KIT
Karlsruher Institut für Technologie WS2023/24

Elektronische Eigenschaften von Festkörpern
Prof. Dr. Le Tacon, TTProf. Dr. Willke

Tutorial 6

1. **Magnetism and Hund's rule**

   a) What forms of magnetism have you encountered up to now? Describe their origin briefly in one sentence.

   b) The electron configuration of elementary Chromium Cr is $[Ar]3d^54s$. In ionic bonding Chromium donates at first its electron of the outer 4s shell. Afterwards, if more electrons have to be donated to reach the intended valence, they are taken from the 3d shell. The experimentally determined value of the magnetic moment of the Cr^{3+} ion is $\mu = 3.8\,\mu_B$. Determine the quantum numbers S, L and J of the Cr^{3+}-ion in its ground state. Using the determined quantum numbers, calculate the magnetic moment μ in units of μ_B. How does this compare?

   c) Using Hund's rules, give the electronic ground state of the following ions:

   (1) Pr^{3+}
   (2) Eu^{2+} in configuration $[Xe]4f^7$
   (3) Eu^{3+} in configuration $[Xe]4f^6$
   (4) Tb^{3+}
   (5) Er^{3+}

   State the corresponding terms in spectroscopic notation $^{2S+1}L_j$.

2. **Heisenberg Exchange Interaction**

In the lecture, we introduced the Heisenberg model

$$H_{ex} = J \cdot \vec{S} \cdot \vec{I}$$

Where $\vec{S}$ and $\vec{I}$ are two electron spin ½. Additionally we set $\hbar = 1$.

   a) Calculate the Eigenenergies of the spin system and give the respective eigenstates.

Hints: Use $\vec{S} = (S_x, S_y, S_z)$ and rewrite the equation in terms of the ladder operators $S_\pm = S_x \pm iS_y$, (use $S_xI_x + S_yI_y = \frac{1}{2}[S_+I_- + S_-I_+]$. The ladder operator changes the respective spin state, e.g. $S_+|\downarrow\uparrow\rangle = |\uparrow\uparrow\rangle$.). Next, let the Hamiltonian act on the states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$. Not all of them will be Eigenstates, but use the states discussed in the lecture to find the correct energies and ground state.

   b) How does this compare to the ground state of a pure Zeeman Hamiltonian?
   $$H_{Zeeman} = g_e\mu_B B_z \cdot (S_z + I_z)$$
   Draw a qualitative diagram that shows the transition between the energies calculated in a) to the limit where $E_{Zeeman} \gg E_{Ex}$. What happens to the ground state?

   c) Which of these levels are least susceptive to magnetic field noise? Think of possible applications.

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d) The figure below shows a scanning tunneling microscopy image of ordered layers of magnetic molecules, called cobalt phthalocyanine [adapted from PRL 103, 257202 (2009)]. The (super-)exchange interaction between vertically stacked molecules was determined to be J~18 meV. What magnitude would a magnetic field need to have to reach this value for spins with s=1/2 and a moment of $1\,\mu_B$? What is the magnetic dipolar contribution, assuming that both spins point out of plane?
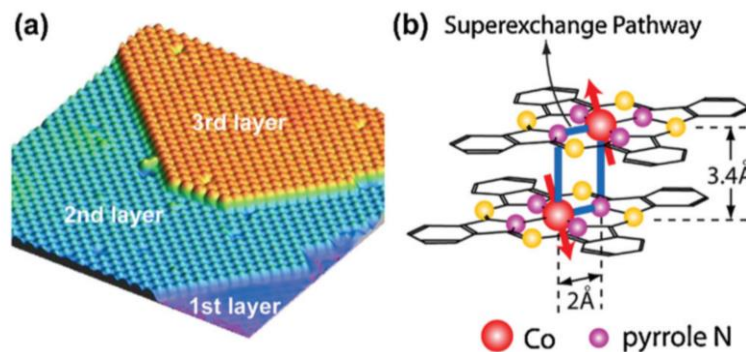
3. Magnetic Dipole Interaction

The potential energy between two magnetic dipoles μ_1 and μ_2 is given by:

$$E_{DD} = -\frac{\mu_0 \mu_1 \mu_2}{4\pi r^3}[3(\boldsymbol{S_1}\cdot\hat{r})(\boldsymbol{S_2}\cdot\hat{r}) - \boldsymbol{S_1}\cdot\boldsymbol{S_2}]$$

a) Express the energy as an effective magnetic field acting on one of the spins.

b) Calculate the maximum strength of the magnetic field that is produced by an atom of magnetic moment $\mu_1=\mu_B$ at the site of an neighboring atom (nearest neighbor only). Typical nearest neighbor distances r_0 for the ferromagnets Fe can be calculated by the following information: Fe has a bcc lattice with $a = 2.866$ Å

c) Compare the maximum energy of the dipole-dipole interaction to the thermal energy of the dipoles at the Curie temperature of these materials.

d) Does this mean that magnetic dipole-interaction is always smaller than magnetic exchange interaction? What parameter is crucial here?
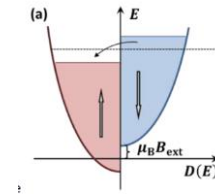
4. Pauli paramagnetism

a) In the lecture we derived the term for χ_{Pauli} by approximating the spin density as a simple rectangle in the DOS diagram. Do a proper calculation of the resulting magnetism using a redistribution of the spin densities as an integral:

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$$n_+ = \frac{1}{2V} \int_0^\infty D(E + \mu_B B_{\text{ext}}) f(E)\, dE$$

$$n_- = \frac{1}{2V} \int_0^\infty D(E - \mu_B B_{\text{ext}}) f(E)\, dE$$

b) In order to see why the Pauli paramagnetism is temperature independent, one can write it in a form that resembles the Curie-law. Write it in that form by using the Fermi-"temperature" $E_F = k_B T_F$. Make an argument why it is still temperature independent and compare experimental temperatures to T_F.

c) E_F is 7 eV for pure copper. How large is T_F? How is then the "fraction" of temperature dependence? How large is χ_{Pauli}? Copper is still diamagnetic, how can this happen?

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