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

Theoretical Material Science: exercise sheet 10

Return: Monday, June 30 in the exercise

Exercise 23 (8 points): *Lattice Vibrations*

Consider a monatomic fcc lattice with lattice constant a and atoms of equal mass M, which interact only with their direct neighbors via a central potential $\tilde{\phi}(|\mathbf{R}_n - \mathbf{R}_{n'}|)$.

(a) Show that the squared-frequencies for the three modes with wave vector k are the eigenvalues of the following matrix:

$$D^{\nu}_{\mu}(\mathbf{k}) = \frac{1}{M} \sum_{\mathbf{R}} \sin^2\left(\tfrac{1}{2}\mathbf{k}\cdot\mathbf{R}\right)\left(A\delta_{\mu,\nu} + BR_\mu R_\nu\right),$$

with summation over the 12 nearest neighbors of $\mathbf{R} = 0$,

$$A = 2\tilde{\phi}'(d)/d, \qquad B = 2\left(\tilde{\phi}''(d)/d^2 - \tilde{\phi}'(d)/d^3\right),$$

with d the nearest neighbor distance.

(b) Derive the relationship between $\tilde{\phi}'(d)$ and hydrostatic pressure p. Consider the case with $A = 0$, which corresponds to the low pressure limit.

(c) Calculate the eigenmodes and eigenfrequencies for $\mathbf{k} = k(1,0,0)$ and $\mathbf{k} = (k/\sqrt{2})(1,1,0)$ (with $k \in 0, 2\pi/a$), and plot the resulting dispersion relations as functions of k.

(d) Which symmetries do the (1, 0, 0) and (1, 1, 0) axes have? What is their relationahip to the eigenmodes?

Exercise 24 (4 points): *Specific heat in the Debye-model*

(a) Show that the overall number of phonon modes of a single polarisation with wave vector smaller than k can be written as

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

(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 ω_D with the help of

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

(c) Determine the contribution of the phonons to the specific heat in this model. Write the resulting integral in dimensionless form.

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

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

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: Festk?rpertheorie, 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