Antiferromagnetic versus Non-Collinear Arrangement of Chromium Clusters of Various Sizes

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Motivation:

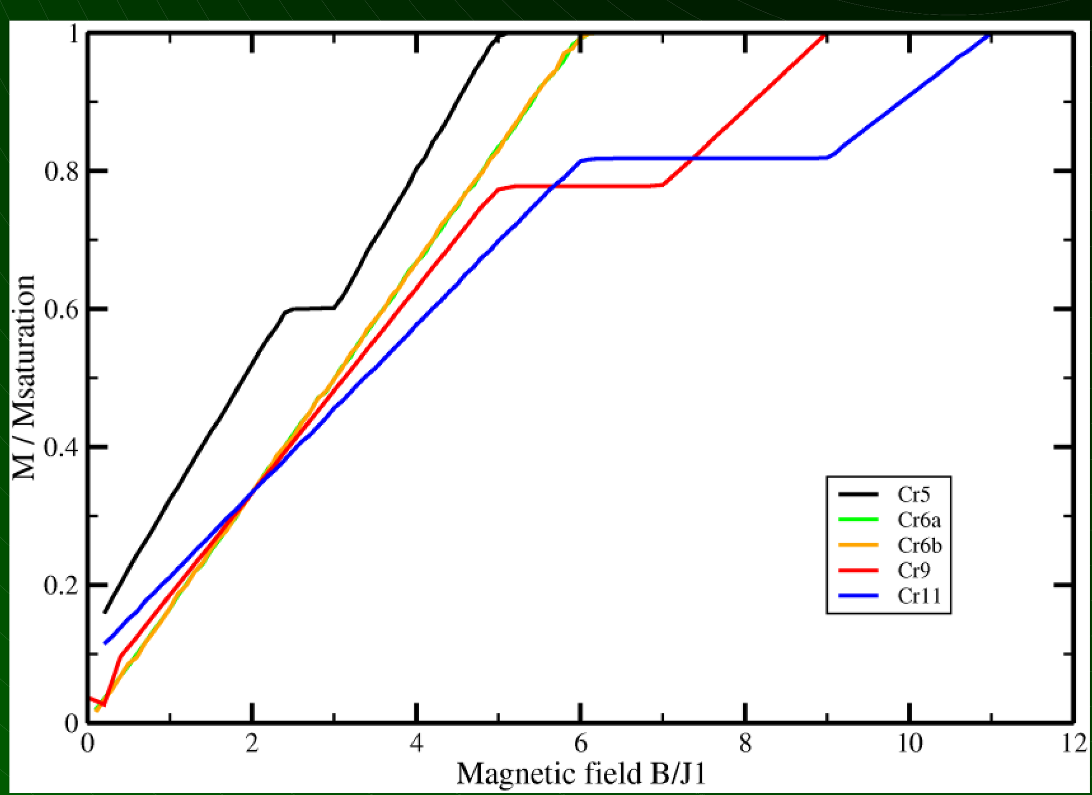
- Frustrated systems and their degenerated ground states
- Clusters of anti-ferromagnetic interacting atoms – super-paramagnetic states

Goals:

- Determine the intensity of the magnetic field that restores the collinearity of frustrated clusters
- Investigate the dependence of the total magnetization as a function of the field B
- Investigate the influence of the next-nearest neighbor interactions J2 in the presence of a magnetic field B

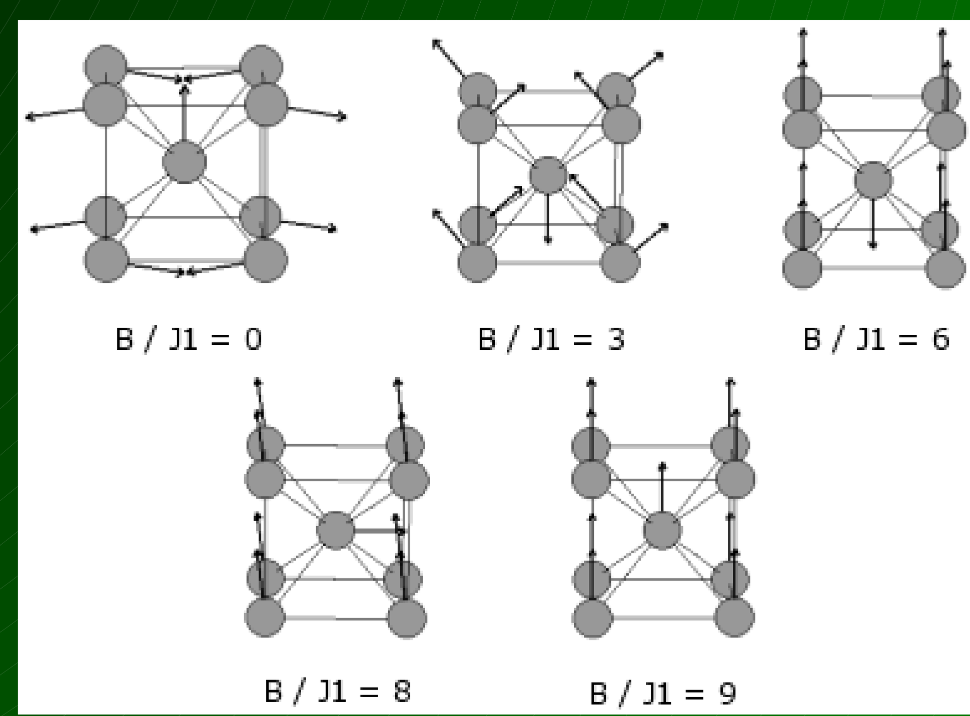
We use a Heisenberg potential with both nearest (J1) and next-nearest neighbor interactions (J2) in Monte Carlo simulations at zero temperature to determine the magnetic field value B that restores the collinearity of atomic moments in frustrated clusters, [1, 2]. Rather amazing is that the simulations with the classical potential predict magnetization plateaus – a quantum mechanical phenomenon [3].

$$H = -J_1 \sum_{<nn>} s_i s_j - J_2 \sum_{<nnn>} s_i s_j - B \sum_i s_i$$

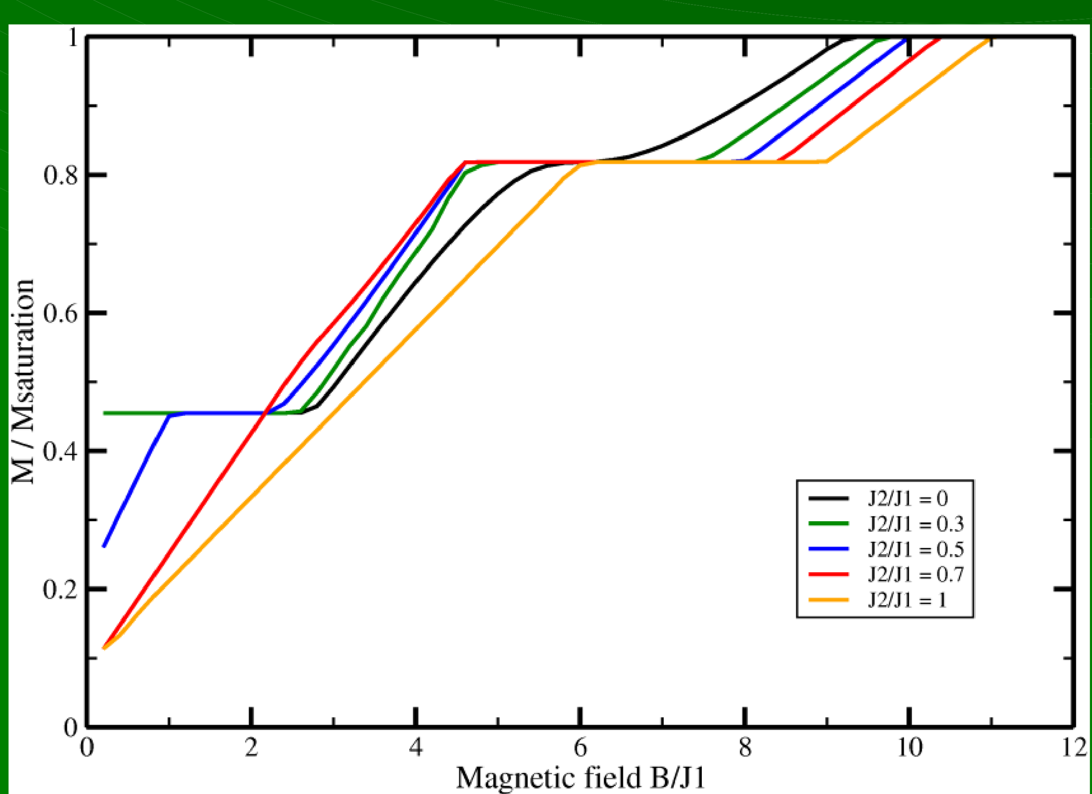


Magnetization plateaus are observed for various sizes N of the chromium clusters. For each cluster size there are specific B_1, B_2 satisfying the following relations:

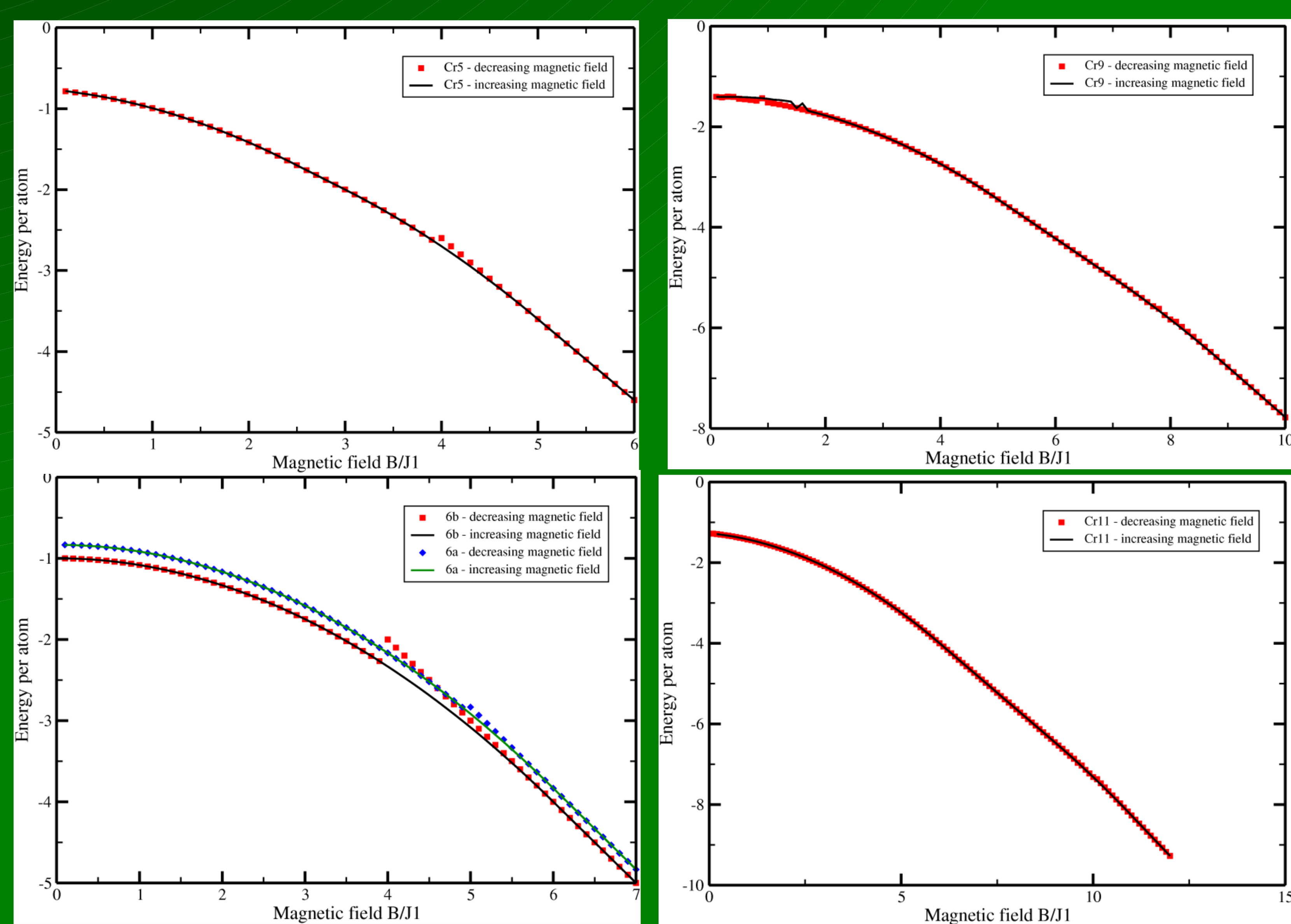
- M ~ B for $B < B_1$
- M is constant for $B_1 < B < B_2$ (the magnetic susceptibility vanishes)
- M approaches $M_{saturation}$ for large B



Cr9: The spin orientations change with the magnetic field B increase. The "B / J1 = 6" picture displays the orientation of the spins in the area of the plateau.



Cr11: The magnetization characteristics of the chromium clusters change when varying the strength of the next neighbors coupling. For small J2 a spin gap is observed.



The dependence of the energy per atom from the magnetic field changes with the size of the system. In small systems a phase transition is observed while in large systems it disappears. The bottom left picture shows that this function varies also with the topology of the cluster (6a is a topological ring but 6b is a topological ladder).

Findings:

- Quantum-mechanical effects (magnetization plateaus) appear in the frame of classical Monte Carlo simulations with the Heisenberg hamiltonian
- In small Cr clusters the phase transition from the aligned state at a high magnetic field to a non-collinear state at a lower field becomes continuous with the size increase
- The configuration topology plays a role for specific sizes

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2. A. Proykova and D. Stauffer, C.E.J. of Physics, 3 (2005) 209-220
3. H. Kageyama, K. Yoshimura, R. Stern, N.V. Mushnikov, M. Kato, K. Kosuge, C.P. Slichter, T. Goto and Y. Ueda, Phys. Rev. Lett., 82 (1999) 3168-3171