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Theorie zu Magnetismus, Supraleitung und Elektronische Korrelation in Festkörpern

Sommersemester 2019

Blatt 6

(Abgabe: 28.05.2019)

Aufgabe 1 (**Hund's rules**) (5=2+2+1 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

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

(2) $$L = S|2l+1-n|,$$

(3) $$J = S|2l-n|.$$

Aufgabe 2 (**Boundaries for the Heisenberg antiferromagnet**) (5=2+1+1+1 Punkte)

We want to show that the ground state energy E_0 of the antiferromagnetic Heisenberg model,

$$H = \frac{1}{2}\sum_{i,j} |J_{ij}| \vec{S}_i \vec{S}_j,$$

is bounded by the following inequality

$$-\frac{1}{2}S(S+1)\sum_{i,j}|J_{ij}| \le E_0 \le \frac{1}{2}S^2 \sum_{i,j}|J_{ij}|.$$

To do this proceed in the following way:

a) The eigenvectors of a hermitian matrix form a complete orthogonal basis. Derive from this fact that the largest (smallest) possible diagonal matrix element of any hermitian matrix equals the largest (smallest) eigenvalue.

b) Show that the smallest diagonal matrix element of $\vec{S}_i\vec{S}_j$ is given by $-S(S+1)$.

c) Derive from a) and b) a lower bound for E_0.

d) Find an upper bound via a variational ansatz. Use an appropriate trial for the groundstate.