

Condensed Matter Theory Seminar

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Keeping the theory on the ball: Using DMRG to solve large magnetic spherical molecules

We discuss recent advances to solve the Heisenberg model on ever larger molecules using the density-matrix renormalization group (DMRG), to which a short pedagogical introduction is given. Results are discussed for the undoped C₆₀ buckminsterfullerene, which can be thought of to be at a crossover point between frustration and order. Another application is the 60-site tetrahedra-based sodalite cage. It has a threefold degenerate, symmetry-broken ground state, which is in addition characterized by three nearly disconnected parts. This is in stark contrast to most other spherical molecules, which normally have a unique ground state that respects the spatial symmetries.

References: [1] doi: 10.21468/SciPostPhys.10.4.087 [2] arXiv:2111.04549

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