Aufgaben zur Vorlesung Theorie zu Magnetismus, Suprateitung und Elektronische Korrelation in Festkörpern
SS 2018

Aufgabenblatt 4
(Abgaben datum: Mo., 14. May, 2018, 12:00 (PM))

Aufgabe 4.1: Hund’s rules (10 Punkte)

Given \( n \) electrons residing in a shell of orbital angular momentum quantum number \( l \) of an isolated ion with the total spin

\[
\vec{S} = \sum_{i=1}^{n} \vec{s}_i,
\]

the total orbital angular momentum

\[
\vec{L} = \sum_{i=1}^{n} \vec{l}_i,
\]

and overall total angular momentum

\[
\vec{J} = \vec{S} + \vec{L},
\]

the magnitudes \( S \), \( L \) and \( J \) in the ground states are defined by the three Hund’s rules as follows:

1) \( S \) has the largest possible value (Hund’s first rule)
2) \( L \) has the largest possible value permitted by the first rule (Hund’s second rule)
3) \( J = |L - S| \) for less than half-filled shells and \( J = L + S \) for more than half-filled shells (Hund’s third rule)

Show that:

The Hund’s rules can be summarized in the following formula’s

\[
S = \frac{1}{2}[(2l + 1) - |2l + 1 - n|], \quad (1)
\]

\[
L = S|2l + 1 - n|, \quad (2)
\]

\[
J = S|2l - n|. \quad (3)
\]
Consider a system of $N$ atoms with intrinsic magnetic moment $\mu$. The Hamiltonian for this system with external magnetic field $\vec{B}$ is given as

$$H = H_0 - \mu B \sum_{i=1}^{N} \cos \alpha_i,$$

with $H_0$ being the Hamiltonian without external field and $\alpha_i$ is the angle between the external field $\vec{B}$ and the magnetic moment of the $i$-th atom.

Show that:

a) The induced magnetic moment is given by

$$M = N \mu \left( \coth \theta - \frac{1}{\theta} \right),$$

with $\theta = \mu B / k_B T$.

Hint:

$$\coth x = 1 / \tanh x$$

b) The magnetic susceptibility per atom is given by

$$\chi = \frac{\mu^2}{k_B T} \left( \frac{1}{\theta^2} - \frac{1}{\sinh^2 \theta} \right).$$

(5)

c) For high temperature $T$ the susceptibility $\chi$ obeys the Curie law, i.e. $\chi \propto T^{-1}$. Find the corresponding Curie constant $C$ which fulfills $\chi = C / T$ for high temperatures.

Hint:

$$\frac{1}{\sinh^2 x} \approx \frac{1}{x^2} - \frac{1}{3} \quad \text{for } |x| \ll 1$$