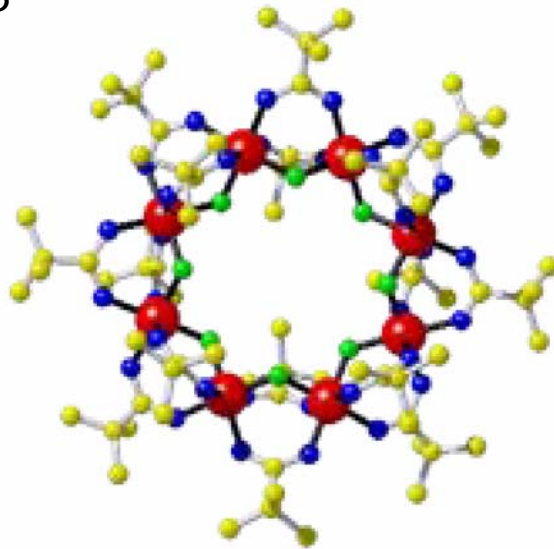


The spectra of antiferromagnetic molecular nanomagnets

Imke Schneider

Cr_8



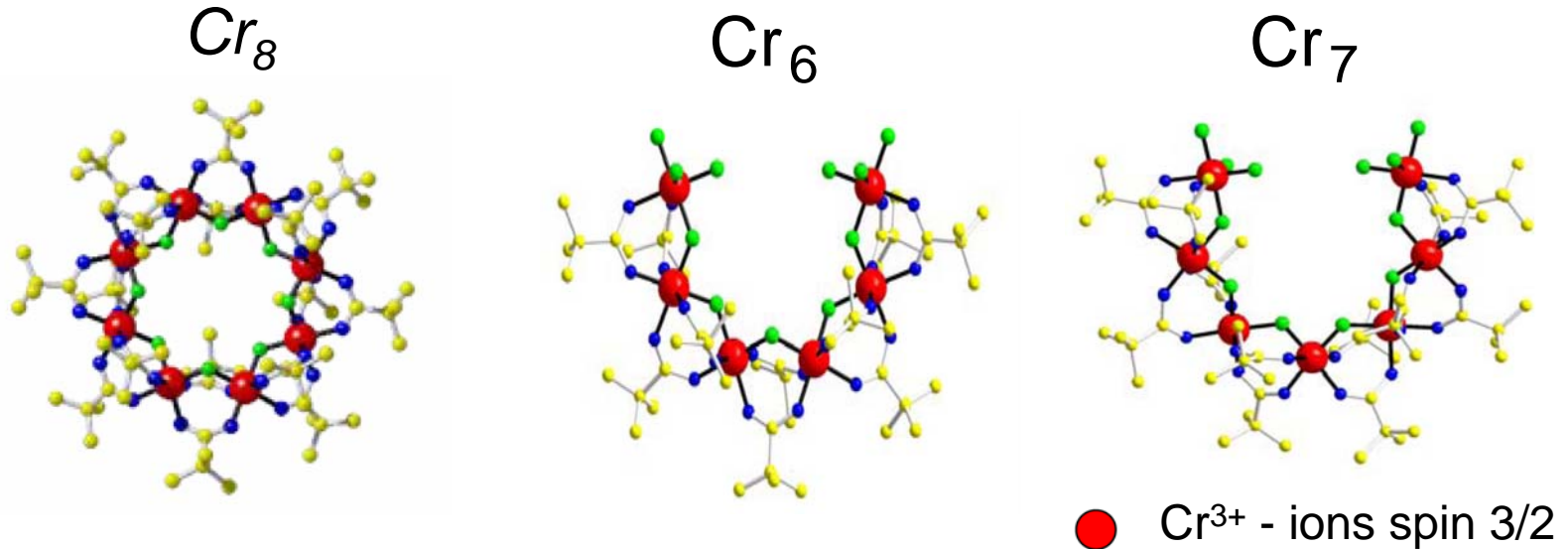
Anna Machens
Oliver Waldmann
Sebastian Eggert



Cr³⁺ - ions
spin 3/2

Figure courtesy of A. Machens

Horseshoe molecules



Effective model: Heisenberg chain

$$H = -J \sum_{i=1}^{N-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

$$Cr_6: J = -1.18 \text{ meV}$$

$$Cr_7: J = -1.27 \text{ meV}$$

Boundaries strongly affect spectra !

SU(2) symmetry of the isotropic Heisenberg chain

Hamiltonian:
$$H = -J \sum_{i=1}^{N-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} \quad \mathbf{S}_i^2 = s(s+1)$$

\mathbf{S}_i : Spin operator on site i with spin $s = 3/2$

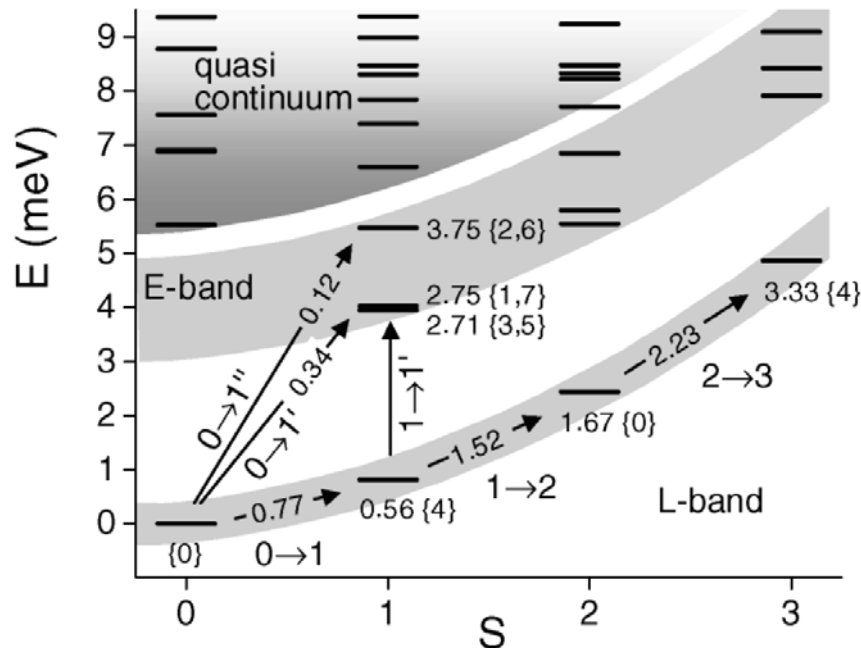
Total spin S and S^z are good quantum numbers

Group eigenstates in multiplets of $2S + 1$ degenerate states

Rotational bands in the Spectrum of Cr₈

Energy spectrum of Cr₈ vs total spin S

Arrows: observed transitions by inelastic neutron scattering



Rotational bands:

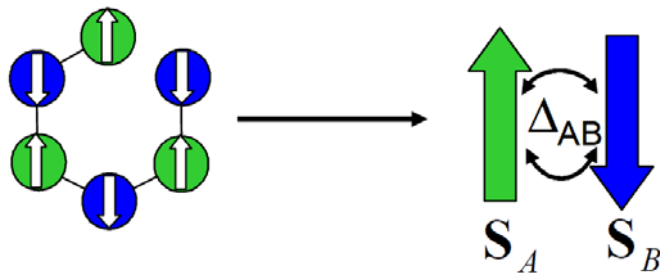
$$E(S) \propto S(S + 1)$$

Fig. taken from O. Waldmann et al. PRL 91, 2003

The H_{AB} - model (I)

Semiclassical approximation

applicable for bipartite lattices: $H_{AB} = \Delta_{AB} \mathbf{S}_A \cdot \mathbf{S}_B$



$$\mathbf{S}_A = \sum_{i=1,3,5,\dots} \mathbf{S}_i$$

$$\mathbf{S}_B = \sum_{i=2,4,6,\dots} \mathbf{S}_i$$

$$E(S) = \frac{\Delta_{AB}}{2} (S(S+1) - S_A(S_A+1) - S_B(S_B+1))$$

For fixed \mathbf{S}_A and \mathbf{S}_B :

Rotational bands $E(S) \propto S(S+1)$ shifted by constants

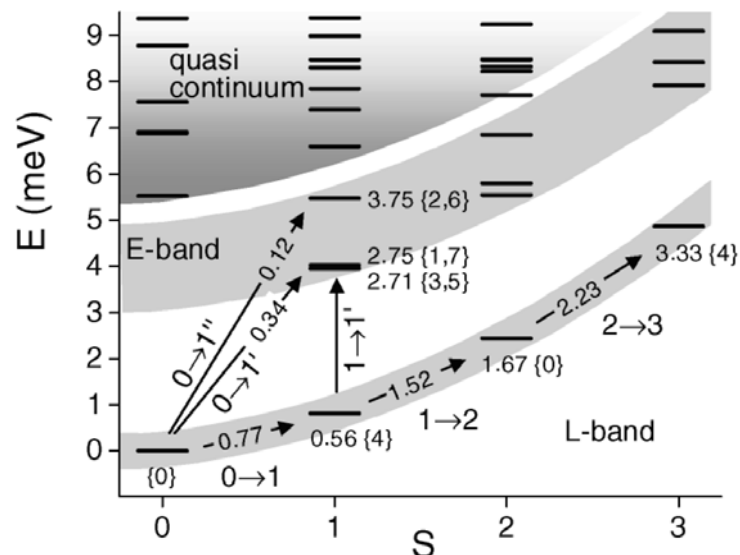
The H_{AB} – model (II)

$$E(S) = \frac{\Delta_{AB}}{2} (S(S + 1) - S_A(S_A + 1) - S_B(S_B + 1))$$

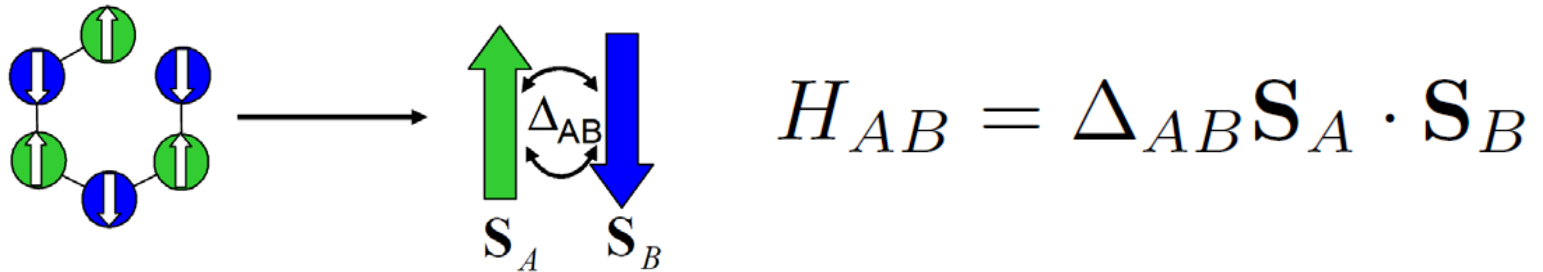
L- Band: $S_A = S_B = Ns/2$

E-Band: $S_A = Ns/2 - 1$ and $S_B = Ns/2$ or vice versa

Spectrum of Cr8
vs total spin S



The H_{AB} – model (III)



Coupling constants adjusted by matching the ferromagnetic state

$$\Delta_{AB} = \frac{4}{N} \quad \text{even + p.b.c}$$

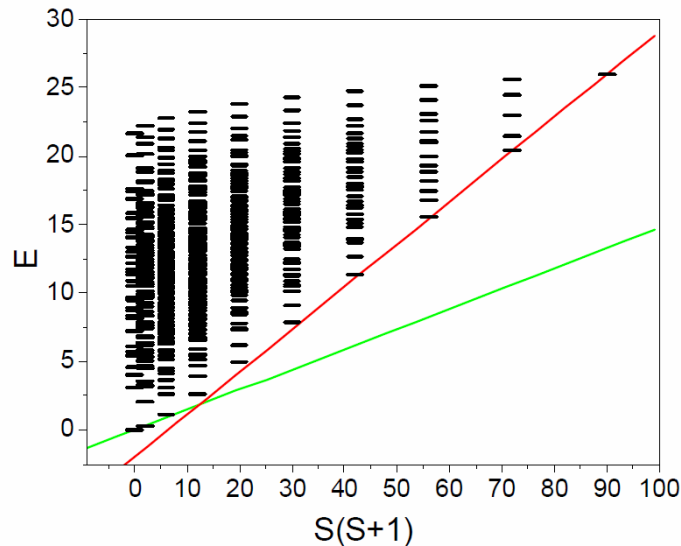
$$\Delta_{AB} = \frac{4(N-1)}{N^2} \quad \text{even + o.b.c.}$$

$$\Delta_{AB} = \frac{4}{N+1} \quad \text{odd + o.b.c.}$$

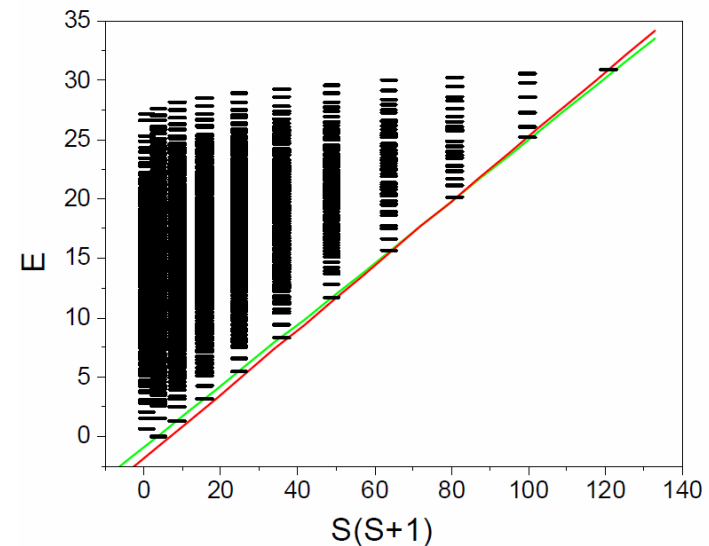
The even odd effect in the spectra

Striking difference between excitation spectra of Cr_6 and Cr_7

$N = 6$



$N = 7$



General feature for various spin values and system sizes:
Strong curvatures for even chains

Possible attempts to solve the puzzle

- Nonlinear Sigma model: Occurrence of edge spin for open boundaries which couple differently for even and odd chain lengths
- Valence bond picture: Again occurrence of edge spins
- Bosonization: different dimerization degrees

Why does H_{AB} model fail for even chains with open boundaries?