Technische Universität Berlin
Institut für Theoretische Physik
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Exercises: Dr. Christian Carbogno, Henrik Kowalski et al.

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http://www.itp.tu-berlin.de/menue/lehre/lv/ss_2017/pflichtveranstaltungen_masterstudium/theoretische_physik_vi_vertiefung_theoretische_festkoerperphysik_i_ii/

Theoretical Material Science: Exercise Sheet 11

Please hand in solutions by: Tuesday, July 11, start of the exercise class

Exercise 25 (12 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? Plot the results. 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 $Ga_{0.75}Mn_{0.25}As$ 8-atom supercell from part c). Consider only the Mn atoms as nearest neighbors (ignore the Ga and As atoms). How many nearest neighbours are there? What would be the simplest antiferromagnetic state? (Draw.)

f) Take a look at the pre-computed results from the 16 atom supercell that contains the ferromagnetic and antiferromagnetic state. What is the energy difference $E_{\mathsf{FM}} - E_{\mathsf{AFM}}$? Use the difference to compute the interaction parameter in your Hamiltonian and calculate the Curie temperature. For a simple cubic lattice and a classical nearest-neighbour Ising Hamiltonian $-J\sum_{\langle i,j\rangle} S_i S_j$ with $S_i = \pm 1$, Monte Carlo results give $k_B T_C = J/0.221654$.