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

June 20, 2012

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

Theoretical Material Science: Exercise Sheet 11

Please hand in solutions by: Wednesday, June 27, start of the exercise class

Exercise 25 (8 points): *Lattice vibrations*
Consider a monatomic fcc lattice with lattice parameter a and atoms of equal mass M. Each atom interacts with its nearest neighbours only, 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 $\mathbf{k}$ are eigenvalues of the following matrix:

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

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

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

with d the nearest neighbour distance.

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

c) Calculate the eigenmodes and eigenfrequencies for $\mathbf{k}$=k(1,0,0) and $\mathbf{k}$=$k/sqrt2$(1,1,0) (where k in $[0, \frac{2\pi}{a}]$), 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 relationship to the eigenmodes?

Exercise 26 (4 points): *Magnetism: Free energy and susceptibility*
The magnetic Helmholtz free energy F is defined by the fundamental statistical mechanics rule:

$$e^{-F/k_BT} = \sum_n e^{-E_n(H)/k_BT}\,.$$

If one rewrites this expression in the form

$$e^{-\beta F} = \sum_n e^{-\beta E_n} = \sum_n \langle n|e^{-\beta\kappa}|n\rangle = \mathrm{Tr}\; e^{-\beta\kappa}\,, \qquad (\beta = \frac{1}{k_BT})\,,$$

then it is easy to deduce Curie's law directly at high temperature without going through the algebra of Brillouin functions, for when $\kappa \ll k_BT$, one can expand $e^{-\beta\kappa} = 1 - \beta\kappa - (\beta\kappa)^2/2 - \cdots$. Here, we have used κ to denote the Hamiltonian to distinguish it from the magnetic field.
Evaluate the free energy to second order in the field, using the fact that

$$\mathrm{Tr}\,(\mathbf{J}_{\mu}\mathbf{J}_{\nu}) = \frac{1}{3}\,\delta_{\mu\nu}\;\mathrm{Tr}\,\mathbf{J}^2\,,$$

and extract the high-temperature susceptibility

$$\chi = \frac{\mu_0}{V}\frac{(g\mu_B)^2}{3}\frac{J(J+1)}{k_BT}\,, \qquad (k_BT \gg g\mu_BH)\,.$$

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