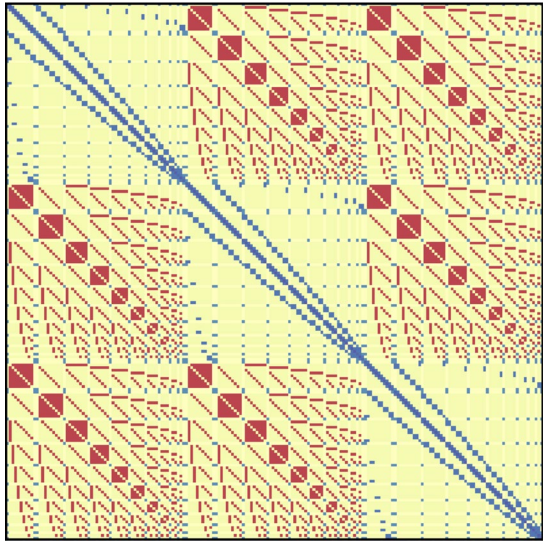
BLUE WATERS
SUSTAINED PETASCALE COMPUTING

Allocation: BW Professor/250 Knh

PI: Bryan Clark

University of Illinois at Urbana-Champaign

Physics & Engineering



The XXZ0 Hamiltonian has an exponentially degenerate ground-state space. Each of the exponential states in this ground state can be represented as a product state over three spins (here represented as red, blue, and green). Shown is one prototypical three-coloring ground state on the kagome lattice.

SIMULATING THE EMERGENT PHENOMENA ARISING FROM STRONGLY CORRELATED SYSTEMS

Research Challenge

New algorithms are needed in order to understand exotic quantum phenomena. While the rules of quantum mechanics are simple, the resulting phenomena that arise from these rules are difficult to simulate and complicated due to quantum entanglement. Evaluating physically interesting Hamiltonians is exponentially costly due to the needed system size. To avoid this exponential cost we have developed a method that starts with interesting physics encoded in a wave-function and automatically find Hamiltonians that support them. A universal property of complicated quantum systems is the wide array of competing phases that comes from similar Hamiltonians. We seek a unifying explanation for the menagerie of phases by examining a class of materials called frustrated magnets; these are insulating materials whose spin degrees of freedom reside on lattices (grids) such as the triangular or kagome lattice. We numerically probe a transition in a class of physical systems coined the many-body localized phase, a phase where statistical mechanics to break down, between the many-body localized phase and the ergodic phase, where statistical mechanics still operate.

Methods & Codes

- The Eigenstate-to-Hamiltonian construction (EHC), an inverse technique of encoding interesting physics in a wave-function and automatically determining a physically reasonable Hamiltonian.
- A highly parallel exact diagonalization code for XXZ Hamiltonians on a frustrated kagome lattice.
- A novel Shift and Invert MPS algorithm (SIMPS) to compute interior eigenstates of a large, $2^{32} \times 2^{32}$, matrix in the many-body localized phase.

Why Blue Waters

Without computation at the scale of Blue Waters, this project would not have been possible. The examination of many-body localized phase involves studying samples with disorder. To extract any physics requires averaging many thousands of disordered samples that we run in parallel.

Results & Impact

- EHC, opens up an entirely novel approach to solving condensed matter problems and changes the search for interesting physics from a search in the dark to a targeted one. Typical forward approach is exponentially slow: 50 sites is intractable even on Blue Waters. EHC is a quadratic algorithm: **thousands** of sites can be simulated using the inverse approach.
- We have discovered a new Hamiltonian, the XXZ0 point, which has an exponential number of ground states that can be represented as all possible ways of coloring the kagome lattice with three colors.. We showed in a concrete example five explicit phases surrounding the XXZ0 point, including the enigmatic spin-liquid.
- We discovered that many-body localized eigenstates at low temperature can tell that there is an ergodic phase above them at higher temperatures. This allows us to learn about the transition using the many-body localized eigenstates that are easier to probe.