{T}\vec{y}. \tag{4}$$

where $\tilde{T}$ is a symmetric $N \times N$ matrix.

(c) Prove that all eigenvalues of $\tilde{T}$ are non-negative. What is the physical consequence of this fact?

(d) Make the ansatz $\vec{y}(t) = e^{i\omega t}\vec{z}$ and solve the eigenvalue problem in the case $m_2 = \ldots = m_N =: m$ and $m_1 = m(1+\mu)$. The inverse L^{-1} of the matrix $L = kT - m\omega^2 I$ is called Green's function of the harmonic chain. Show that the eigenvalue problem is of the form

$$(I - m\omega^2 L^{-1}\Lambda)\vec{x} = 0, \tag{5}$$

where Λ is the matrix with μ at position $(1,1)$ and 0 otherwise. The determinant of the matrix $I - m\omega^2 L^{-1}\Lambda$ is a rational function $f(\omega, \omega_j)$ of ω and the frequencies ω_j, $j = 1, \ldots, N$, of the problem with $\mu = 0$. Calculate $f(\omega, \omega_j)$. Analyse the postions of the roots of f graphically.

(e) Discuss the special cases of $\mu = -1$ and $\mu \to \infty$. What is the physical meaning?

19. **Two-atomic molecules (4 points)**

Consider a gas consisting of N two-atomic molecules, each of which has 6 degrees of freedom. Neglect the translational and rotational degrees of freedom. Let ν_0 be the frequency of oscillation. Calculate the contributions to the energy U and specific heat c_V caused by the oscillation. Plot U and c_V as a function of temperature T.