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

June 27, 2012

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

Theoretical Material Science: Exercise Sheet 12

Please hand in solutions by: Wednesday, July 4, start of the exercise class

Exercise 27 (9 points): *Antiferromagnet in the mean field approximation*
We consider the magnetic interaction of adjacent spins on a bcc lattice consisting of N particles. If every spin interacts only with its nearest neighbour, we can divide the lattice into two sublattices A and B such that interactions only occur between spins of *different* sublattices. Each spin of sublattice A will only interact with its 8 nearest neighbours of sublattice B and vice versa. We describe this with the Hamiltonian

$$\hat{H} = -B_0 \left(\sum_{i \in A} \hat{s}_z^{(i)} + \sum_{j \in B} \hat{s}_z^{(j)} \right) + J \sum_{\langle i,j \rangle} \hat{s}_z^{(i)} \hat{s}_z^{(j)}, \tag{1}$$

where J is a positive constant and $\langle i,j \rangle$ denotes that i and j are nearest neighbours.

a) What is the ground state in the absence of the external magnetic field B_0?

b) In the mean field approximation we replace the operator product $\hat{s}_z^{(i)} \hat{s}_z^{(j)}$ by $\hat{s}_z^{(i)} m_B + m_A \hat{s}_z^{(j)} - m_A m_B$, where m_A and m_B are the average values of s_z in the corresponding sublattices. This approximation leads to the new Hamiltonian

$$\hat{H}^{\mathsf{MF}} = -\sum_{i \in A} \hat{s}_z^{(i)} B_A^{\mathsf{eff}} - \sum_{j \in B} \hat{s}_z^{(j)} B_B^{\mathsf{eff}} + H_0. \tag{2}$$

Determine B_A^{eff}, B_B^{eff}, and H_0.

c) In the mean field approximation, the probability that the spin on site i in sublattice A takes the value s_i (with $s_i = \pm\frac{1}{2}$) is given by $P(s_i) = \frac{1}{z_i} \langle s_i | e^{-\beta H^{\mathsf{MF}}} | s_i \rangle$, where β is the inverse temperature. Determine the normalization constant z_i. Use your result to show that the partition sum is

$$Z = \left[2 \cosh\left(\frac{\beta B_A^{\mathsf{eff}}}{2} \right) 2 \cosh\left(\frac{\beta B_B^{\mathsf{eff}}}{2} \right) e^{-2\beta H_0} \right]^{N/2}. \tag{3}$$

d) The expectation value for the magnetization in sublattice A is $m_A = \frac{1}{N/2} \sum_{i \in A} P(s_i) s_z^{(i)}$. Argue that (and why) solutions for the magnetization satisfy $m_A = -m_B$ in the absence of the external field B_0. In this case, show that

$$m_A = \frac{1}{2} \tanh(4\beta J m_A) \tag{4}$$

and draw the graphic solution of this fixed point equation. What is the corresponding equation for m_B? What is the critical temperature T_C above which the magnetization disappears?

e) Perform the low temperature limit: Approximate $\tanh(x) \approx 1 - 2e^{-2x}$ for large x and approximate m_A by the result of part a). Show that, in this case, $m_A \approx \frac{1}{2}(1 - 2e^{-2T_C/T})$.

f) Evaluate the magnetic susceptibility. To that end, perform the same limits as in part e), but in the presence of an external magnetic field B_0.

Please turn over!⟶

Exercise 28 (3 points): *Exact ground state energy of a simple antiferromagnet*
Show that the ground state energy of the four spin antiferromagnetic nearest-neighbour Heisenberg linear chain (ring boundary conditions),

$$H = J(\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_4 + \mathbf{S}_4 \cdot \mathbf{S}_1) \tag{5}$$

is

$$E_0 = -4JS^2 \left[1 + \frac{1}{2S}\right]. \tag{6}$$

Hint: Write the Hamiltonian in the form

$$H = \frac{1}{2}J[(\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4)^2 - (\mathbf{S}_1 + \mathbf{S}_3)^2 - (\mathbf{S}_2 + \mathbf{S}_4)^2]. \tag{7}$$

- **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