# The 3rd OCU Intn'l Seminar on QC/QCC-on-QCs*

## Date: Mar. 29-30, 2016
## Venue: OCU Faculty of Science, Meeting Room
## * QC/QCC-on-QCs: Quantum Chemistry/Quantum Chemical Calculations on Quantum Computers

## Program:

*** Note:** We have had a piece of bad news. Dr. James Whitfield, Univ. of Vienna won't be able to come because the final process of arranging the flights wasn't successful on Japan side. The seminar has been supported by OCU.

## March 29 (Tue.)
## 14:00-15:30 (including a ten-minute coffee/tea break)

Chiranjib Mitra, Associate Professor
Dept. of Physic, Physical Science, IISER Kolkata (Indian Institute of Science Education and Research Kolkata), India

"Probing quantum phase transitions using tools of quantum information processing "

**Outline of the lecture:**

Abstract

The macroscopic entanglement properties of a low dimensional quantum spin system is investigating by studying its magnetic properties at low temperatures and high magnetic fields. The temperature and magnetic field dependence of entanglement from the susceptibility and magnetization data is performed and comparison is made with corresponding theoretical estimates. Extraction of entanglement has been made possible through the macroscopic witness operator, magnetic susceptibility. The spin system studied is a chain, which exhibits dimerisation and yields fascinating entanglement properties when the temperature and magnetic field are varied. These spin systems exhibit quantum phase transition (QPT) at low temperatures, when the magnetic field is swept through a critical value. We show explicitly, using tools used in quantum information processing (QIP), that quantum phase transition (QPT) can be captured experimentally using quantum complementary observables. We also report heat capacity as an entanglement witness. Entanglement properties of the same quantum spin system has also been investigated by heat capacity measurements performed down to very low temperatures (400 mK), for various applied magnetic field values. The experimentally extracted results for the value of heat capacity at zero field matches perfectly with the theoretical estimates of entanglement from model Hamiltonians. We also report experimentally quantified quantum discord in the same spin system.

References

[1] Diptaranjan Das, Harkirat Singh, Tanmoy Chakraborty, Radha Krishna Gopal and Chiranjib Mitra, Experimental detection of quantum information sharing and its quantification in quantum spin systems, New Jour. Phys., 15, 013047 (2013).
[2] Harkirat Singh, Tanmoy Chakraborty, Diptaranjan Das, H S Jeevan, Y Tokiwa, Philipp Gegenwart, Chiranjib Mitra, Experimental quantification of entanglement through heat capacity, New Journal of Physics, 15, (2013) 113001.
[3] Harkirat Singh, Tanmoy Chakraborty, Prasanta K Panigrahi, Chiranjib Mitra, Experimental estimation of discord in an antiferromagnetic Heisenberg compound Cu $(NO_3)2$ 2.5 $H_2O$, Quantum Information Processing, 14, (2015) 1-11.
[4] Spin chains: Long-distance relationship, Chiranjib Mitra, Nature Physics, 11, (2015) 212.

## 15:30-16:30 (no coffee/tea break)

Elham Hosseini, Postdoctoral Fellow
Dept. of Chemistry & Molecular Materials Science, Graduate School of Science, Osaka City Univ.
“Quantum control in molecular spin qubits” (provisional)
Outline of the lecture:

1. Introduction to quantum control
2. Implementation of quantum control in molecular spin qubit systems

## 16:40-17:40 (no coffee/tea break)

Kenji Sugisaki, Assistant Professor
Dept. of Chemistry & Molecular Materials Science, Graduate School of Science, Osaka City Univ.
"Quantum chemistry on quantum computers: General survey and what can we do?"
**Outline of the lecture:**
1. Recent advance in CSF-based full-CI calculations
2. A method of free complement: Beyond the full-CI calculations

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## March 30 (Wed.)

## 9:30-11:00 (including a ten-minute coffee/tea break)

Nike Dattani, Dr., Research Scientist, Dept. of Chemistry, The Univ. of Oxford.
Research Fellow, Fukui Institute for Fundamental Chemistry, Kyoto University
“Reducing multi-qubit interactions in adiabatic quantum computation without adding auxiliary qubits” (provisional)

**Outline of the lecture:**
Quantum annealing has recently been used to determine the Ramsey numbers R(m,2) for 3 < m < 9 and R(3,3) [Bian et al. (2013) PRL 111, 130505]. This was greatly celebrated as the largest experimental implementation of an adiabatic evolution algorithm to that date. However, in that computation, more than 66% of the qubits used were auxiliary qubits, so the sizes of the Ramsey number Hamiltonians used were tremendously smaller than the full 128-qubit capacity of the device used. The reason these auxiliary qubits were needed was because the best quantum annealing devices at the time (and still now) cannot implement multi-qubit interactions beyond 2-qubit interactions, and they are also limited in their capacity for 2-qubit interactions. We present a method which allows the full qubit capacity of a quantum annealing device to be used, by reducing multi-qubit and 2-qubit interactions. With our method, the device used in the 2013 Ramsey number quantum computation could have determined R(16,2) and R(4,3) with under 10 minutes of runtime.
http://arxiv.org/abs/1508.07190

Most recent publications (2015):
Dec. 2: http://arxiv.org/abs/1512.01141
Oct. 26: http://arxiv.org/abs/1510.07420
Sept. 23: http://arxiv.org/abs/1509.07041
Aug. 28: http://arxiv.org/abs/1508.07190
Aug. 28: http://arxiv.org/abs/1508.07184
Aug. 19: http://arxiv.org/abs/1508.04816
**FeynDyn (QUAPI on GPUs):** http://tinyurl.com/FeynDyn
http://oxford.academia.edu/NikeshDattani

## 11:10-12:00 (no coffee/tea break)

Mr. Satoru Yamamoto, Grad. Student
Dept. of Chemistry and Molecular Materials Science, Graduate School of Science, Osaka City Univ.
"Adiabatic quantum computation on molecular spin (MSQ) quantum computers"
**Outline of the lecture:**
1. ESR-based spin Hamiltonian and spin manipulation
2. MSQ based AQC: Implementation of pulse sequences for factorization

**Contact: Kazunobu Sato, Professor**
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