# STRONGLY CORRELATED SYSTEMS THROUGH COMPUTATION

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**Executive Summary:** Condensed matter physics maps microscopic degrees of freedom to emergent behavior. Computational simulations are essential in making this connection particularly in the context of strongly correlated systems where analytical tools are difficult to apply. Unfortunately, simulating quantum mechanics scales exponentially with system size requiring significant computational resources and novel algorithms. In the last year, the condensed matter systems we've considered include many-body localization, where the concept of temperature breaks down; pair density waves, which are essential to understanding superconducting materials; and spin-liquids in frustrated magnetism which have non-abelian anyons. In addition, we have developed novel algorithms including a new inverse approach and machine-learning inspired wave-functions. We have posted/published eight papers using Blue Waters including two that have been published in the prestigious journals of Physical Review X and Physical Review Letters. The use of Blue Waters has been critical in accomplishing the computational tasks described above.

## Description of Research Activities and Results

### Many-Body Localization

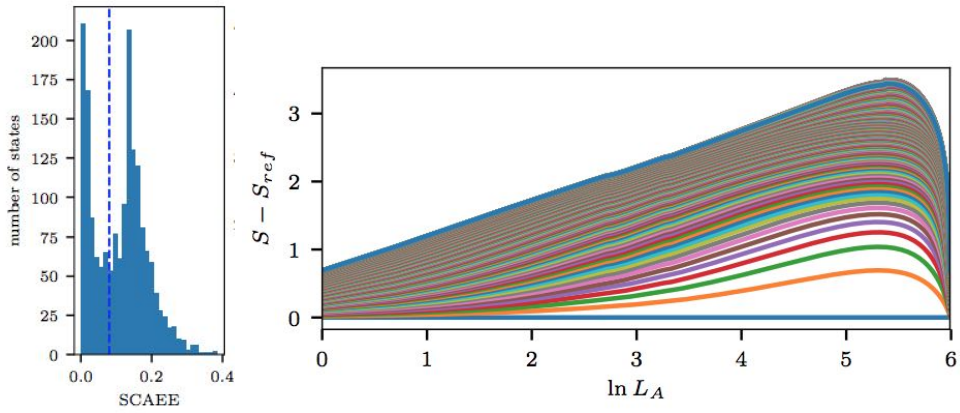
*Why it matters:* Historically there are two qualitative categories of phases - quantum phases (i.e. superconductivity, anti-ferromagnetism, etc.) and thermal phases (liquid, solid, etc.). Recently, it has been realized that there is a third qualitative category of phase - eigenstate phases. The two canonical examples of an eigenstate phase are the many-body localized (MBL) phase and the ergodic phase. The MBL phase is a phase

of matter where the concept of temperature itself breaks down and the system fails to thermalize even at what would be infinite temperature. The existence of a new category of phase means that all the questions physicists have sorted out about thermal and quantum phases over the last five decades are still open in this new eigenstate phase. For example, even whether the concepts of first and second order transitions makes sense in this context is still unclear.

*Key Challenge:* Currently the two main challenges in this field are to understand the nature of the transition and to discover eigenstate phases which go beyond the many body localized phase. Numerically, the difficulty in accomplishing this results from needing many disordered realizations of interior eigenstates of exponentially (in system size L) large matrices. The eigenstates are separated by a distance of of 2^{-L}. Typical system sizes range from L=10 to L=100. At the lower end of this range (10<L<22), these eigenstates can be captured using exact diagonalization whereas in the upper end of this range they require new algorithms we have developed such as the SIMPS approach.

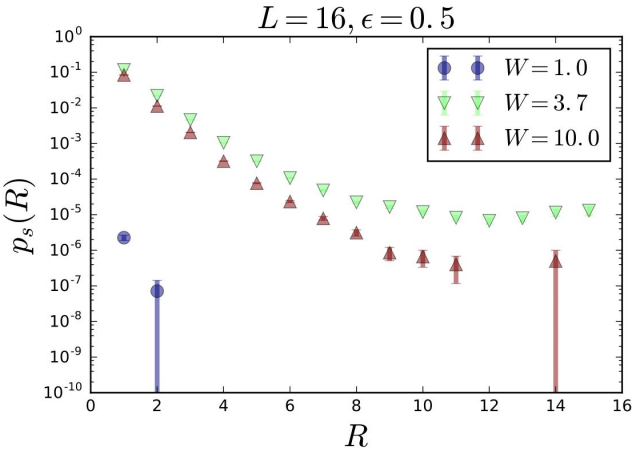
*Accomplishment*: To begin with, we took last year's work on understanding the mobility edge and shepherded it through the review process; it has now been published in Physical Review B. This work on the mobility edge made the surprising discovery that states underneath the mobility edge know about the ergodic phase which exists above them.

In addition, this year we posted (and published in Physical Review B) a work which discovered an eigenstate phase which goes beyond the many-body localized phase. The MBL phase is characterized by a many body spectrum whose eigenstates are all area law. The new phase we discovered is characterized by an emulsions of states some of which are area law and some of which are log-law. This is the first numerically validated example of an eigenstate phase which is neither many-body localized nor ergodic.




*Caption:* (Left) Figure showing a histogram of states as a function of entanglement in the spin-disordered Hubbard model at L=8 in a particular quantum number sector. Note the bimodal nature of the histogram indicates that the eigenstates have both area-law entanglement (peaked around zero) and non-area law entanglement (peaked around 0.2) (Right) Difference in entanglement between a ground state and a series of finite energy-density eigenstates on a logarithmic scale (each eigenstate in the graph is higher in energy by U). Note the fact that the lines are straight at high energy give evidence for the existence of logarithmically entangled eigenstates.

We have also made significant progress on an ongoing project to understand the MBL-ergodic transition. In order to understand this transition it is important to measure a series of rare resonances which are believed to drive the transition. This year we have computed an extensive number of exact eigenstates on smaller systems over disorder strengths that span both the ergodic and the MBL phases. To understand the structure of these resonances we have started to analyze the eigenstates' two-site quantum mutual information. Preliminary data (shown below) suggests the formation of long range resonances appears in a scale invariant fashion close to the ergodic MBL transition. As part of the work this year we need to better understand this result in terms of the l-bits, etc.



*Caption: Preliminary results showing* probability of finding strong quantum mutual information bonds (resonances) of range R. Three different disorder strengths are presented: W=1.0 is ergodic, W=3.7 is at the transition, and W=10.0 is MBL. We can see evidence of the scale invariance of the resonances' structure at long ranges.

*Why Blue Waters:* For the calculations concerning the resonant bonds of ergodic and MBL eigenstates, a million eigenstates for each point of the phase diagram mapped (3 energy densities and 24 different disorder strengths) were necessary, due to long resonances being extremely rare events. The large scale of parallelism achieved by Blue Waters was essential for the realization of this project. The same feature will be essential to proceed with this and other projects we have planned for this year.

Spin-liquids and frustrated magnets

*Why it matters:* One of the most difficult quantum materials to understand are insulators whose spin degrees of freedom interact on a frustrated lattice (for example, the kagome or triangular lattice). Such quantum materials are often very sensitive to minor changes in their underlying Hamiltonian induced by changes in properties such as doping or pressure. This results in a wide myriad of possible phases. These phases range from the pedestrian, such as anti-ferromagnets, to the exotic, such as the quantum spin liquid. It is critical to understand better how frustration drives the existence of these phases as well as become better at predicting which parameters lead to which phases. In addition, quantum spin liquids have potential applications in quantum computing.

*Key Challenges*: The key challenge in this area is that the cost to compute properties of a Hamiltonian scales exponentially with the system size. This is particularly problematic given that many Hamiltonians must be considered to work out an entire phase diagram. To make progress then, one must either (1) pay the exponential cost or find good approximations for measuring properties of the Hamiltonian or (2) find special Hamiltonians which one can solve for more efficiently.

*Accomplishments*: This year, we have made progress in both of these areas as well as made direct connection to experiment.

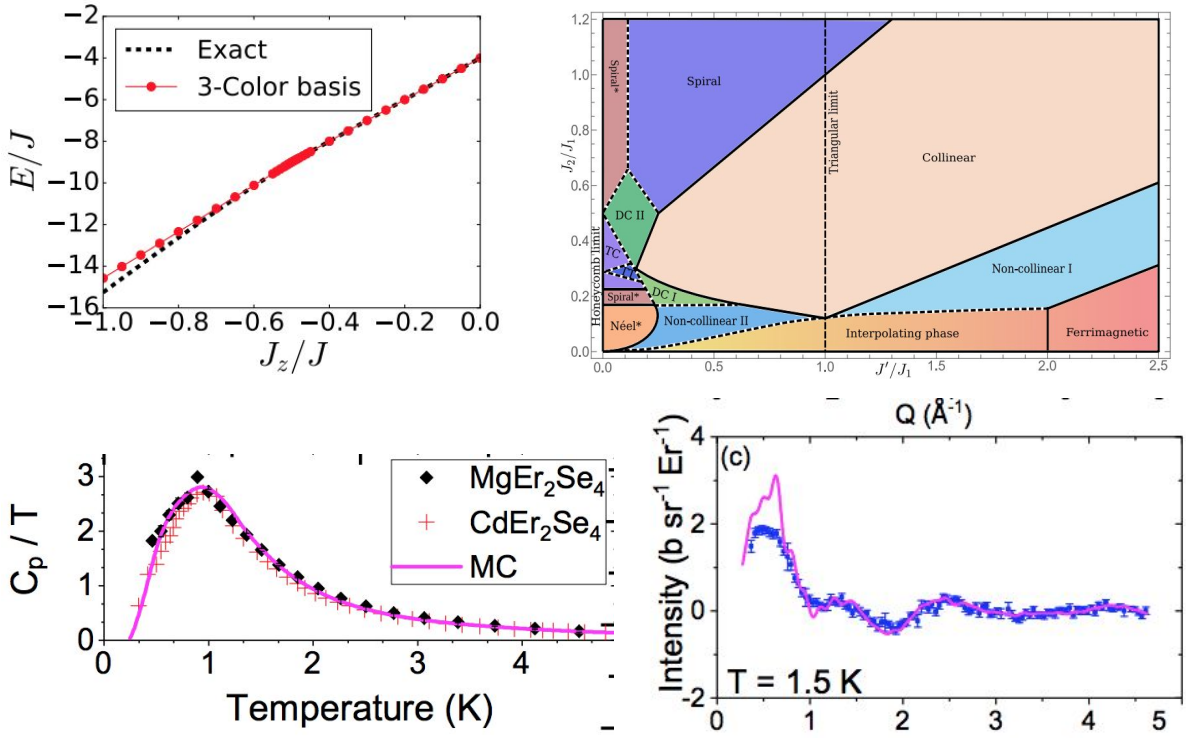
(1) We recently discovered a special Hamiltonian, H=XX+YY- ½ ZZ, which has an exponential number of degenerate ground states. This Hamiltonian connects to the most interesting phase in frustrated magnets, the quantum spin liquid. In addition, we numerically were able to show that this degenerate Hamiltonian connected to four additional phases. This gives good evidence that almost all of the phases on the

kagome lattice are actually sourced by this point. This gives a new important qualitative understanding of frustration. While much of this work was accomplished in 2017, we shepherded this result through the review process this year and it has now appeared in Physical Review Letters.

In addition, we have produced a follow-up work where we were able to analytically connect the exponentially degenerate point to all phases at high and low magnetization sectors on the kagome lattice as well as a number of other lattices. While we were eventually able to show this analytically, the key to accomplishing this was a serendipitous numerical discovery that this Hamiltonian was entirely described by the degenerate subspace. This work has been posted at https://arxiv.org/abs/1808.08633.

(2) In addition this year, we made progress on finding spin-liquids and determining the phase diagram of classical and quantum spins on the stuffed honeycomb lattice. Concerning the classical spins, we have determined the entirety of the phase diagram and found 13 phases! Four of these phases intersect in a quatri-critical point which becomes a quantum spin liquid on melting. This work is now published in Physical Review B. In terms of the model with quantum spins, we have found the existence of two spin-liquids: a Dirac spin-liquid and a chiral spin liquid. In addition, we have been able to determine seven other phases in the overall phase diagram. The current remaining questions (to be addressed this year) is to refine the locations of the transitions in these phases and to track down which PSG the Dirac spin liquid falls under.

(3) Finally, we have been collaborating with Greg MacDougall to determine the nature of the new spinel spin-ice candidate, MgErSe4. This material appears largely classical and has a ground state which has a non-trivial zero temperature entropy suggesting that it is a spin-ice. We did a numerical comparison with this experiment and showed that the typical Hamiltonian was not a good representation of this material as there was no way to use a classical Hamiltonian and simultaneously match the neutron scattering and specific heat data. Instead, some amount of quantum mechanical interactions must be included. This work has been posted at https://arxiv.org/abs/1703.04267




*Caption:* (top left) Evidence that the degenerate subspace of the XXZ0 Hamiltonian exactly represents the exact state at large Jz. Here we compare the ground state energies from exact diagonalization and diagonalization in the three-color basis as a function of Jz for the 36d cluster for Sz = 14. (top right) Classical phase diagram of the stuffed Honeycomb lattice showing 13 different phases as a function of J' and J2. (bottom) Comparison of Monte Carlo (solid line) with experiment (data points) for the specific heat (left) and the neutron scattering intensity (right). The comparison is good for the specific heat but poor for the intensity indicating that there has to be additional quantum terms.

*Why Blue Waters:* Each of these frustrated magnetism projects require a significant number of simulations to either span a phase diagram (like the stuffed Honeycomb projects) or to tune parameters to match experimental data (like the spin-ice project). In addition, at least for the cases where exact diagonalization is required it takes approximation a wall-clock day distributed over 10 nodes to get a state. Without the node-hours on Blue Waters we would not have enough time to span over the necessary part of the phase diagram.

<u>Pair Density Waves/Hubbard Models</u>

*Why it matters:* An outstanding question in the field of superconductivity is an explanation of the intertwined orders of the high temperature superconductor materials, such as LBCO. One proposal to describe this order is known as pair density wave

(PDW) order. We are considering a model which analytic arguments suggest should have pair density waves and majorana modes (a key ingredient for topological quantum computing). A better understanding of this state could lead to new insights and a deep understanding of superconducting materials.

*Key Challenge:* The key physics challenge is to numerically validate that this model has a pair density wave and majorana edge modes. In practice, the difficulty in accomplishing this is to find the relevant parameters (the phase space is large) and to overcome the fact that the system is gapless causing most methods to have increased computational complexity to solve. For example, we are attempting to use DMRG whose complexity scales logarithmically with system size.

*Accomplishments*: Despite the finite size problem, we've discovered 4 degenerate excited states that show evidence of hosting a topological edge mode. It contains a nearly localized edge mode with a superconductor in the bulk. Further work must be done to fully understand if these are indeed Majorana modes and how the ground state differs.

*Why Blue Waters*: The state of the art technique for studying this model, density matrix renormalization group (DMRG), is most adept for gapped 1D systems. Our system is effectively 1D, but is gapless – requiring a logarithmically scaling cost to evaluate larger systems. Additionally, we are plagued with finite size effects which require a large parameter search space to find a state that can realize the long range physics. The ability to parallelize many simulations simultaneously using Blue Waters allows for an efficient time frame for searching the parameter space.

<u>Machine Learning and Wavefunctions</u>

*Why it matters:* The key task of condensed matter physics is to start with a Hamiltonian and produce a ground state wave-function. Progress on this front directly affects every field of condensed matter physics.

*Key Challenge:* Unlike classical physics where there is always a polynomial relationship between the physical world and what can be classically simulated, in quantum physics simulations are exponentially more costly then the real world (this is actually why quantum computers are so powerful).

*Accomplishments:* Our accomplishments in this area are two-fold. First, we finished a result where we inverted this entire process - we can now take wave-functions and

generate all the Hamiltonians which give it. The process is, surprisingly enough, polynomial in system size. We have used this technique to invert a number of interesting wave-functions including a descendant of a spin-liquid on a ladder. This work has now appeared in Physical Review X.

Secondly, we have been using ideas from machine learning to generate improved wave-functions. In our first work on this we have developed a way to use machine learning techniques for fermion systems. In particular, we use a deep neural network to produce a configuration dependent set of single particle orbitals; we label our new wave-function the neural net backflow. This significantly improves the energetics on the Hubbard model giving us a (variance extrapolated) result that is within a percent of the exact energy.

*Why Blue Waters:* Optimizing wave-functions is computationally very expensive but embarrassingly parallel. The use of Blue Waters is essential to be able to get results back in a quick enough wall-clock time that we can iterate on the wave-functions and parameters.

List of publications/presentations associated with this work


Changlani, H. J., Kochkov, D., Kumar, K., Clark, B. K., & Fradkin, E. (2018). Macroscopically degenerate exactly solvable point in the spin-$1/2$ kagome quantum antiferromagnet. *Physical Review Letters*, *120*(11), 117202. https://doi.org/10.1103/PhysRevLett.120.117202

Changlani, H. J., Pujari, S., Chung, C.-M., & Clark, B. K. (2018). Resonating quantum three-coloring wavefunctions for the kagome quantum antiferromagnet. *ArXiv:1808.08633 [Cond-Mat]*. Retrieved from http://arxiv.org/abs/1808.08633

Chertkov, E., & Clark, B. K. (2018). Computational inverse method for constructing spaces of quantum models from wave functions. *Physical Review X*, *8*(3), 031029. https://doi.org/10.1103/PhysRevX.8.031029

Luo, D., & Clark, B. K. (2018). Backflow transformations via neural networks for quantum many-body wave-functions. *ArXiv:1807.10770 [Cond-Mat, Physics:Physics]*. Retrieved from http://arxiv.org/abs/1807.10770

Reig-i-Plessis, D., Geldern, S. V., Aczel, A. A., Kochkov, D., Clark, B. K., & MacDougall, G. J. (2017). Deviation from the dipole-ice model in the new spinel spin-ice candidate, MgEr$_2$Se$_4$. *ArXiv:1703.04267 [Cond-Mat]*. Retrieved from http://arxiv.org/abs/1703.04267

Sahoo, J., Kochkov, D., Clark, B. K., & Flint, R. (2018). Classical phase diagram of the stuffed honeycomb lattice. *Physical Review B*, *98*(13), 134419. https://doi.org/10.1103/PhysRevB.98.134419

Villalonga, B., Yu, X., Luitz, D. J., & Clark, B. K. (2018). Exploring one-particle orbitals in large many-body localized systems. *Physical Review B*, *97*(10), 104406. https://doi.org/10.1103/PhysRevB.97.104406

Yu, X., Luo, D., & Clark, B. K. (2018). Beyond many-body localized states in a spin-disordered Hubbard model. *Physical Review B*, *98*(11), 115106. https://doi.org/10.1103/PhysRevB.98.115106

**Presentations**:

“Infinite Temperature Quantum Mechanics - How Short Quantum Circuits Lead to the Breakdown of Statistical Physics and other stories about Many Body Localization” - Colliquium at UIUC by B. Clark

“Hunting for Hamiltonians” - APS 2018 March Meeting by E. Chertkov

“Artificial Neural Networks as Variational Ansatz” - APS 2018 March Meeting by D. Kochkov

“Exploring one-particle orbitals in large many-body localized systems” - APS 2018 March Meeting by B. Villalonga

“The Wellspring of all phases on the kagome lattice.” - PQI Sympsium by B. Clark

“The Wellspring of all Phases on the Quantum Kagome Antiferromagnet” - Blue Water’s Symposium by B. Clark

“Hunting Hamiltonians and Beyond” - Gordon Research Conference by B. Clark (*poster)*

“The Mother of All States on the Kagome Quantum Antiferromagnet” - International Conference on Magnetism by B. Clark (*poster*)

“The Search for Topological Edge Modes in Pair-Density Waves” - 2019 MagLab Theory Winter School by R. Levy (*poster*)

Plan for next year
We are requesting 250,000 node hours next year split into Q1: 30% , Q2: 20%, Q3: 30%  Q4: 20%

Our plans for next year involve continuing/new projects on a variety of these themes.

***Many Body Localization***

*Tackling the transition:*  Maybe the most important question remaining about the many-body localized phase is understanding the transition between the MBL and ergodic phases. While there is precise phenomenology describing the structure of the integrals of motion (IOM) of MBL systems, the breakdown of the locality of these IOMs at the transition is not yet well understood. In addition, the computation of the local IOMs of MBL systems is a challenging task for large systems. We are developing an efficient algorithm that presents successful preliminary results in computing local approximate IOMs (up to a very small error) of infinite MBL systems. Also, our algorithm shows the breakdown of the locality of the IOMs close to the transition. We expect to gain knowledge about the transition, as well as insight on the mechanism for the break down of the locality of the IOMs through this project. We plan to obtain IOMs for at least 1000 disorder realizations, at least 20 disorder strengths, and about 30 IOMs per case. Each of the runs involves exactly diagonalizing of the order of 10 large matrices (up to computational constraints) that take to 10 minutes each, running on a single core. This gives us an estimate of about 30,000 node hours needed on Blue Waters.

*Many-body localization in two dimensions:* Studies on many-body localization have mainly focused in the past on one-dimensional systems, due to the difficulty of computationally accessing highly excited eigenstates of two dimensional models. During the past year, we have developed an algorithm that efficiently approximates MBL eigenstates in arbitrary dimensions. We plan to study the MBL phase in two-dimensional systems, where its existence is an open question. Using our newly developed selected CI variant, we will do this by accessing about 1000 eigenstates on three different system sizes on at least 20 different points of the phase diagram. Each run of the algorithm to access an eigenstate involves iteratively solving about 100 eigenvalue problems on about 100 increasingly larger subspaces of an exponentially large Hilbert space, which overall takes about 20 core hours. Our estimate is that we will need 30,000 node hours to complete this project.

*Hamming distance localization of MBL eigenstates:* Our algorithm developed for two dimensional systems presents an efficient way of analyzing the spread in Hamming distance of the dominant configurations of the eigenstates, both in one- and two-dimensional systems. It is believed that MBL eigenstates are localized in Hamming distance, and this analysis would provide and empirical measurement over large systems. We expect to run this algorithm for at least 1000 eigenstates over at least 10 points over the one-dimensional phase diagram. This gives us an estimate of 15,000 node hours needed.

In total, our MBL projects require approximately 75,000 node hours.

***Spin Liquids and Frustrated Magnetism***

Stuffed Honeycomb: This year we will finish the stuffed honeycomb project determining which PSG the spin liquid supports. To accomplish this, we need to do variational Monte Carlo simulations on all the different PSG on the stuffed honeycomb lattice. Our collaborators have recently catalogued the available PSG and identified 12 of them. We then need to optimize these 12 PSG (they each have around 6 parameters) on a series of system sizes that allow us to extrapolate to the thermodynamic limit (L=32, 144, 648). The optimization of the largest size is expected to take 8000 node hours (this is extrapolating from runs we've done on 144 sites and using the fact that the algorithm scales cubically). Checking the 12 PSG then will take 96,000 node hours.

***Machine Learning for Quantum Many-Body Problems***

We have recently developed a new variational code based on the tensorflow framework that optimizes machine learning wave-functions on GPU. I understand that, recently, Blue Waters has updated tensorflow to a new enough version that we can now run efficiently all the features of this code on Blue Waters. Machine learning wave-functions are a new class and there remains a number of interesting problems and benchmarking to solve using these techniques. Our focus this year will be on using these wave-functions to understand the spin-liquid on the kagome lattice which is still controversial. Because it is only recently that everything seems to work on scale at Blue Waters and given the historical difficult of solving the kagome Heisenberg model, it has been difficult to determine how many node-hours this particular project will need. We roughly expect that we will need to do systematic studies up to 5 hidden layers with a couple different neurons per layer to extrapolate to the exact limit. Previous studies

on kagome find that a width of 8 is required to get results near the thermodynamic limit. Assuming we do a periodic bulk 8x8 system with 3 sites per unit cell, this gives 192 sites. This should take about 400 node hours per optimization run and therefore 30,000 node hours for the complete systematic study. Assuming we want to do three different parameters (the J2=0 which is most interesting but may be at a critical point) and two values at positive and negative J2, this gives 90,000 hours to accomplish this work using the xk nodes that provide GPU support.

**Pair Density Waves**

This year we will aim to finish our project on finding pair density waves and majoranas in Kondo Heisenberg chains. Preliminary results have suggested that the correlation lengths for the pair density waves are such that ladder of length L>256 are required to observe or rule out the existence of topological edge modes. We've identified several ranges of parameters which appear to have the smallest correlation lengths. If we tune three parameters around this regime (the perpendicular and parallel Heisenberg terms across the ladder as well as the diagonal term) using four points in each direction gives 64 phase points to consider seriously. Each of these phase points requires approximately 500 node hours to run requiring in total 32,000 node hours. Because these are run with DMRG, they require the high memory XE nodes**.**

**Triangular Hubbard Models**

The Hubbard model is one of the paradigmatic models of strongly correlated systems. While there has been significant study of the square Hubbard model, there is still a number of open questions about Hubbard models on different lattices. Interestingly, recent experimental and theoretical work (using DMRG) has suggested the existence of a chiral spin liquid phase on the triangular Hubbard model. As the DMRG only can simulate ladders, this has yet to be confirmed in the bulk. We will accomplish this using variational Monte Carlo (VMC) techniques, which allow a study of very large system sizes through VMC's efficient parallelization. Our preliminary optimization runs takes approximately 1000 node hours (parallelized over 10 nodes) per simulation. The triangular Hubbard model has a single parameter U/t which needs to be tuned throughout the phase diagram. Previous studies suggest that the chiral spin liquid phase, if it exists, has a range of approximately 1 (in units of U/t) but it's exact location is controversial. Therefore we will need increments of approximately 0.2 between U/t=4 and U/t=10 with approximately 2 different wave-functions each (Slater-Jastrow and a CPS wave-function). This gives 60,000 node hours total.

In total these calculations will require 353,000 node hours total with 90,000 node hours being on the GPU nodes. We are therefore requesting the maximum allowed 250,000 node hours. In practice, using some of the discounted time on Blue Waters may allow us to recover some of the additional node hours we need (this discounted time will also help compensate for the fact that many of these estimates are conservative assuming everything goes smoothly and no new exciting or confusing physics phenomena arise which need to be explored). Alternatively we will make what partial progress is possible given the allocated node hours applying for additional node hours elsewhere to complete the projects.