Néel probability in antiferromagnetic ferric wheels Fe_6 and Fe_{10}

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9.7 cm

Antiferromagnetic ferric wheels Fe_n, $n = 6, 10, 18$, are profound examples of molecules consisting of transition-metal ions bridged by oxo-groups with complete compensation of single-ion spins, so the total spin $S = 0$. On the other hand these aggregates can be very well described as finite spin systems with dihedral symmetry group (D_n) and Hisenberg-like interactions between the nearest neighbours. The two first rings (Fe_6 and Fe_{10}) are investigated with application of group-theoretical and combinatorial methods followed by *exact* determination of states with given S and the total magnetization $M = 0$. The largest ferric wheel (Fe_{18}) is a subject of the so-called 'combinatorial explosion' (there are more than 10^{14} basic spin configurations) and left out in the present stage of calculations. Having determined eigenstates of a given Heisenberg Hamiltonan (for states with $M = 0$ and labelled by one-dimensional irreps of the symmetry group) we are able to investigate their properties such as the probability of finding a system in the classical antiferromagnetic ground-state, hence in the Néel state. The global Néel probability is also taken into account, i.e. we analyze all states with maximal sublattice magnetization (15/2 i 25/2 for $n = 6, 10$, respectively) and the total magnetization $M = 0$. The Néel probability (not global) shows exponential decreasing with respect to the energy per spin E for all values of the total spin S, so it can be written as $\ln p_N = -(\alpha E + \beta)$, $\alpha, \beta > 0$. Both coefficients depend exponentially on S, but their sum is constant (in good approximation).

13.4 cm

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