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Tunnelling transport through a Mn_{12} molecular magnet in an external magnetic field. L. MICHALAK, C.M. CANALI, Kalmar University, Sweden, V.G. BENZA, Universita' dell' Insubria, Italy, M.R. PEDERSON, NRL, U.S.A. — Recent single-electron-transistor experiments with Mn_{12} as a central island exhibit a puzzling behaviour in the tunnelling conductance as a function of the external magnetic field, such as the lack of magnetic hysteresis. We describe the system in terms of a phenomenological giant spin model with two charge states: the N-electron state (neutral molecule) and the $(N+1)$-electron state (one extra electron added). The parameters of the model, such as the total spin and the magnetic anisotropy barrier, are calculated by state-of-the-art DFT. The addition of the tunnelling electron's spin to the giant spin is represented in terms of Schwinger bosons. We compute transport by means of a quantum rate equation in the sequential tunnelling regime, which is appropriate for experimental conditions. We find that the model cannot display hysteresis in the differential conductance as a function of the magnetic field when the coupling with the leads is the only source of relaxation. Coherence effects and cotunnelling are further analyzed by means of a master equation for the full density matrix. DFT calculations can also shed light on the influence of the tunnelling electron orbital degree of freedom on the tunnelling amplitudes.

C.M. Canali
Kalmar University, Sweden

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