

Theoretical Material Science: exercise sheet 13

This is a voluntary exercise for the holidays.

Exercise 28: Free energy of an Ising ferromagnet

We regard the Hamiltonian of spins in a bcc-lattice, where each spin has 8 neighbours:

$$\hat{H} = -B_0 \sum_i \hat{s}_z^{(i)} - J \sum_{\langle i,j \rangle} \hat{s}_z^{(i)} \hat{s}_z^{(j)},$$

where J is a positive constant. Note the difference to the Hamiltonian of exercise 26. This time we have a minus sign in front of the coupling term, which will make a ferromagnetic state favourable and sublattices needless. Perform the mean field approximation. Evaluate the partition sum and then show that the Free Energy $F := -\frac{1}{\beta} \ln Z$ is

$$F = \frac{N}{\beta} \{ \beta H_0 - \ln [2 \cosh(\beta B_{eff})] \}$$

with the inverse temperature $\beta = \frac{1}{k_B T}$. Use the same definitions for B_{eff} and H_0 as in exercise 26. Show that the critical temperature is $T_C = \frac{8J}{2Nk_B}$. Write the Free Energy without external field as

$$F = N \left[\frac{T_C}{2} \left(\frac{M}{M_\infty} \right)^2 - T \ln \left(2 \cosh \frac{T_C}{T} \frac{M}{M_\infty} \right) \right].$$

Exercise 29: Landau theory and critical exponents

Critical exponents describe how physical quantities behave near a phase transition. Remarkable about them is that they don't depend on microscopic details of the system, but only on universal properties like dimension and the range of the interactions. In Landau theory we assume that there exists a functional L depending on the coupling constants of a given hamiltonian and on the *order parameter* η , (here: magnetization). We further assume that the system will choose the state, where L takes its absolute minimum with respect to η . The Landau functional approximates the free energy. Expand the result of exercise 28 to fourth order in m around $m = 0$ and to first order in T around $T = T_C$, keep B_0 only to first order to identify the constants in the Landau functional:

$$L = at\eta^2 + \frac{1}{2}b\eta^4 - B_0\eta. \quad (1)$$

a and b are phenomenological parameters, $t = \frac{T-T_C}{T_C}$ is the reduced temperature. The magnetization η can take values between $-1/2$ and $1/2$.

- a) Consider the system without external field H . Draw sketches of $L(\eta)$, where magnetization is
 - favoured but without preferred direction,
 - favoured with preferred direction,
 - not favoured.
- b) Derive equation 1 with respect to η . Determine the minimum of $L(\eta)$ in the absence of the external field H . Which arrangements of the parameters a , b and t are required to favour/not favour magnetization?

Please turn over! →

- c) The critical exponent β describes how the magnetization at $H = 0$ depends on the reduced temperature t near $t = 0$:

$$\eta \sim t^\beta \quad \text{around } T = 0.$$

Show that $\beta = 1/2$.

- d) The critical exponents γ and γ' describe how the magnetic susceptibility $\chi_t(H) = \left. \frac{\partial \eta(H)}{\partial H} \right|_{t \text{ const.}}$ depends on the external field H :

$$\chi_{t>0}(H) \sim t^{-\gamma} \quad \text{around } H = 0,$$

$$\chi_{t<0}(H) \sim t^{-\gamma'} \quad \text{around } H = 0.$$

Show that $\gamma = \gamma' = 1$. For this, use the derivative of an inverse function and that the magnetization η at $H = 0$ is known.

• **Webpage of the lecture:** <http://www.itp.tu-berlin.de/menue/lehre/lv/ss08/wpfv/tfkp/>

• **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