# QLCI Workshop on Applications of Quantum Computing to Chemistry and Biology

## Friday 2/21

**QLCI Session 1 (Joint with Sanibel Symposium Plenary 9)**

10:45-11am Chair Jim Freericks

**11:00 – 11:35 am Sofia Economou**

**Variational quantum eigensolvers for quantum chemistry simulations**

Quantum chemistry is one of the most interesting applications of quantum computers. Prior to the development of a universal quantum computer, near-term quantum simulators could implement the solution of chemistry problems that are beyond the capabilities of classical computers. To achieve this ambitious goal, it is paramount to develop algorithms that exploit the strengths of the quantum processor while also making use of classical resources. A notable example of such algorithms is the variational quantum eigensolver (VQE). A crucial aspect of VQE is the creation of a good variational ansatz, which allows for relatively shallow circuits and a low number of classical optimization parameters. In this talk, I will give an overview of VQEs for chemistry applications and present ADAPT-VQE, a novel algorithm which realizes efficient ansatze on quantum computers.

**11:35am – 12:10pm Lex Kemper**

**Physics of Spin Systems using Quantum Computing**

Quantum hardware has advanced to the point where it is now possible to perform simulations of physical systems and elucidate their ground states and excitation spectra. In this talk, I will overview some of our recent results on this topic, focusing mainly on systems of interacting spins and their properties as seen through a quantum computing lens. First, I will discuss our recent results on measuring magnons in the Heisenberg chain based on circuit that constructs the Lehmann representation of an operator. Although this approach is straightforward mathematically, the noise characteristics of the current generation of hardware causes rapid deterioration of the signal to noise ratio as a function of system size. Nevertheless, we are able to show that relatively modest noise mitigation together with Fourier transform filtering enables one to extract the magnon spectra. Second, I will overview our results on the quantum calculation of the topological phase transitions in the Kitaev model based on an adaptation of tensor network approaches. Finally, time permitting, I will overview our recent work on

measuring the thermodynamic partition function on quantum computers based on time evolution of a thermal density matrix.

**12:10pm – 12:55pm Nathan Wiebe**

**Advances in quantum chemistry simulation algorithms**

Within the last several years there have been major strides in quantum hardware that have made the promise of quantum computing much closer than anyone would have believed a mere 5 years ago. Similarly, quantum simulation algorithms have undergone a revolution. In this talk, I will provide an overview of quantum simulation algorithms as well as some of the major developments that have caused the cost of quantum simulation to be reduced by a factor of roughly 10 Billion or more. In particular, I will review recent algorithmic developments including interaction picture simulation methods, improved methods for Trotter-Suzuki simulations and stochastic integrator techniques and discuss how these techniques can be used to further reduce the cost of quantum chemistry simulation.

**Break for Lunch 12:55 – 2:25**

**QLCI Session 2 (Joint with Sanibel Symposium Plenary 10 and MAGNA Worshop)**

2:25 – 2:35 Chair Beverly Sanders

**2:35 – 3:10 Dominika Zgid**

**Creation of sparse Hamiltonians optimal for quantum computing using classical-quantum hybrid schemes**

We have developed a procedure that allows us to perform embedding calculations using a classical-quantum hybrid scheme. The impurity Hamiltonian is immediately parametrized to recover the self-energy of a realistic system in the limit of high frequencies or short time. The effective interactions parametrizing the fictitious impurity Hamiltonian are local to the embedded regions thus providing a sparse Hamiltonian resulting in a low circuit depth that is excellent for quantum computing. We show that this impurity Hamiltonian can lead to excellent total energies and self-energies that approximate the quantities of the initial realistic system very well. Moreover, we show that as long as the effective impurity Hamiltonian parametrization is designed to recover the self-energy of the initial realistic system for high frequencies, we can expect a good total energy and self-energy.

**3:10 – 3:45 Silas Hoffman**

**Topological Quantum Computation in electronic and quantum spin systems**

Majorana bound states (MBSs) realized at the ends of one-dimensional topological superconductors are useful in quantum information processing owning to their robustness to disorder and non-Abelian statistics. Although several signatures of MBSs

have been identified, definitive evidence in semiconducting nanowires has been elusive. In this talk, I consider a quantum spin chain as an alternative system supporting MBSs, pointing out salient differences in their signature and qubit construction between the electronic and spin realizations.

**3:45 – 4:20 Daniel Crawford**

**Machine Learning Meets Response Properties**

The successes of reduced-scaling coupled-cluster approaches are well known for reaction energies, thermodynamic constants, dipole moments, etc. — properties that depend primarily on the quality of the ground-state wave function. However, much more challenging are higher-order properties such as polarizabilities, hyperpolarizabilities, optical rotations, magnetizabilities, and others that also require accurate representation of the derivative of the wave function with respect to external electromagnetic fields. This lecture will provide an overview of our recent efforts to improve the description of such perturbed wave functions, from the development of field-aware densities to streamline local pair-natural orbital methods, to applications of regression techniques to learn the coupled cluster wave function from lower levels of theory, to the use of neural networks for real-time coupled cluster simulations of absorption spectra.

**Coffee Break 4:20 – 4:40**

**Dine and Dance 7pm**

## Saturday 2/22

**QLCI Session 3** (Chair: Erik Deumens)

**8:45am-9:35am Nick Rubin**

**Quantum chemistry Google's gate model quantum processor**

Simulation of quantum chemistry is a likely first application for noisy intermediate scale quantum (NISQ) computers in the post supremacy age and for fault tolerant quantum computers. We discuss the various strategies for representing and simulating electronic structure statics and dynamics with gate model quantum computers and provide perspective on progress towards exponential speedups based on current hardware performance demonstrated through the quantum supremacy experiment. As an example calculation we present the largest experimental implementation of the variational quantum eigensolver to date and demonstrate we can approach chemical accuracy for small molecular simulation problems on current devices.

**9:35am – 10:25 Yunseon Nam**

**Quantum beasts and where to stab at them**

A host of dozen-qubit quantum computers are coming online today and the race towards practical quantum computing is on. To make the best use out of existing and upcoming quantum computers, a community-wide effort, from the quantum software design to hardware manufacturing, is essential. In this talk, I will first outline the way that IonQ helped pave in this collaborative effort. Specifically, I will focus on the co-design aspect, where quantum algorithms, compilations, and controls are considered in harmony to best harness the power of trapped-ion quantum computers. Viewed through the lens of quantum applications, I will also address current and potential future efforts at IonQ that may be of interest by a wider community of prospective near-term quantum computer users.

**Coffee Break 10:25 – 10:40**

**QLCI Session 4** (Chair: Chenglong Li)

**10:40 – 11:30 Cyrus Umrigar**

**Near FCI energies from the Semistochastic Heatbath Configuration Interaction method: Application to the G1 set and the chromium dimer**

The Semistochastic Heatbath Configuration Interaction (SHCI) method [1, 2, 3, 4, 5] is a fast and memory-efficient Selected Configuration Interaction plus Perturbation Theory (SCI+PT) method that can provide near Full Configuration Interaction (FCI) energies for a variety of systems. Two key innovations are:

1. It takes advantage of the fact that the Hamiltonian matrix elements for double excitations depend only on the four orbitals whose occupations change to make the determinant selection in both the variational and the perturbative steps much faster. A similar idea is used to speed up the selection of 1-body excitations as well. This enables a procedure in which only the important determinants are ever looked at, resulting in orders of magnitude saving in computer time.

2. It overcomes the memory bottleneck of the perturbative step by evaluating the perturbative energy correction using a 3-step semistochastic approach.

The method has been applied to challenging molecular systems with more than 2 billion variational determinants and trillions of perturbative determinants, and to the homogeneous electron gas using more than 30,000 orbitals. Correlating 28 valence and semicore electrons, an accurate potential energy surface is obtained for the chromium dimer. Applications to the G1 set of molecules are also described.

References

[1] A. A. Holmes, N. M. Tubman and C. J. Umrigar, J. Chem. Theory Comput. 12, 3674 (2016).

[2] S. Sharma, A. A. Holmes, G. Jeanmairet, A. Alavi and C. J. Umrigar, J. Chem. Theory Comput. 13, 1595 (APR 2017).
[3] A. A. Holmes, C. J. Umrigar and S. Sharma, J. Chem. Phys. 147 (OCT 28 2017).
[4] J. Li, M. Otten, A. A. Holmes, S. Sharma and C. J. Umrigar, J. Chem. Phys. 149, 214110 (2018).
[5] J. Li, Y. Yao, A. Holmes, M. Otten, S. Sharma and C. J. Umrigar, Phys. Rev. Research 2, 012015(R) (2020).

**11:30 – 12:20 Victor Batista**

**Quantum simulation of molecular vibronic spectra on a superconducting bosonic processor**

The efficient simulation of quantum systems is a primary motivating factor for developing controllable quantum machines. A controllable bosonic machine is naturally suited for simulating systems with underlying bosonic structure, exploiting both quantum interference and an intrinsically large Hilbert space.

**Break for lunch (12:20-2)**

**QLCI Session 5** (Chair: Hai-Ping Cheng)

**2pm – 2:50pm Bert de Jong**

**Advancing Chemical Sciences on Near-Term Quantum Computers**

In recent years significant advances have been made to deliver quantum computing as a platform enabling scientific discovery. One of the early fields to adopt this technology is chemical sciences, but many more fields are now exploring the opportunities that quantum hardware can bring. While progress has been made in hardware, software, and algorithms, much work is still to be done to make scientific quantum computing a reality. In this talk, I will discuss some of the advances made by the QAT4Chem Quantum Algorithms Team and the BES Quantum Project, and discuss planned efforts in the Accelerated Research in Quantum Computing Teams AIDE-QC and FAR-QC, and the high-energy physics QuantiSED effort led out of Lawrence Berkeley National Laboratory. These programs involve quantum algorithm developers, mathematicians, and computer scientists with a mission to deliver algorithmic, computational, and mathematical advances to enable scientific discovery on quantum computers.

**2:50 – 3:40pm Sabre Kais**

**Quantum Information and Computation for Complex Chemical Systems**

I will present the challenging problems in quantum computing for complex chemical systems focusing on electronic structure calculations and open quantum dynamics. I will present three related approaches to electronic structure calculations: The quantum circuit model, the adiabatic quantum computing model and the quantum machine learning approach. Then I will present our recent developed quantum algorithm for evolving open quantum dynamics on quantum computing devices. Finally, I will discuss

the opportunities, open questions and challenges in the field of quantum information for quantum chemistry.

**Coffee break 3:40 – 3:55**

**QLCI Session 6** (Chair: Beverly Sanders)

**3:55 – 4:45 Jim Freericks**

**Crossing the Chasm: Practical quantum chemistry on a quantum computer**

In this talk, I will discuss strategies for explicitly carrying out quantum chemistry calculations on current and near term quantum computers. I will also discuss methodologies to embed large molecules on quantum computers in hybrid quantum-classical computations. Much of the talk will be a discussion of different options that need to be explored, but I will discuss some of the subtleties involved in using unitary coupled cluster based on my own work.

**4:45 – 5:45 Discussion (all speakers): Perspectives**

**Dinner 7pm Solarium**