Possible Inversion Symmetry Breaking in the $S = 1/2$ Pyrochlore Heisenberg Magnet

Imre Hagymási,[1] Robin Schäfer,[1] Roderich Moessner,[1] and David J. Luitz[1]

[1] *Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany*

We address the ground-state properties of the long-standing and much-studied three-dimensional quantum spin liquid candidate, the $S = \frac{1}{2}$ pyrochlore Heisenberg antiferromagnet. By using $SU(2)$ density-matrix renormalization group (DMRG), we are able to access cluster sizes of up to 128 spins. Our most striking finding is a robust spontaneous inversion symmetry breaking, reflected in an energy density difference between the two sublattices of tetrahedra, familiar as a starting point of earlier perturbative treatments. We also determine the ground-state energy, $E_0/N_{\text{sites}} = -0.490(6)J$, by combining extrapolations of DMRG with those of a numerical linked cluster expansion. These findings suggest a scenario in which a finite-temperature spin liquid regime gives way to a symmetry-broken state at low temperatures. [1]

References:

[1] I. Hagymási, R. Schäfer, R. Moessner, and D. J. Luitz, Phys. Rev. Lett. **126**, 117204 (2021).