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].

Magnetization plateaus are observed for various sizes N of the chromium clusters. For each cluster size there are specific B1, B2 satisfying the following relations:
- M \sim B for B < B1
- M is constant for B1 < B < B2 (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.

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