Evolution of the thermodynamics for mixed Heisenberg spin tetramers

P. Dyszel and J. T. Haraldsen

[1]Department of Physics, University of North Florida

ABSTRACT:
Molecular magnets provide a playground of interesting phenomena and interactions that have direct applications for quantum computation and magnetic systems. A general understanding of the underlying geometries for molecular magnets therefore generates a consistent foundation for which further analysis and understanding can be established. Using a Heisenberg spin-spin exchange Hamiltonian, we investigate the evolution of magnetic excitations and thermodynamics of quantum spin tetramer with mixed spins and produce exact general solutions for the energy eigenstates and spin decomposition, which can be used to determine the heat capacity and magnetic susceptibility. We show how the thermodynamic properties change with coupling parameters and how the underlying ground state governs the Schottky anomaly. Overall, we feel these calculations can help with the general analysis and characterization of molecular magnet systems.

GENERAL METHODS:
For this study, the Heisenberg model is used to explore the general effects of the exchange parameters on the thermodynamic properties of the antiferromagnetic spin XXYY tetramer. The spin Hamiltonian is the starting point for this process:

$$\mathcal{H} = J[\alpha_1'(\mathbf{S_1}\cdot\mathbf{S_2}) + \alpha_1(\mathbf{S_3}\cdot\mathbf{S_4}) + \alpha_2(\mathbf{S_1}\cdot\mathbf{S_3} + \mathbf{S_1}\cdot\mathbf{S_4} + \mathbf{S_2}\cdot\mathbf{S_3} + \mathbf{S_2}\cdot\mathbf{S_4})]$$

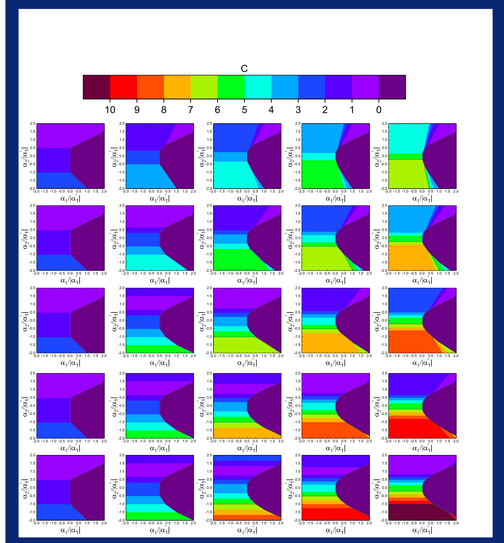
Here, The energy states can be found by knowing the total spin (S_T) of the tetramer, the total spin for the individual dimer states (S_{d1} and S_{d2}), and the individual spins (S_i) for each of the atoms making up the tetramer.

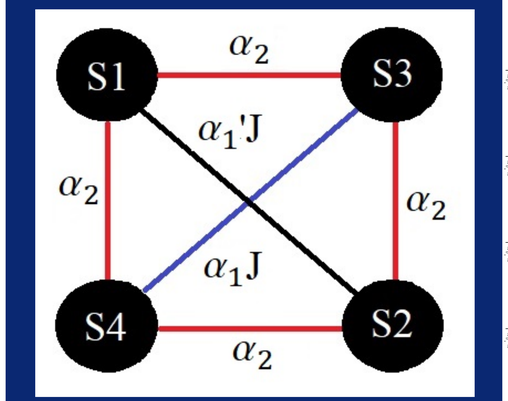
$$E = \frac{J}{2}[S_T(S_T+1)\alpha_2 + S_{d1}(S_{d1}+1)(\alpha_1'-\alpha_2) + S_{d2}(S_{d2}+1)(\alpha_1-\alpha_2) - [S_1(S_1+1) + S_2(S_2+1)]\alpha_1' - [S_3(S_3+1)+S_4(S_4+1)]\alpha_1] - m_z\mathbf{B}$$

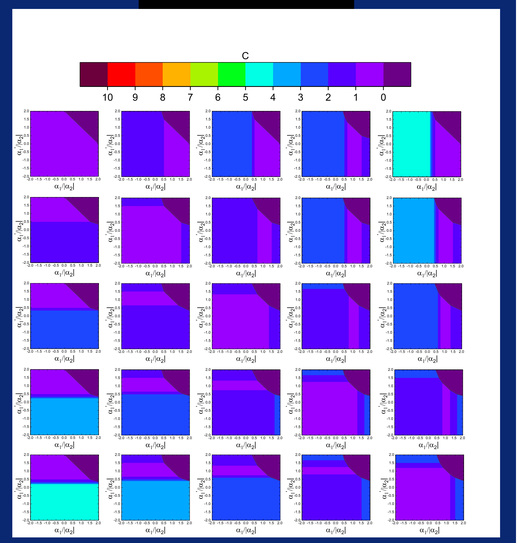
From the energy states, the phase diagrams and thermodynamic properties can be determined exactly for the model through the calculation of the partition function.

We examine the change in the thermodynamic properties of mixed spin tetramers with various exchange interactions

Take a picture to **go to** the **UNF Materials Theory website**







Heat Capacity and Phase Diagrams for various spin configurations