Technische Universität Berlin
Institut für Theoretische Physik
Lecture Course: Prof. Dr. Matthias Scheffler, Dr. Patrick Rinke, Dr. Alex Tkatchenko
Exercises: Dr. Volker Blum

June 13, 2012

http://www.itp.tu-berlin.de/menue/lehre/lv/ss12/
wahlpflichtveranstaltungen/theoretische_festkoerperphysik_i_ii_theoretical_material_science/

# Theoretical Material Science: Exercise Sheet 10

**Please hand in solutions by: Wednesday, June 20**, start of the exercise class

**Exercise 23** (8 points): *Phonon dispersion relation for the diatomic chain*
Consider a one-dimensional ring with $2N$ alternating atoms of masses $M^A$ and $M^B$. Let the potential between any two neighbouring atoms be the same as that caused by a classical elastic spring with spring constant $C$. For simplicity, the atoms are assumed to move only in one dimension along the ring. Complications arising due to the curvature of the ring can be neglected. Please follow the derivation outlined below (quantum case).

a) What does the Hamiltonian of this problem look like? Use as coordinates the displacement of the atoms, $q_s^{A/B}$ from their equilibrium positions along the ring.

b) Go to a Fourier representation by using

$$q_s^{A/B} = \frac{1}{\sqrt{N}} \sum_k Q_k^{A/B} e^{iksa} \; . \tag{1}$$

$a$ is the distance between two atoms of the same kind. Which $k$ points are involved in the summation? Find the operators $P_k^A$ and $P_k^B$ which, together with $Q_k^A$ and $Q_k^B$, fulfill the canonical exchange relations.

c) Write the Hamiltonian in these new coordinates. What is noticeable about the $k$-summation?

d) Make the ansatz $Q_k^E = \alpha Q_k^A + \beta Q_k^B$. Calculate

$$\dot{Q}_k^E = \frac{[Q_k^E, H]}{i\hbar} \; . \tag{2}$$

e) From

$$\ddot{Q}_k^E = \frac{[\dot{Q}_k^E, H]}{i\hbar} \, , \tag{3}$$

derive an eigenvalue equation for $\omega_k$. Discuss $\omega_k$ for the limiting cases of $k \to 0$ and $k \to \pi/a$.

**Exercise 24** (4 points): *Specific heat in the DEBYE approximation*

a) Show that the overall number of phonon modes for one polarisation direction with wave vector smaller than $k$ can be written as

$$N = \left( \frac{L}{2\pi} \right)^3 \frac{4\pi k^3}{3} \; . \tag{4}$$

b) For the Debye dispersion $\omega = ck$, derive an expression for the density of states $D(\omega) = dN/d\omega$ and calculate the Debye frequency with the help of

$$\int_0^{\omega_D} D(\omega) d\omega = N \; . \tag{5}$$

c) Determine the contribution of the phonons to the specific heat in this approximation. Write the thereby appearing integrals dimensionless.

d) Find a meaningful approximation for the integral in c). Use

$$\sum_{s=1}^{\infty} \frac{1}{s^4} = \frac{\pi^4}{90} \; . \tag{6}$$

**Please turn over!**⟶

- **Webpage of the lecture:**
  http://www.itp.tu-berlin.de/menue/lehre/lv/ss12/wahlpflichtveranstaltungen/theoretische_festkoerperphysik_i_ii_theoretical_material_science/
  http://th.fhi-berlin.mpg.de/sitesub/lectures/spring_2012/
- **Lecture:** Tue. & Wed., 10:00 h -12:00 h (sharp!) in room EW 203, TU Berlin
- **Exercise:** Wed., 14:00 h in room EW 229
- **Literature:**
  - Ashcroft, Mermin, David: Solid state physics, Saunders College, Philadelphia, 1981
  - Kittel: Quantum theory of solids, Wiley, New York, 1963
  - Ziman: Principles of the theory of solids, Cambridge University Press, Cambridge, 1964
  - Ibach, Lueth: Solid-state physics: an introduction to principles of materials science, Springer, Berlin, 1995
  - Madelung: Festkörpertheorie, Springer, Berlin, 1972
  - Scherz: Quantenmechanik, Teubner, Stuttgart, 1999
  - Dreizler, Gross: Density functional theory: an approach to the quantum many-body problem, Springer, Berlin, 1990
  - Parr, Yang: Density-functional theory of atoms and molecules, Oxford University Press, Oxford, 1994
  - Anderson: Basic notations of condensed matter physics, Benjamin/Cummings, London, 1984
  - Marder: Condensed matter physics, Wiley, New York, 2000
  - Martin: Electronic Structure, Cambridge University Press, Cambridge, 2004
  - Kohanoff: Electronic Structure Calculations for Solids and Molecules: Theory and Computational Methods, Cambridge University Press, Cambridge, 2006
- **"Übungsschein"-criteria:**
  - Regular and active participation in the exercises
  - Presentation of homework tasks and
  - 50% of the homework points.
  - Active participation in computational exercises
- **Consultation hours:**
  - Prof. Dr. Matthias Scheffler, Dr. Alex Tkatchenko, Dr. Patrick Rinke: by appointment
  - Dr. Volker Blum: Available Wed. 16:00 (after the exercise class) or by appointment