Quantum Information for Quantum Chemistry (11frg014)

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The development and use of quantum computers for chemical applications has potentially revolutionary impact opportunities to change the way computing is done in future generations. The workshop brought together leading scientists from the fields of quantum information, quantum computing and quantum chemistry to exchange ideas and discuss ways to develop quantum algorithms and experimental realization and to push forward the quantum information revolution in the field of chemistry.

The main Objectives of meeting are:

- To advance our understanding of chemical processes using theoretical concepts and frameworks from quantum information. To build bridges between the communities of chemical physics and quantum information.
- To create a chain of tools for mapping quantum chemistry calculations onto a quantum algorithm. To develop calculations suitable for current and near-term quantum information processors but extendable to future devices.
- To overcome the challenges of experimental quantum simulation by developing new methods to suppress errors due to faulty controls and noisy environments. To create a toolbox of decoupling pulses and optimized error correction for integration with quantum algorithms for chemical systems.

At the meeting, Kais present an overview of the field of quantum information and computation in chemistry, discussed recent developments and open problems with emphasis on scientific progress made in this field. Presentation from the participants highlights the following topics:

- *Implementation of adiabatic quantum optimization at D-Wave*:
  D-wave has developed a hardware platform which implements an adiabatic quantum optimization algorithm[1]. The past few years have been spent characterizing this hardware tool, obtaining experimental data from the computer, and describing these experimental results using open quantum system models. The results have been extremely promising and now the quantum nature of the building blocks of the processor are well understood, focus has turned to using the hardware for real world applications. One of these applications is in the field of quantum simulation. At the workshop, Gildert and Rose presented an overview of the hardware in order to inform the other participants of the capability of this tool as a simulator[1]. Three presentations were given, the first describing the underlying Ising physics of the system, the second gave an introduction to the topology, processor architecture and fabrication processes. The final presentation covered characterizing and controlling an adiabatic quantum processor. The presentation and subsequent discussion session also included some very recent results suggesting how their system may be of use in quantum chemistry, and quantum random walks and the modeling of specific processes such as those occurring in photon capture in photosynthetic compounds. In particular Aspuru-Guzik discussed the first experimental realization of a quantum annealing

protocol towards the study of lattice folding instances. Moreover, the challenges to be overcome are: Efficient mapping of lattice-folding free-energy functions into a spin-glass classical Hamiltonian and fully programmable device able to implement arbitrary coupling define each computational instances.

- *Experimental quantum photonics*:
  One of the main objectives of the experimental quantum photonics is to build a photonic quantum simulator that is capable of exploring new physical phenomena in quantum chemistry, solid-state physics and other physical systems[2]. Quantum simulations are attracting much attention as it seems that the controlled manipulation of a few tens of qubits is already sufficient to provide insight into quantum systems that cannot be treated with classical computers. The main challenge, however, is the necessary level of coherent quantum control of individual qubits for the physical realization of quantum simulators. Walther group at Vienna[2] use the particular advantage of photons, the single particle quantum control and tunable measurement-induced interaction, to accomplish efficient quantum simulation of novel physical phenomena. This work aims to go significantly beyond state-of-the-art in developing new techniques for the generation and manipulation of multi-photon entanglement to break the ground for unimagined quantum control of ten or more individual photons. The results of these experiments will be crucial to demonstrate the feasibility of quantum simulation as a new promising application for optical quantum computers. In particular, Aspuru-Guzik and Walther discussed the demonstration of valence bond theory in chemical binding of conjugated chemical systems.

- *Decoherence, correlation and quantum annealing*:
  Kyriakidis has focused on two topics. One is on the controlled creation and manipulation of correlated states whose decoherence and relaxation times are, by virtue of their physical correlation, much greater than the more commonly used states for quantum information processing. He identified two such promising states. One is the formation meron spin textures [3] in quantum dots. These textures were previously thought to exist only in bulk 2D electron systems, and only bound in pairs. He has shown that both these assumptions are false. In fact, isolated merons can condense into the ground states of multi-electron strongly interacting quantum dots. The advantage in terms of quantum information processing is that these states possess a topological degree of freedom – the winding number; these can be used as logical qubits that may be impervious to local decohereing fluctuations.

  The second such state is a fermionic Fock state [4], again in quantum dots. Certain finite quantum systems can be open to particle exchange with a reservoir. In this case, the particle number of the system is not a good quantum number and one can speak of a coherent superposition of states with different particle numbers. He has shown [4] that these states, if they can be formed, will possess a coherence impervious to *any* single particle perturbation of the system – bosonic scattering (i.e., phonons, or lattice vibrations), particle exchange with the bath, etc.

  The second focus of his work concerns adiabatic quantum computation and its efficacy for quantum simulation of physical systems and processes. He look in particular at how the choice of interpolation function affects the performance of the computation. He has developed heuristics to derive optimal trajectories and have applied these to the factoring problem. His preliminary results indicate that optimizing the trajectories can dramatically and qualitatively improve the scaling of the computation with system size. It is currently an open question over how many decades this improved scaling can be maintained. It is also an open question as how transferable these promising results are to other important problems in quantum simulations.

- *Lie theory of unitary group and quantum information*:
  In this talk Love discussed the Cartan decomposition of the unitary groups $SU(2^n)$ with applications in quantum information theory. Sequences of Cartan decompositions have been used to prove bounds on the number of non-trivial entangling two qubit gates required to synthesize an arbitrary unitary operator on n qubits. He described a particular alternating sequence of Cartan decompositions that reproduce the best known results on synthesis of quantum circuits over CNOT gates: the quantum shannon decomposition. Concomitant with the existence of a Cartan decomposition is the existence of a Cartan involution that enables one to constructively obtain the factors at each stage of the decomposition, and ultimately to obtain the entire circuit for an arbitrary unitary matrix. Also, he described an implementation of the best-known sequence of Cartan decompositions for this purpose, and give performance data.

Factorization of 8 qubit circuits is feasible with desktop computing resources, but of course the exponential scaling of the dimension of the group with the number of qubits sets sharp limits on applying these techniques to larger circuits.

These decompositions of unitary operators may be viewed as parameterizations - and may be used in quantum information in contexts outside the circuit model. He described one such application, the computation of mixed state entanglement by a convex roof optimization over the space of ensembles realizing the mixed state density matrix. Applications of this technique include the calculation of entanglement in FMO complexes and in the recently available D-Wave superconducting quantum annealing processors.

- *Quantum algorithms and their implementation*:
Papageorgiou review recent work at Columbia University concerning quantum algorithms and their quantum circuit implementation to study the simulation of a system evolving with Hamiltonian H. They are interested in the cost of quantum algorithms approximating e^{-iHt}, with error ε. They consider algorithms based on high order splitting formulas. These algorithms approximate e^{-iHt} by a product of exponentials and obtain upper bounds for the number of required exponentials with significant speedups relative to previously known results. They also study the estimation of the ground state energy of a system with relative error ε. Deterministic classical algorithms have cost that grows exponentially with the system size. The problem depends on a number of state variables d. They exhibit a quantum algorithm that achieves relative error ε using a number of qubits $C'd\log\varepsilon^{-1}$ with total cost $Cd\varepsilon^{-(3+\delta)}$, where $\delta > 0$ is arbitrarily small. This is joint work of A. Papageorgiou, I. Petras, J. F. Traub and C. Zhang[5]. Improving the cost estimates for Hamiltonian simulation the ground state energy estimation is an open problem. They anticipate improved estimates by taking into account the initial state. Their technique for deriving an approximate ground state can be extended to other eigenvalue estimation problems. Characterizing these problems and deriving cost of the respective algorithms is another open problem. Finally Papageorgiou discuss very recent work of A. Aho and J. Briceno on the design of QuID, a high-level programming language for describing quantum circuits, and a QuID compiler. QuID contains high-level features (modular code, looping, branching) and uses Dirac notation when possible. QuID outputs "quasm"(quantum assembly language) code but the design of the compiler is target agnostic. It uses an abstract internal representation of the quantum circuit. Currently QuiD can express basic quantum circuits, the quantum Fourier transform and diagonal operators. The compiler outputs quasm code with Pauli, single qubit rotations, Hadamard, CNOT and Toffoli gates. Extensions of the language will include other unitary operators and libraries. Extensions of the compiler will include the ability to select the set of elementary quantum gates and quantum circuit templates. Code optimization and error correction are parts of the future work.

References

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