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ATYPICALLY ENTANGLED PHASES AND NEW METHODS FOR THE QUANTUM MANY-BODY PROBLEM

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EXECUTIVE SUMMARY

This work focuses on: (1) developing new machine-learning approaches to simulate the quantum many-body problem, and (2) elucidating novel phenomena in ayptically entangled phases. (The many-body problem, in brief, involves understanding the collective behavior of large numbers of interacting particles. Entanglement deals with the phenomenon of particles that remain correlated even when separated by great distances.) One new machine-learning approach [1] simulates difficult quantum many-body electronic systems by combining deep neural networks with ideas originally developed by Feynman [2] about backflow. Using this new approach, the research team extrapolated to near exact energies on difficult quantum many-body systems and competed favorably with other state-of-the-art methods. One important atypically entangled phase is the spin-liquid; the team has discovered an expanded spin-liquid regime in the phase diagram of the stuffed honeycomb model.

RESEARCH CHALLENGE

Entanglement makes quantum mechanics both interesting and difficult to simulate. Einstein once described entanglement in quantum mechanics as "spooky action at a distance," and phases of matter ranging from spin-liquids to eigenstate phases have exotic properties because of their atypical entanglement. Entanglement is also responsible for causing the cost of exactly simulating quantum many-body systems to scale exponentially with system size; every two years researchers can simulate one more electron.

The research team's problem is twofold: to identify, classify, and find phases with interesting entanglement, as well as to develop new methodologies based on ideas from machine learning to overcome the barriers to efficient simulation. The two phases of atypical entanglement the group is most interested in are spin-liquids and eigenstate phases.

Spin-liquids [3] are phases of matter whose entanglement is so complicated that they can't be constructed with short quantum circuits. In spin-liquid materials, the electron "fractionalizes," splitting into multiple pieces. Spin-liquids support anyons, which are important for constructing quantum memories and quantum computers. While the theory of spin-liquids is well established, the key question is to bring these spin-liquids into the real world by finding physical systems that support them.

Eigenstate phases [4] of matter are a recently discovered class of physical systems whose eigenstates have atypical entanglement. The entanglement of a typical eigenstate is boring; all particles are uniformly entangled with each other. On the other hand, in eigenstate phases, the entanglement in each eigenstate is highly structured. In addition to weird entanglement, these states of matter never equilibrate—the equivalent of a never-cooling cup of coffee. Eigenstate phases might be the key to allowing quantum computers to run at higher temperatures. The key question the team is addressing here is to increase the number of known eigenstate phases.

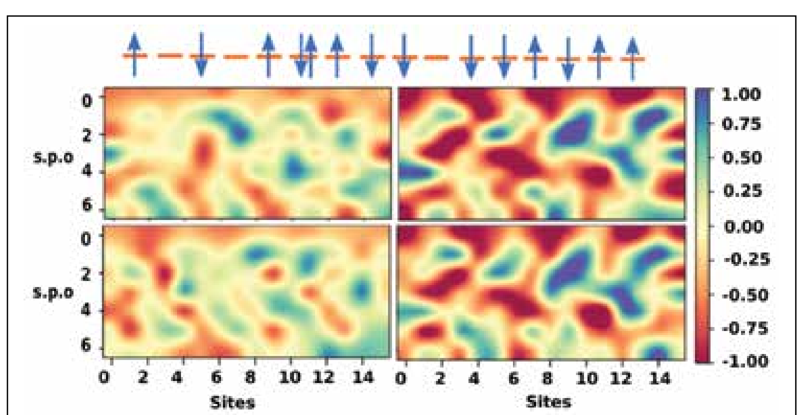

Figure 1: Matrix to diagonalize without (left) and with (right) neural network added to the wave function for spin-up (top) and spin-down (bottom) electrons. The neural network wave function restores the symmetry between the spin-up and spin-down electrons, which is known to exist in the exact wave function. Reproduced from [6].

METHODS & CODES

To find spin-liquids, the team has taken a two-fold approach. In one case, the researchers have mapped out a very general phase diagram of the stuffed honeycomb lattice that interpolates between a triangular and honeycomb lattice. To accomplish this, they have to find the lowest eigenvector of matrices, which are 68 billion by 68 billion using a parallel exact diagonalization code the team developed. In an alternative approach, they have searched for a numerical Hamiltonian that best fits the collaborators' experiment on a spin-ice material [5].

The team has approached better quantum mechanical simulations in two ways: by using deep neural networks and also by using an inverse approach. In the first case, they use deep neural networks to represent the quantum wave function. Wave functions map electron positions to scalar amplitudes. To generate this amplitude, they take a configuration and have a deep neural net generate a matrix whose determinant is then evaluated [6]. This builds on other approaches [7] that have neural networks directly generate the amplitude. In the second case, the researchers have tackled the quantum many-body problem using an inverse approach that avoids the exponential cost of the forward method [8]. The team's algorithm takes a targeted set of properties (encoded as a wave function) and outputs the Hamiltonians that might have generated it. This turns out to be extremely useful because it is easy to write down wave functions with interesting and exotic physics.

RESULTS & IMPACT

The research group has determined that the phase diagram of the stuffed honeycomb lattice supports nine different phases. One of these phases is a spin-liquid phase that significantly expands the known spin-liquid regime on the triangular lattice [9]. This increases the chance that experimentalists might be able to find spin-liquid behavior in real materials.

In eigenstate phases, the team has discovered an entirely new type of eigenstate phase [10], making it the second nontrivial concrete example of this type of phase. This phase has eigenstates with two different types of intermixed eigenstates: some of the eigenstates have entanglement that grows logarithmically with system size, and some are constant. The implications of this discovery is that whether the system equilibrates (*i.e.*, the coffee cup cools) depends sensitively on the starting conditions of the system.

The two algorithms the team has developed have significantly improved the regime of simulatable systems. The machine learning methodology extrapolates to the correct answer on difficult Hubbard systems in the regime where the researchers believe superconductivity exists and competes favorably with other state-of-the-art methods including the density matrix renormalization group. The inverse approach the team has developed has allowed them to find a whole class of Hamiltonians that support a spin-liquid-like state.

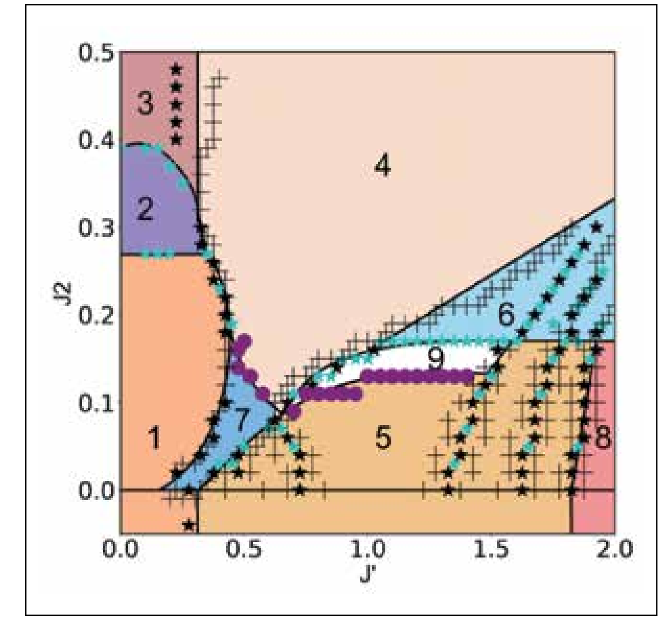

Figure 2: Phase diagram of the Heisenberg model on the stuffed honeycomb model including all nine phases. Phase nine is the spin-liquid phase. Dots and stars indicate different types of fidelity dips signaling a change in the phase.

WHY BLUE WATERS

Without Blue Waters, the research team would not have been able to perform these calculations. The stuffed honeycomb simulations required diagonalization of huge matrices at over 200 different phase points. For the eigenstate phases, the researchers needed ~100 different realizations for each of five different disorder strengths. Even testing and benchmarking the new algorithms was a significant undertaking computationally; for example, the deep neural network approaches scales of N^4, where N is the size of the system. Without being able to run these simulations in parallel, the team would not have been able to obtain results.

PUBLICATIONS & DATA SETS

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