SIMULATING THE EMERGENT PHENOMENA ARISING FROM STRONGLY CORRELATED SYSTEMS

Allocation: Blue Waters Professor/250 Knh
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EXECUTIVE SUMMARY

This work focuses on using simulations and developing new algorithms to understand exotic quantum phenomena. For example, a key goal in condensed matter physics is to find Hamiltonian models with interesting physics; we developed a novel inverse algorithm to accomplish this [1]. Instead of the typical forward method of guessing at Hamiltonian models that might produce interesting physics, we start with the interesting physics encoded in a wave-function and automatically find Hamiltonians that support them. Additionally, we have discovered a new special Hamiltonian that sources almost all the phases on frustrated magnetism materials, explaining the menagerie of observed phases there [2] and connecting to the enigmatic spin-liquid [3] on the kagome.

RESEARCH CHALLENGE

The rules of quantum mechanics are simple. The phenomena that arise from these rules is both difficult to simulate (with an exponential cost in system size) and results in complicated phenomena. Both these properties are the result of quantum entanglement.

We address three key research problems in our work:

(1) A key goal in condensed matter is to find models (i.e., Hamiltonians) with interesting physics. A typical approach toward accomplishing this is to try many different Hamiltonians until a good one is found; this is inefficient, especially since each Hamiltonian is exponentially costly to simulate. We developed a novel approach to tackle this key problem.

(2) One universal property of complicated quantum systems is the panoply of competing phases that comes from similar Hamiltonians. Is this a cosmic accident or is there a unifying explanation for this menagerie? We focus on resolving this question via a class of materials called frustrated magnets [4,5]; these are insulating materials whose spin degrees of freedom reside on lattices, such as the triangular or kagome lattice.

(3) Recently, it has been realized that a class of physical systems, coined the many-body localized phase [6,7], have exotic entanglement at high temperature causing statistical mechanics to break down. We numerically probe the transition between this many-body localized phase and the ergodic phase where statistical mechanics still operate.

METHODS & CODES

(1) Our approach to this problem was to develop an inverse technique: start with some targeted interesting physics encoded in a wave-function and automatically determine a physically reasonable Hamiltonian from which those physics might arise. Our new algorithm, the Eigenstate-to-Hamiltonian Construction (EHC), uses a quantum covariance matrix that is a quantum generalization of the typical covariance matrix from statistics.

(2) We considered the XXZ Hamiltonian on the frustrated kagome lattice and computed its phase diagram. This was done using a highly parallel exact diagonalization code that we developed.

(3) We used a novel algorithm our group recently developed, SIMPS [8], to compute interior eigenstates of a $2^{32} \times 2^{32}$ Hamiltonian matrix in the many-body localized phase and measured their properties at a temperature slightly beneath the ergodic phase.

RESULTS & IMPACT

1) Our algorithm, 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. While the typical forward approach is exponentially slow, EHC is a quadratic algorithm. Although 50 sites is intractable [9] in the forward method—even on Blue Waters—thousands of sites can be simulated using the inverse approach.

(2) While most Hamiltonians have unique ground states, we have discovered a new Hamiltonian, the XXZ0 point [10], which has an exponential number of ground states that can be represented as all possible ways of coloring the kagome lattice with three colors. This Hamiltonian then becomes the source for the menagerie of competing phases because they all have identical energy in the ground state. We showed in a concrete example five explicit phases surrounding the XXZ0 point, including the enigmatic spin-liquid.

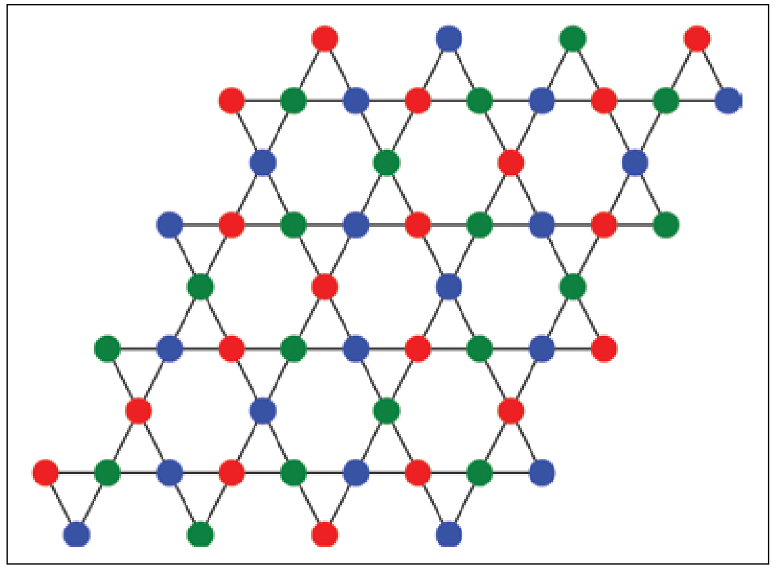

Figure 1: Our algorithm, Eigenstate-to-Hamiltonian Construction (EHC), generates Hamiltonians as a linear combination of null vectors of the quantum covariance matrix. Shown here is a color plot of the quantum covariance matrix that EHC computed for a wave-function of singlet dimers.

(3) 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.

WHY BLUE WATERS

Without Blue Waters, we would not have been able to perform these calculations. It was an essential component to benchmarking EHC on a series of examples and will become even more important as we begin to enumerate a long list of interesting wave-functions. Our discovery of the macroscopically degenerate point relied on having enough computational power to explore a region of phase space that no one had ever considered before. Then, once it was discovered, it required thousands of phase points to validate that it was connected to the spin-liquid phase. Without computation at the scale of Blue Waters, this would not have been possible. Finally, the examination of the 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 on Blue Waters.

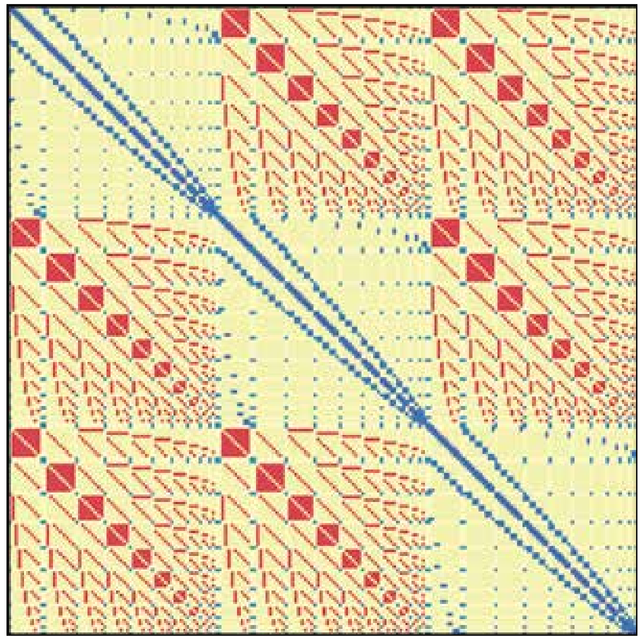

Figure 2: The XXZ0 Hamiltonian has an exponentially degenerate ground-state space. Each of the exponential states in this ground state can be represented as a product state over three spins (here represented as red, blue, and green). Shown is one prototypical three-coloring ground state on the kagome lattice.

PUBLICATIONS & DATA SETS

Claes, J., and B. Clark, Finite-temperature properties of strongly correlated systems via variational Monte Carlo. *Physical Review B*, 95:20 (2017), DOI:10.1103/PhysRevB.95.205109.

Pekker, D., et al., Fixed points of Wegner-Wilson flows and many-body localization. *Physical Review Letters*, 119:7 (2017), DOI:10.1103/PhysRevLett.119.075701.

Changlani, H.J., et al., Macroscopically Degenerate Exactly Solvable Point in the Spin-1/2 Kagome Quantum Antiferromagnet. *Physical Review Letters*, 120:11 (2018), DOI:10.1103/PhysRevLett.120.117202.

Villalonga, B., et al., Exploring one-particle orbitals in large many-body localized systems. *Physical Review B*, 97:10 (2018), DOI:10.1103/PhysRevB.97.104406.

Chertkov, E., and B.K. Clark, A computational inverse method for constructing spaces of quantum models from wave functions. *arXiv:1802.01590* (2018).

Yu, X., D. Luo, and B.K. Clark, Beyond many-body localized states in a spin-disordered Hubbard model with pseudo-spin symmetry. *arXiv:1803.02838* (2018).

Sahoo, J., et al., Classical phase diagram of the stuffed honeycomb lattice. *arXiv:1805.09831* (2018).