The 4th OCU Joint International WS/Seminar on QC/QCC-on-QCs*,# and WS on AI Applications to Univ. Education/Administration#

Date: Mar. 29-30, 2017
Venue: Takahara Memorial Hall, Osaka City University
*** QC/QCC-on-QCs: Quantum Chemistry/Quantum Chemical Calculations on Quantum Computers**

Program

Note:
*Prof. Man-Hong Yung, Department of Physics, South University of Science and Technology, Guangdong Sheng, China won't be able to come and participate in the WS as an invited speaker this time.

The WS/Seminar has been sponsored by Graduate School of Science, Osaka City University.

Invited speakers:

- Dr. Ryan Babbush, Google Inc., Venice, CA, USA
- Dr. Jarrod McClean, Lawrence Berkeley National Laboratory, Berkeley, CA, USA
- Prof. Joonsuk Huh, Department of Chemistry, Sungkyunkwan University, Seoul, Korea
- Dr. Hiroyuki Nakashima, Quantum Chemistry Research Institute, Kyoto, Japan
- Dr. Yusaku Kurokawa, Quantum Chemistry Research Institute, Kyoto, Japan
- Dr. Kenji Sugisaki, Department of Chemistry, Graduate School of Science, Osaka City University
- Dr. Satoru Yamamoto, Department of Chemistry, Graduate School of Science, Osaka City University
- Mr. Atsuroh Hiroe, Watson Division, IBM Japan, Ltd., Tokyo, Japan

* Prof. Man-Hong Yung, Department of Physics, South University of Science and Technology, Guangdong Sheng, China

Session “QC/QCC-on-QCs: Quantum Algorithms”

March 29 (Wed.)

9:30-10:45

Dr. Ryan Babbush, Google Inc., Venice, CA, USA
"Towards Practical Quantum Chemistry on a Quantum Computer"
Outline of the lecture:
Abstract
As small quantum computers come increasingly close to viability there has been substantial renewed interest in quantum algorithms for modeling chemistry and strongly correlated materials due to low qubit requirements and industrial importance. I will discuss these algorithms and recent work which has dramatically reduced their asymptotic cost. However, while industrial efforts to engineer a quantum memory will soon produce a quantum computer with more physical qubits than can be simulated classically, we are still many years away from having the same number of error-corrected logical qubits. This raises the question of whether shallow (and somewhat noisy) quantum circuits can be used to study classically intractable fermionic systems. I will discuss the promising possibility that parameterized quantum circuits could be trained to model such systems if optimized with respect to a variational principle. Finally, I will review a recent experimental demonstration of these algorithms and discuss prospects for larger demonstrations in the next several years.
References

10:45-12:00

Dr. Hiroyuki Nakashima, Quantum Chemistry Research Institute, Kyoto, Japan
Hiroyuki Nakashima and Hiroshi Nakatsuji
“Solving the Non-BO Schrödinger equations and analytical potential curves of small molecules with the free complement method”
Outline of the lecture:
Abstract:
Most of quantum chemistry has been developed within Born-Oppenheimer approximation where nuclei are treated classically. On the other hand, the non-Born-Oppenheimer (Non-BO) Schrödinger equations are truly exact quantum mechanical equations including all the quantum effects of electron and nuclear motions. In the present study, we tried to solve the Non-BO Schrödinger equations of small molecules accurately with the free complement method, which guarantees to converge to the exact solutions of Schrödinger equation. We also proposed a method to describe an analytical potential curve from the Non-BO wave function.

12:00 – 13:00 (Lunch break)

13:00-14:15

Dr. Jarrod McClean, Lawrence Berkeley National Laboratory, Berkeley, CA, USA
"Hybrid quantum-classical computation for chemistry and materials"
Outline of the lecture:
Abstract:
Quantum computers promise to dramatically advance our understanding of new materials and novel chemistry. Unfortunately, many proposed algorithms have resource requirements not yet suitable for near-term quantum devices. In this talk I will focus on the application of quantum computers to hard problems in the application area of chemistry and materials, and discuss the challenges and opportunities related to current algorithms. One particular method of interest to overcome quantum resource requirements is the variational quantum eigensolver (VQE), a recently proposed hybrid quantum-classical method for solving eigenvalue problems and more generic optimizations on a quantum device leveraging classical resources to minimize coherence time requirements. I will briefly review the original VQE approach and introduce a simple extension requiring no additional coherence time to approximate excited states. Moreover, we show that this approach offers a new avenue towards mitigation of decoherence in quantum simulation requiring no additional coherence time beyond the original algorithm and utilizing no formal error correction codes. The geometry of this algorithm and it possible extensions to other application specific error correction will be discussed.

14:15-15:30

Dr. Yusaku Kurokawa, Quantum Chemistry Research Institute, Kyoto, Japan
Yusaku I. Kurokawa, Hiroshi Nakatsuji
"Solving the Schrödinger Equation of Harmonium Systems with the Free-Complement Local-Schrödinger-Equation method"
Outline of the lecture:
Abstract:
The Free Compliment Local-Schrödinger-Equation (FC-LSE) method is a general method to solve the Schrödinger Equation of any systems. We have applied it to solve the Schrödinger Equation of two- and three-electron harmonium systems. The results agreed with the Cioslowski's energies to five digits in the atomic unit. In the lecture, we review the FC method, and show the application to these harmonium systems.

15:30-16:30

Dr. Satoru Yamamoto, Department of Chemistry and Molecular Materials Science, Graduate School of Science, Osaka City University
"Computational Control and Measurement Approaches for Electron Spin Resonance Based Quantum Computers"
Outline of the lecture:
Abstract:
We have studied quantum computing (QC) based on electron spin resonance techniques, aiming the implementation of molecular spin quantum technology. In relevant QC experiments, there are two subjects; (1) to identify the time evolution and (2) to apply arbitrary quantum operations. To tackle those, we have developed the

experimental and computational approaches which enable us to tackle the issues above.

16:30-17:30

Dr. Kenji Sugisaki, Department of Chemistry and Molecular Materials Science, Graduate School of Science, Osaka City University
"Quantum chemical calculations of open shell molecules on quantum computers"
Outline of the lecture:
Abstract:
An overview of the full configuration interaction (full-CI) calculations of open shell molecules on quantum computers will be provided. We will propose two relevant quantum algorithms to construct the wave function consisting of one configuration state function, which is suitable for the initial guess wave function in the quantum phase estimation algorithm-based full-CI calculations of open shell molecules with many unpaired electrons.

March 30 (Thu.)

9:30-10:40

Prof. Joonsuk Huh, Department of Chemistry, Sungkyunkwan University, Seoul, Korea

“Quantum simulation of molecular spectroscopy”

Outline of the lecture:
Abstract:
The intrinsic nature of parallelism of quantum states is anticipated to give extraordinary computational power to quantum processors for certain problems. A linear optical network is one of the simplest quantum processors that it could reveal the (computational) quantum supremacy against classical machines. A photon-sampling problem in a linear optical network, so-called Boson Sampling, is a specially designed mathematical problem, which is expected to be intractable for any classical machine. In my talk, I will present what we can do with the photonic quantum simulator (non-universal quantum computer) practically. Boson Sampling is generalized with Gaussian input states to simulate the molecular vibronic spectroscopy [1-5].
[1] J. Huh, G. G. Guerreschi, B. Peropadre, J. R. McClean, and A. Aspuru-Guzik. Boson Sampling for Molecular Vibronic Spectra. Nature Photon. 9 (2015): pp 615-620.
[2] J. Huh and M.-H, Yung, Hierarchy in Sampling Gaussian-correlated Bosons, Preprint: arXiv:1608.03731.
[3] Y. Shen, J. Huh, Y. Lu, J. Zhang, K. Zhang, S. Zhang and K. Kim, Quantum simulation of molecular spectroscopy in trapped-ion device, Preprint: arXiv:1702.04859

[4] D. G Olivares, B. Peropadre, J. Huh and J. J. García-Ripoll,
Quantum emulation of molecular force fields: A blueprint for a superconducting architecture
Preprint: arXiv:1611.08101
[5] B. Peropadre, J. Huh and C. Sabin, Dynamical Casimir effect for boson sampling,
Preprint: arXiv:1610.07777

Session “AI Applications to Univ. Education/Administration” (in Japanese)

10:45-12:00
講演者：広江　淳良氏、ワトソン事業部、IBMジャパン
講演題目：“ワトソンで何ができるか“
Mr. Atsuroh Hiroe, Watson Division, IBM Japan, Ltd., Tokyo, Japan
“What can Watson do in the university education and administration?”

Outline of the lecture:

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