Ground state and thermodynamics of the S=1/2 pyrochlore Heisenberg antiferromagnet

We consider the S=1/2 antiferromagnet on the pyrochlore lattice, a strongly frustrated spin system which is a spin liquid candidate. Using a combination of exact diagonalization, high temperature series expansion and DMRG for large clusters of up to 128 spins, we find robust evidence for a spontaneously broken inversion symmetry in the ground state. Extrapolating the finite size groundstate energies, as well as high temperature series, we determine the groundstate energy per site to be -0.490(6)J, in very good agreement with the perturbative treatment by Tsunetsugu. At finite temperatures, down to T=0.25J, we obtain converged results in the thermodynamic limit, with no signs of this inversion symmetry breaking, which appears to happen at much lower temperatures.

[1] Possible Inversion Symmetry Breaking in the S=1/2 Pyrochlore Heisenberg Magnet Imre Hagymási, Robin Schäfer, Roderich Moessner, and David J. Luitz Phys. Rev. Lett. 126, 117204 (2021)

[2] Pyrochlore S=12 Heisenberg antiferromagnet at finite temperature Robin Schäfer, Imre Hagymási, Roderich Moessner, and David J. Luitz Phys. Rev. B 102, 054408 (2020)