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

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

Theoretical Material Science: exercise sheet 12

Return: Monday, July 14 in the exercise

Exercise 26 (1+2+2+2+1+1 points): *Antiferromagnet in mean field approximation*
We consider the magnetic interaction of adjacent spins in a bcc lattice consisting of N particles. If every spin interacts only with its nearest neighbour, we can divide the lattice in 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

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

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 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. Conducting the mean field approximation leads to the new Hamiltonian

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

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

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

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

d) The expectation value for the magnetization in sublattice A is $m_a = \frac{1}{N/2} \sum_{i \in A} P(s_i) s_z^{(i)}$. Convince yourself that solutions for the magnetization satisfy $m_A = -m_B$. Show that in absence of the external field B_0

$$m_A = \frac{1}{2} \tanh\left(4\beta J m_A\right) \qquad (1)$$

and draw the graphic solution of this fixed point equation. What is the corresponding equation for m_B? What is the Curie 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 reult of part a). This leads to $m_A \approx 1 - 2e^{-\beta T_C}$.

f) Evaluate the magnetic susceptibility. Therefore perform the same limits as in part e), but in presence of the external magnetc field B_0.

Please turn over!⟶

Exercise 27 (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,

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

is

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

Hint: Write the Hamiltonian in the form:

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

- **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