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

July 4, 2012

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

Theoretical Material Science: Exercise Sheet 13

Classroom exercise – be there and explore

Exercise 29 (optional points): *Dilute magnetic semiconductors*
Having a semiconducting material that is ferromagnetic at the same time could open up a new field of electronics (*spintronics*). Unfortunately, there are some small difficulties, like finding a ferromagnetic semiconductor with a Curie temperature above room temperature. But this should be an easy task for theory – right?

The system ($Ga_{1-x}Mn_x$)As is perhaps the most studied ferromagnetic semiconductor material. The basic structure is zincblende. A few Ga atoms are replaced by Mn, with x between 2 % and 10 % in experiment. (For much more Mn, the material becomes unstable and forms a different structure.) The highest reported Curie temperature is T_C=173 K (for 8 % Mn).

a) In GaAs, Mn substitutes a (formally) three-fold positive Ga ion. Consider an *isolated* Mn^{3+} ion. Which electronic occupation and spin state do you expect? Remind yourself of the crystal field splitting diagram of a Mn^{3+} ion in a tetrahedral environment. Draw the levels and their occupation.

b) As theorists, we can easily introduce any amount of Mn and keep the zincblende structure. In a key paper on GaMnAs (Ohno *et al.* APL **69**, 363 (1996)), the lattice parameter for GaAs is given as a_{GaAs}=5.66 Å (x=0), and that for *hypothetical* zincblende MnAs a_{MnAs}=5.98 Å (x=1). Use Vegard's law to estimate lattice parameters for x=0.25, 0.125, and 0.03125.

c) Use DFT-LDA to compute the total and the atom- and angular-momentum-resolved partial density of states for ferromagnetic $Ga_{0.75}Mn_{0.25}As$ in a cubic 8-atom unit cell at the lattice parameter found above. Where are the Mn d levels in relation to all other states? Is there a gap in any of the spin channels? How many occupied spin-up and spin-down Mn d-levels are there? What is the difference to the "simple" Mn^{3+} ion?

d) $Ga_{0.75}Mn_{0.25}As$ is not quite "dilute". Using pre-computed results for a 64-atom cell ($Ga_{\frac{31}{32}}Mn_{\frac{1}{32}}As$), investigate if the results for the smaller supercell prevail.

e) Write down a (classical) nearest-neighbour only interaction Hamiltonian for the simple cubic $Ga_{0.75}Mn_{0.25}As$ 8-atom supercell above. How many nearest neighbours are there? What would be the simplest antiferromagnetic state? (Draw.)

f) Create a supercell geometry that can contain this antiferromagnetic ground state (16 atoms total). What type of primitive lattice do the lattice vectors define? Compute the total energy once for a ferromagnetic state and once for an antiferromagnetic state. What is the energy difference $E_{\mathsf{FM}} - E_{\mathsf{AFM}}$? Use the difference to compute the interaction parameter in your Hamiltonian.

g) For the interaction parameter derived from task f), calculate the Curie temperature. For a simple cubic lattice and a classical nearest-neighbour Ising Hamiltonian $-J\sum_{\langle i,j\rangle} S_iS_j$ with $S_i = \pm 1$, Monte Carlo results give $k_BT_C = J/0.221654$. Do you think that this is the highest T_C that one can achieve?

Outlook: We have only really investigated T_C for a single arrangement of Mn atoms on the lattice. One question of real interest is, could we predict a specific Mn arrangement for which T_C would be highest? We do not have the time to do so in this exercise, but we have prepared a few more supercells in the outlook part to illustrate the idea. Take a look, while the (long) calculation of part f) is running.

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