atoms, leading to a metastable compositional depth profile which includes the Sb-enriched region. The atoms in this region phase-separate laterally into pure Sb clusters and 50-50 GaSb, the former of which crystallize as observed here, forming the "seeds" which will drive the formation of nanopatterns on the surface.

Further analysis is needed to investigate the influence of compositional variations on the direct ion-impact energy and momentum transfer to the surface atoms. Such information is critical for determining the mechanisms and parameters relevant to generalized models of surface nanopatterning [6,7], allowing the prediction of pattern parameters and surface properties as functions of experimental parameters such as ion species, incident energy, or choice of surface component materials.

WHY BLUE WATERS

The work completed involved conducting MD simulations of 3 million atoms for nearly 50 million time steps. On a conventional supercomputing cluster this would take multiple years to complete. Large output data files were written at a fairly high frequency, necessitating a high-performance file system to minimize the impact on the overall simulation time. Production runs on Blue Waters were able to simulate up to 10 million time steps on 128 nodes in just 48 hours, allowing the majority of the production runs to be completed in less than two months actual time.

SIMULATING STRONGLY CORRELATED SYSTEMS: FROM FRUSTRATED MAGNETS TO MANY-BODY LOCALIZATION

Allocation: Blue Waters Professor/250 Knh
PI: Bryan Clark[1]
Collaborators: Hitesh Changlani[1], Eduardo Fradkin[1], Krishna Kumar[2], David Luitz[1], and Xiongjie Yu[1]

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EXECUTIVE SUMMARY

The key problem in condensed matter physics is connecting microscopic details to emergent phenomena. My group has used Blue Waters to develop this connection. We have focused on three main emergent phenomena: many-body localization, spin liquids, and superconducting systems. We describe the former two in this report.

Frustrated magnets arise from geometrically frustrated lattices, such as the Kagome lattice. We find strong numerical evidence for a chiral spin liquid in a natural spin system on the Kagome lattice under a magnetic field. Many-body localization is a phenomenon where statistical mechanics breaks down and quantum mechanics survives at infinite temperature. Using a **newly developed** method we show the saturation of entanglement for many-body localized states.

INTRODUCTION

Frustrated Magnets

In many cases, the electrons in a material are localized in space. The important physics can be captured by viewing the electrons simply as spins which decorate a geometric lattice and want to anti-align. On a square lattice there is a simple pattern which satisfies all electrons; every other electron points up (respectively down). In contrast, when the electrons are on a triangular lattice, this is no longer the case. Instead, while two electrons can be anti-aligned, the third electron must be aligned with one of the other two, causing geometric frustration. One of the most frustrated lattices is the Kagome lattice, which consists of corner sharing triangles. This inherent frustration makes it possible for exotic phases to arise. One such phase is the chiral spin liquid.

Many-Body Localization

Many-body localization is a phenomenon where statistical mechanics [1,2] breaks down and quantum mechanics manifests itself at finite (even infinite) temperature. This is particularly surprising as quantum phenomena are typically only prevalent at zero temperature. From a technological point of view, this phase is important because it may allow for the construction of a quantum computer and quantum memory that is robust to thermal noise.

METHODS & RESULTS

Frustrated Magnetism

Our approach to understanding electrons on the Kagome lattice was to perform an exact quantum simulation (using exact diagonalization) for the largest system size possible given our computational constraints. We simulate a system of spins with the nearest neighbor XY interactions under a magnetic field. Our computational ability allows us to simulate 48 spins requiring finding the lowest eigenvector of hundreds of matrices each of which are of size 377 million by 377 million. In doing so, we find ample numerical evidence that this system forms a chiral spin liquid.

The strongest evidence for the presence of a chiral spin liquid is as follows: A normal state of matter is insensitive to the topology on which the system lives. A magnet on a sphere, a donut, or a cylinder looks roughly the same. Topological states of matter such as spin liquids know the topology of their system and can "feel" the effect of distant boundaries. In our simulations, we slowly twist the boundaries of the system so that the spins interact differently across them. Once we make a full twist, the geometry of the system returns to where it started and amazingly enough, the system does not. Instead, the system picks up an additional quantized phase. The presence of this phase is a key signal of the topological phase of matter and shows that our system is a chiral spin liquid.

Spin liquids are important for two reasons. First, they are the prototype for a phase of matter which stretches beyond the theoretical boundaries of the typical way physicists describe phases—the Landau paradigm. Secondly, they have the potential to be essential for the implementation of quantum computers that are robust to errors.

Many-Body Localization

Unfortunately, in the field of many-body localization, exact methods are limited to 22 sites. More sites are needed to better understand the phase, so we have developed a **novel** density matrix renormalization group (DMRG) algorithm (called the Shift and Invert MPS, or SIMPS). We applied this new algorithm to the disordered Heisenberg model scaling to an order of magnitude more sites than previously possible. With this capability we were able to measure the probability of entanglement, show the saturation of entanglement, and generate thousands of local excitations.

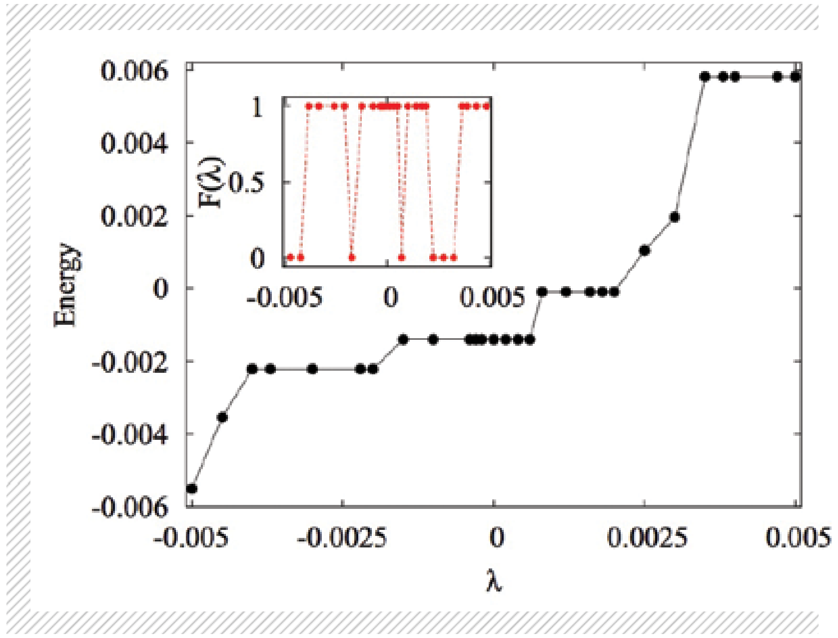

FIGURE 1: Example of sweeping the target energy lambda of a SIMPS run. Each dot corresponds to the eigenstate energy identified. The inset shows the overlap of nearest neighbor eigenstates. The fact that they are always one or zero validates that each state is individually an eigenstate.

WHY BLUE WATERS

Frustrated Magnetism

Blue Waters was essential to "numerically prove" the existence of our chiral spin-liquid. Because of symmetry constraints, 48 spins was the smallest number of spins for which one could reasonably

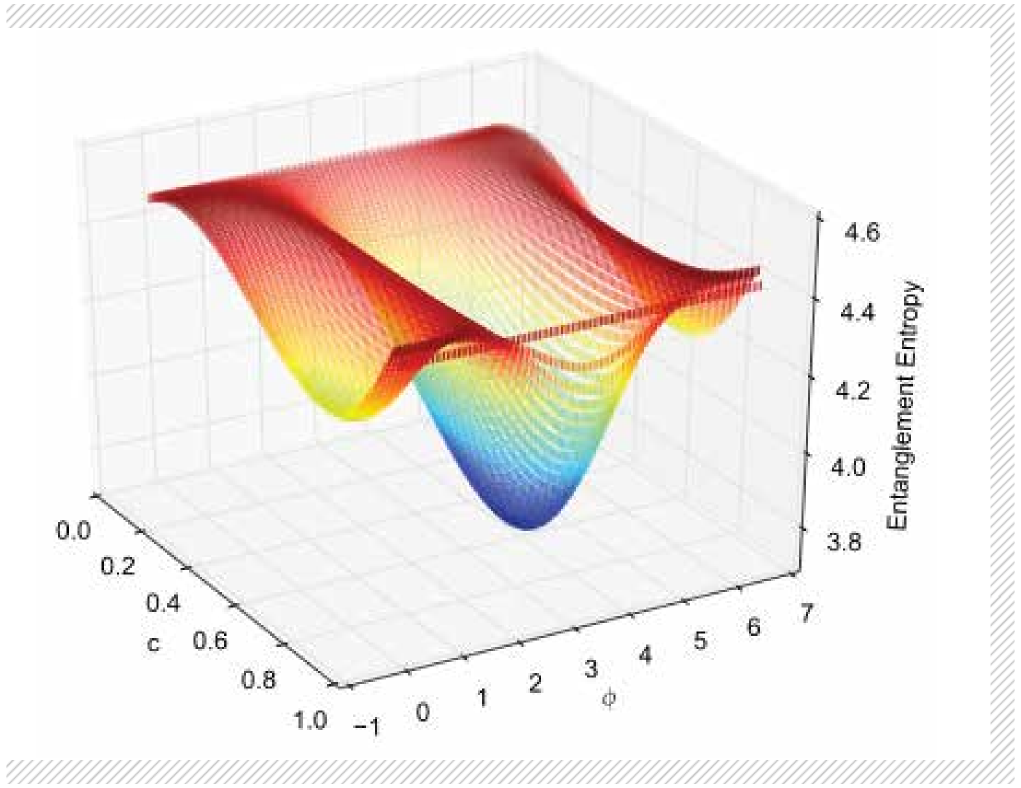

FIGURE 2: Renyi entanglement entropy for the 42b cluster as a function of c, φ obtained from the reduced density matrix along two topologically non-trivial cuts. The linear combinations corresponding to local minima of the entanglement suggesting the existence of a topological phase.

compute all properties of the topological phase, but computing the entire set of twists required over 100,000 node hours.

Many-Body Localization

Blue Waters was essential to this project because of the multiple layers of computation needed. Many-body localized phenomena involve disordered systems. Therefore, any computation requires an average of over thousands of disordered realization. For each of these disordered realizations, a sweep over multiple target energies lambda is required. Finally, each (lambda, disordered configuration) point requires tens of applications of the SIMPS algorithms to converge to the excitation.

NEXT GENERATION WORK

Frustrated Magnetism

We discovered a chiral spin liquid in our system at a single phase point. We would like to discover whole regions that have spin liquid behavior because that will give us the best chance of finding realizations in nature of these exotic phenomena. Unfortunately, each point in this region requires an entire calculation comparable to the one we have done for the chiral spin liquid. It is only with Track-1 systems that this will become possible.

Many-Body Localization

Our SIMPS methodology currently allows us to access states within the many-body localized region, but fails at the critical point, and understanding the nature of this critical point is key to understanding many-body localization. We are developing new tensor network methodologies which may be able to access this point, but the computational complexity of running them will require the next-generation machines to achieve the system sizes necessary.

PUBLICATIONS AND DATA SETS

Chen, X., et al., Many-body localization transition in Rokhsar-Kivelson-type wave functions. *Phys. Rev. B*, 92:21 (2015), p. 214204.

Yu, X., D. Pekker, and B.K. Clark, Finding matrix product state representations of highly-excited eigenstates of many-body localized Hamiltonians. *arXiv* preprint arXiv:1509.01244 (2015).

Yu, X., D.J. Luitz, and B.K. Clark, Bimodal entanglement entropy distribution in the many-body localization transition, *arXiv* preprint arXiv:1606.01260 (2016).

TRANSIENT TWO-PHASE FLOW AND ELECTRO-MAGNETIC FIELD EFFECT IN STEEL CONTINUOUS CASTING

Allocation: Illinois/200 Knh
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EXECUTIVE SUMMARY

This project aims to advance current state-of-the-art, computationally-intensive models of multiphase phenomena including turbulent fluid flow, particle transport, and MagnetoHydroDynamics (MHD) in the continuous casting of steel. Also, the project applies these current models to gain practical insights into the transient flow phenomena related to defect formations and to improve this important commercial process. In this study, a transient, two-phase Large-Eddy-Simulation model of molten steel-argon gas flow was applied to investigate anisotropic (directionally dependent) turbulent flow in the caster, with and without a double-ruler electro-magnetic field. The model calculations have been validated with plant measurements and applied to understand the mechanism of the flow variations, which is important to surface defect formation in the final product. Also, the effects of the magnetic field on the flow stability in the caster has been quantified with different process parameters.

INTRODUCTION

Continuous casting is used to manufacture more than 95% of steel in the world [1]. Molten steel flows from a tundish container, through a slide gate control valve, and down a vertically bifurcated nozzle into the mold (Fig. 1). Once in the mold, molten steel solidifies against the water-cooled, copper mold walls to form a solid shell. Transient fluid-flow phenomena in the mold are very important to quality and defects in the final product. Abnormal surface flow aggravates level fluctuations, shear instability of the molten slag/steel interface, and vortex formation near the submerged entry nozzle (SEN), which leads to mold slag entrainment. These detrimental flow phenomena in the mold become more complex with argon gas, which is injected into the nozzle to prevent clogging. Furthermore, the argon gas bubbles may become entrapped into the solidifying steel shell, forming other defects. To stabilize and optimize the transient fluid flow in the mold, electro-magnetic fields are often applied, especially at high casting speed [2-4].

FIGURE 1: Schematic of the continuous steel slab-casting process.