Technische Universität Berlin
Institut für Theoretische Physik
Prof. Dr. Matthias Scheffler
Dr. Volker Blum, Dr. Clive Emary
Dipl. Phys. Philipp Zedler

June 10, 2008

http://www.itp.tu-berlin.de/menue/lehre/lv/ss08/wpfv/tfkp/

Theoretical Material Science: exercise sheet 9

Return: Monday, June 23 in the exercise

Exercise 21 (8 points): *Dispersion relation for phonons*

Consider a one-dimensional ring with $2N$ alternating atoms of masses M^A and M^B. The potential between each two neighbouring atoms is the same, e.g. as if caused classically by elastic springs 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).

- 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.
- Go to a Fourier-representation by using

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

  with a 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, fulfil the canonical commutation relations.
- Write the Hamiltonian in these new coordinates. What is noticeable about the k-summation?
- Make the ansatz $Q_k^E = \alpha Q_k^A + \beta Q_k^B$ and calculate

$$\dot{Q}_k^E = \tfrac{1}{i\hbar} \left[Q_k^E, H \right]. \tag{2}$$

- From

$$\ddot{Q}_k^E = \tfrac{1}{i\hbar} \left[\dot{Q}_k^E, H \right] \tag{3}$$

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

Exercise 22 (4 points): *Convergence of lattice sums*
Calculate the lattice sums $A_n^{crystal}$ from Exercie 19 numerically up to neighbour distances of the order o of 15 for simple cubic (SC), face centered cubic (fcc) and body centered cubic (bcc) lattices, and for n = 6, n = 12:

$$A_n^{crystal}(o) = \sum_{\mathbf{R}_I \in \text{crystal of neighbour order } o} \alpha_I^{-n}, \tag{4}$$

$$|\mathbf{R}_I| = \alpha_I c.$$

with c being the nearest neighbor distance. Plot the resulting lattice sums as function of order o and check for convergence. Compare with literature values.

Please turn over!⟶

- **Webpage of the lecture:** http://www.itp.tu-berlin.de/menue/lehre/lv/ss08/wpfv/tfkp/
- **Lecture:** Tue. & Fri., 10:00 a.m.-12:00 p.m. in room EW 203, TU Berlin
- **Exercise:** Mon., 14:00 a.m. in room H 1029
- **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
- **"Übungsschein"-criteria:**
  - Regular and active participation in the exercises
  - Presentation of homework tasks and
  - 50% of the homework points.
- **Consultation hours:**
  - Prof. Dr. Matthias Scheffler: on appointment
  - Dr. Volker Blum: on appointment
  - Philipp Zedler: Wed, 11:00 - 12:00 a.m. in room EW 711
  - Dr. Clive Emary, Wed, 16:00 - 17:00 in room EW 705