# 1 Project Information

**Project title:** A Computational Approach to Strongly Correlated System

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# 2 Executive summary

Our work on Blue Waters involves simulating microscopic quantum systems to find emergent phenomena. This year we have had various accomplishment in frustrated magnetism and many-body localization (MBL). For example, we have discovered a new chiral spin liquid, developed a new algorithm which increases the size that can be studied in MBL by an order of magnitude, and found scale invariance in MBL systems. This has resulted in 7 papers (5 published, 2 preprints) and 5 talks. Next year we will continue work in these fields with a focus on exploring the exotic phases which results from a newly discovered macroscopic degenerate point we've uncovered as well as elucidating the nature of the MBL mobility edge.

# 3 Description of research activities and results

The key challenge in this research is the simulation of emergent quantum mechanical phenomena. The computational cost of simulating quantum mechanics is exponential in the system size. Consequently, significant resources are needed to reach even 30-50 spins or electrons. Approximations, when appropriate, often scale as $N^3$ and require significant computational resources.

Our work on Blue Waters has focused on two areas:

**Frustrated Magnetism:** The key question in the field of condensed matter physics has been the prediction of new phases of matter. Of particular recent interest is the discovery of topological phases. These phases go beyond the canonical ginzburg-landau classification of phases. In addition to their immediate scientific interest, topological phases have potential to be a critical component in building a quantum computer by allowing for robust hardware which doesn't require quantum error correction.

Computational methods are essential for making the connection between the microscopic Hamiltonians and the emergent phases.

*Accomplishments:* In the last year we have used Blue Waters to

- Predict the existence of a new chiral spin-liquid phase in the Heisenberg model at finite magnetization. This is one of the first chiral spin liquids that explicitly breaks translation symmetry. The key challenge in accomplishing this work was that exact techniques were required and the minimum size cluster that made the phase evident was 48 spins. This involved finding the lowest eigenvector of thousands of matrices of size 377 million by 377 million. We would not have had the computational ability to accomplish this without Blue Waters.
- Make progress in understanding the extrapolation between honeycomb and triangular lattices. Two of the most interesting places to look for spin-liquid candidates have been on honeycomb and triangular lattices (often with second nearest neighbor interactions). We have started a project using Blue Waters

to examine the interpolation between these two cases. This project requires exact simulations of $N = 18, 24$, and 32 sites on an entire grid of points. We have completed the $N = 18, 24$ work and started the $N = 32$ calculations. We have only made initial progress on this project because the computational cost eventually required to complete it is beyond our current Blue Waters allocation. This initial progress though has identified a new spin-liquid candidate as well as suggestions of an exotic phase diagram.

- Developed a new method which allows for variational calculation of finite temperature properties. The calculation of ground state properties, while computationally demanding, has been actively developed for the last thirty years. One of the gold-standard approaches in this field is the the use of variational methods. Such methods take as an ansatz, a large class of wave-functions parameterized by a series of parameters $\vec{\alpha}$. Unfortunately, this experience of developing ground state wave-functions has not translated over to the regime of finite-temperature. We have recently shown how to bridge this gap. We have developed a new method that takes as input variational wave-functions and outputs (approximate) finite temperature properties. Typical ground state variational approaches become more accurate as the class of wave-functions approach the ground state. Analogously, our new approach becomes more accurate as the wave-functions in our class more accurately represent $\exp[-\tau H]|R\rangle$ for various product state $|R\rangle$ and various imaginary time $\tau$. This new methodological development is important because it has the potential to open up a regime for the calculation of strongly correlated systems that was previously inaccessible. Blue Waters was essential for this work because this new algorithm is both computationally demanding and parallelizes extremely well. The finite-temperature algorithm needs to essentially do a ground-state optimization for each product state it samples (which current experience suggests is on the order of a few hundred product state). Without the computationally capability of Blue-Waters we would not have been able to test and benchmark this algorithm effectively. This is especially true since we needed results quickly (with respect to wall-clock time) to iterate on various improvements of the algorithm.

**Many-Body Localization:** Many-body localized phases can appear in systems with both interaction and disorder. Typical phases are either a property of the ground state or of the finite-temperature density matrix. Recently a qualitatively new type of phase has been discovered - the many-body localized (MBL) phase. In introductory statistical mechanics we learn that a system at finite-temperature equilibrates. This basic tenant of statistical mechanics breaks down in the MBL phase. MBL systems neither equilibrate nor conduct; heat introduced into the system stays localized. The MBL phase is important because it is the first example we have of a generic breakdown of the laws of statistical mechanics; this means that we can see quantum phenomena even at very high "temperatures." It has even been suggested that MBL phases may be able to stabilize topological phases at high-temperature which may be critical for the design of a quantum computer.

*Accomplishments:* In the last year we have used Blue Waters to

- developed a conceptual new language for describing the MBL phase. Because MBL is a new phenomena, it is still unclear what the correct theoretical description is for the phase. One approach for this has been to describe the phase using the "conserved commuting-operator" description. In recent work, we have offered two complementary descriptions of the phase. In particular, we show that the phase can be described by a MPO with finite bond-dimension as well as showed that the entire spectrum is efficiently representable by $O(n)$ numbers. This is amazing given that, in a typical phase, the spectrum requires $O(4^n)$ numbers. Our description is in the language of matrix-product states (MPS) and matrix-product operators (MPO)

  This work is important because these two complementary descriptions of the MBL phase allow a better understanding of the basic phenomenology of MBL. For example, the lack of conductance is a direct corollary of this description.

  Blue Waters was essential for this work, because a key piece of this work was to show that the bond-dimension of the matrix-product operator saturates as a function of system size (without this, this new description couldn't apply). This could only be done numerically and required solving massive bipartite matching problems for thousands of disorder samples.

- Developed a new algorithm for finding MBL eigenstates. The "order parameter" for a MBL phase is a function of an eigenstate in the middle of the many-body spectrum (this boils down to finding the middle eigenstate of $2^{100}$ eigenstates with the adjoining eigenstates being separated from the target eigenstate by a gap of $2^{-100}$. We spent two years developing an algorithm to accomplish this (which has now been published in PRL). This has completely transformed how people study MBL systems (previously, the biggest system size to be examined was 22 sites; now we can do over a hundred). MBL systems require significant disorder averaging. While this is embarrasingly parallel, it requires significant computational power. Blue Waters was critical for testing variants of this algorithm
- Discovery of a fixed-point and bimodality in the MBL transition. The discovery of the MBL phase meant that there was a transition between this phase and the previously known ergodic phase (where statistical mechanics works). Almost nothing is understand about this transition (it's not even clear if the language used to describe typical transitions applies). We have made two major breakthoughs in understanding the transition. First, we have shown that there is a scale invariance in the phase transition. The discovery of scale-invariance is the key step in being able to understand a transition in the context of the renormalization group. In addition to this discovery of scale-invariance, we resolved an open question showing that at the transition even a single disordered sample could exhibit simultaneously area law and volume law states. Because of the disorder averaging required, we couldn't complete these calculations without the computational power of Blue Waters.

# 4 Publications and Products

Since my last report there have been, using Blue Waters,:

- 7 papers (2 preprints, 5 published)
  - Claes, Jahan, and Bryan K. Clark. "Finite temperature properties of strongly correlated systems via variational Monte Carlo." arXiv preprint arXiv:1612.05260 (2016).
  - Pekker, David, Bryan K. Clark, Vadim Oganesyan, and Gil Refael. "Fixed points of Wegner-Wilson flows and many-body localization." arXiv preprint arXiv:1607.07884 (2016).
  - Yu, Xiongjie, David Pekker, and Bryan K. Clark. "Finding Matrix Product State Representations of Highly Excited Eigenstates of Many-Body Localized Hamiltonians." Physical Review Letters 118, no. 1 (2017): 017201.
  - Kumar, Krishna, Hitesh J. Changlani, Bryan K. Clark, and Eduardo Fradkin. "Numerical evidence for a chiral spin liquid in the XXZ antiferromagnetic Heisenberg model on the kagome lattice at m= 2 3 magnetization." Physical Review B 94, no. 13 (2016): 134410.
  - Yu, Xiongjie, David J. Luitz, and Bryan K. Clark. "Bimodal entanglement entropy distribution in the many-body localization transition." Physical Review B 94, no. 18 (2016): 184202.
  - Pekker, David, and Bryan K. Clark. "Encoding the structure of many-body localization with matrix product operators." Physical Review B 95, no. 3 (2017): 035116.
  - Chen, Xiao, Xiongjie Yu, Gil Young Cho, Bryan K. Clark, and Eduardo Fradkin. "Many-body localization transition in Rokhsar-Kivelson-type wave functions." Physical Review B 92, no. 21 (2015): 214204.
- 5 Talks/poster
  - Condensed Matter Seminar at Iowa State: (2016.12.01)
  - Telluride (2017.07.15)
  - Blue Waters Symposium (2016.06.13)
  - Speaker at PCTS Quantum Coloring (2016.05.05)
  - Laguna Beach Poster (2016.01.15)

# 5 Plan for next year

We are requesting the maximum of 250,000 node hours (in practice the amount we need below is more then this but we will try to fruitfully use the low queue and accomplish as much as possible given the time.) We anticipate Blue Waters usage of Q1: 30%, Q2: 20%, Q3: 20% and Q4: 30%.

Our plan for Blue Water next year involves making progress on these three projects

- **Exploring the source of frustrated magnetism on lattices of triangular motifs.**

  Since the inception of the field of frustrated magnetism, lattices with triangular motifs have been thought to be a good place to look for exotic spin-liquid phases because there is no way to have three spins anti-align on a triangle. This is primarily a classical explanation and doesn't adequately explain why exotic states exist on the kagome lattice but not the triangular lattice. We have recently discovered a more compelling quantum explanation - on lattice with triangular motifs there is an exactly solvable point which leads to exponential degeneracy on the kagome and hyperkagome lattices. This implies the source of many (interesting and exotic) phases on these lattices comes from this point.

  The next step is to perturb this special point in various ways and explore which phases appear. This perturbation step must be done numerically. A machine at the scale of Blue Waters will be necessary for this exploration. We already have preliminary evidence that the most interesting spin-liquid on the kagome lattice (the Z2 SL at Sz=0) is sourced at this point.

  To accomplish this, we will use exact diagonalization. Exact diagonalization involves finding ground states of matrices of 36 spins - in this case, this involves matrices of size 9 billion by 9 billion, although we will often be able to take advantage of some block-diagonal structure in these matrices (usually around 100 blocks). The ground states will be found using Lanczos which scales as the cube of the matrix size. We have recently improved our exact diagonalization code now allowing it to run over approximately 3200 cores (100 nodes) simultaneously getting strong scaling that is approximately 70% efficient (see figure 1). We have done preliminary tests and each phase point can then be computed in approximately 500 walk clock-hours (10 hours per block-diagonal piece of the matrix and approximately 50 pieces). In many cases, this can be attenuated if we know that some blocks are unlikely to be the ground state; on average we find that there are only five important blocks although this is hard to know before-hand. This leaves us with approximately 5000 node hours per phase point. A phase diagram would map out the perturbation of this special point in two directions and would typically involve a $10 \times 10$ grid of 100 points. The perturbation we will consider is magnetic field and $Jz$. It is known that this phase diagram has, at minimum, an interesting chiral phase. As this is above the maximum allowed allocation for Blue Water Professor, we will instead do a preliminary study using a $5 \times 5$ grid of points to determine the coarse features of the phase diagram. This will use 125,000 node hours total.

- **Finish work on emergent lattice**

  We will finish our work looking at the phase diagram of the emergent lattices that form when extrapolating between the honeycomb and triangular lattices. These two lattices can be interpolated into each other by adding an additional point at the center of each honeycomb that is coupled by an interaction $J'$ which is tuned from 0 to 1. In addition, we introduce an additional second nearest neighbor term $J_2$. As mentioned above, we have made significant progress on this problem already this year and already have the complete phase diagram for $N = 18, 24$ sites. Unfortunately, both these system sizes have the problem that the second nearest-neighbor interaction wraps around the boundaries of the lattice so that each site sees itself. This has the potential to fundamentally affects the qualitative features of the phase. We have started running exact diagonalization on the $N = 32$ size systems (the first system size which avoids this wrapping) but need to finish it to complete the work. In particular, we need to focus on two regions of the phase diagram that preliminary work gives evidence for a chiral-spin liquid phase. We estimate finishing this work takes approximately 50,000 node hours.

  In addition, we would like to validate these results on a couple points using ipeps. ipeps works directly in the $N = \infty$ limit and therefore can check whether the $N = 32$ system size affects our results. ipeps involve tensor contraction of a infinite two-dimensional network where all tensors are the same. Unfortunately, ipeps is extremely expensive. There is a parameter in ipeps, the bond dimension $D$,

which specifies the accuracy and which scales as $D^8$. We have done preliminary testing and our runs at $D = 4$ take approximately 50 node hours. State of the art calculations using ipeps use $D = 10$ and then extrapolate to the large $D$ limit from there. Assuming we reach the necessary accuracy at the same point as other studies using ipeps, this means that we will need approximately 75,000 node hours for every phase point. Our hope is to do this validation on at least a single phase point where we see the chiral spin-liquid to remove doubt about its existence.

Total this projects takes 125,000 node hours.

- **Finish work on one-body density matrices in many-body localization** We have recently (in the last few months) started a project where we have been trying to understand the many-body mobility edge. In the MBL phase (describe above), the phase is a function of both disorder strength $W$ as well as energy density $E$. In some cases, at fixed disorder, as a function of $E$, the system can go from MBL to ergodic and back to MBL. This is called a mobility edge. While there is some theory for MBL, there is currently no good theory of the mobility edge. Unfortunately, studying the mobility edge on large systems is essentially impossible because the ergodic phase requires exponential bond-dimensions even using our new MPS algorithms (described above).

  We have therefore been developing an approach to identify features of the mobility edge by looking only at the MBL states. While naively it seems that MBL states should not include information about the ergodic phase, we have recently shown that this is not true. Instead, by looking at the one-body density matrix, one can actually identify that there is an ergodic phase at higher energy density.

  Having made this observation, we now need to do the simulation which gives us many states at low energy density from which we will compute the one-body density matrix. We have recently made modifications to our new MPS code (described above in accomplishments) which have sped it up by an order of magnitude on Blue Waters (we were paying a significant penalty for reading and writing massive matrices to disk and we have resolved this problem somewhat). We have acquired preliminary data to generate a suite of results at $N = 32$ for five different disorders ($W = 2, 3, 6, 8, 15$) as well as three different energy densities (two near $\epsilon = 0.1$ and one at $\epsilon = 0.9$). This took 16,000 node hours. We need to do the same calculation for $N = 64$ (and ideally one point at $N = 128$). The algorithm we developed scales linearly with system size but historically has required a larger bond dimension $D$ at bigger system sizes (the entire algorithm scales as $D^3$ and a rough guess is the bond-dimension needs to go up by 50%). Therefore, we anticipate that this will require 6.75 times the amount of work or 108,000 node hours.

Beyond the CPU time, we have significant storage resource needs. At the moment this is completely dominated by the storage of thousands of vectors which range in size from hundreds of millions to a billion. These vectors come from the result of our exact diagonalization. The computation time described above is essentially involved in producing these vectors. After this computation is done, then various analysis (computing order parameters, overlaps, energy, etc.) is done on these vectors which is a tiny part of the computational effort. Unfortunately, which analysis must be done is hard to predict in advance and even toward the end of the project, we often need to sweep over all these vectors to clean up the analysis of results. At the moment we have been storing these on /projects and are currently using 21 terabytes (most of these were stored before quotas was enforced). We unfortunately need the currently stored vectors as well as new vectors from next year (which will roughly double things) and am requesting 50 terabytes of storage. This storage will mainly stay local to Blue Waters (where we do the analysis runs).

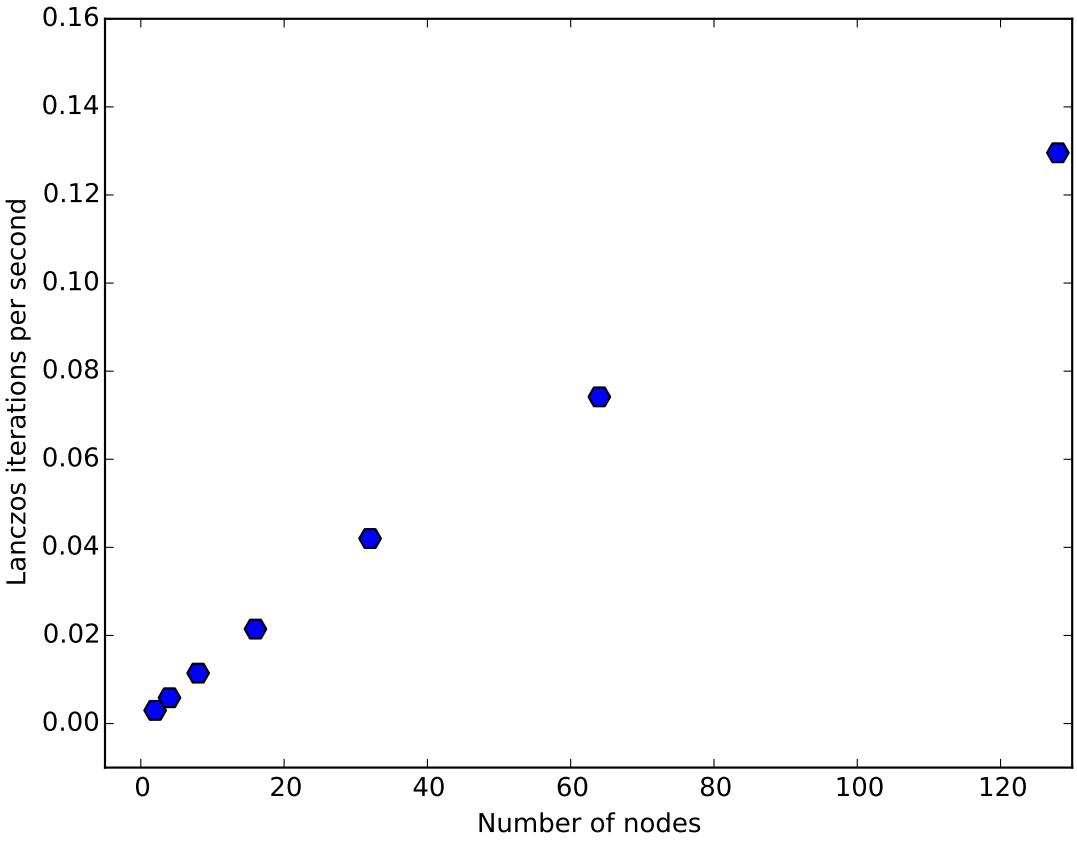


Figure 1: Strong scaling of exact diagonalization code as a function of number of nodes.