Osaka City University
OCU Press Release

August 8, 2016
OCU Public Relations Department

Quantum Computers Can Solve Quantum Chemistry
An Ultrahigh Speed Quantum Algorithm for Solving Intractable Quantum Chemical Calculations by Any Classical Computers.

Summary:
Quantum chemical calculations of large-scale atomic/molecular systems require *exponential CPU time*, called "*notorious exponential explosion*", and thus any modern/classical computers are not allowed to treat relevant problems. Quantum computers enable us to tackle this intractable issue, chemists of Osaka City University (OCU) have reported on Sept. 8, 2016.

A quest for any disruptive algorithm capable of solving *quantum chemical calculations in a polynomial time* has been the focus of contemporary issues in the fields of advanced science and technology. The OCU group of Prof. Takeji Takui, Prof. Kazunobu Sato, Lecturer Kenji Sugisaki and their coworkers of the Graduate School of Science has found an *ultrahigh speed quantum algorithm for solving the Schrödinger equation and performing electronic-structure calculations with full configuration interactions (FCI calculations*). Their paper on the discovery of the quantum algorithm has been published online on the website of *The Journal of Physical Chemistry A*, an international journal of American Chemical Society at 8:00 am on Sept. 8, 2016 (9:00 pm on Sept. 8 (JST) (Cf. Journal/paper information given below).

The quantum algorithm and associated quantum operation circuits (see Fig. below) discovered by the OCU group execute FCI calculations, which are the most suitable approaches for giving optimal solutions of the Schrödinger equation, in polynomial time scale, particularly the most efficient for calculating the electronic structures of open-shell molecular or chemical/physical entities such as single molecule nanomagnets or Mn clusters in the photosynthetic system II. Single molecule nanomagnets are the most important molecular components in spintronics as emerging spin technology, whose electronic spin structures have not fully been elucidated. A difficulty of "*notorious exponential explosion*" in quantum chemistry has been for the first time eliminated.

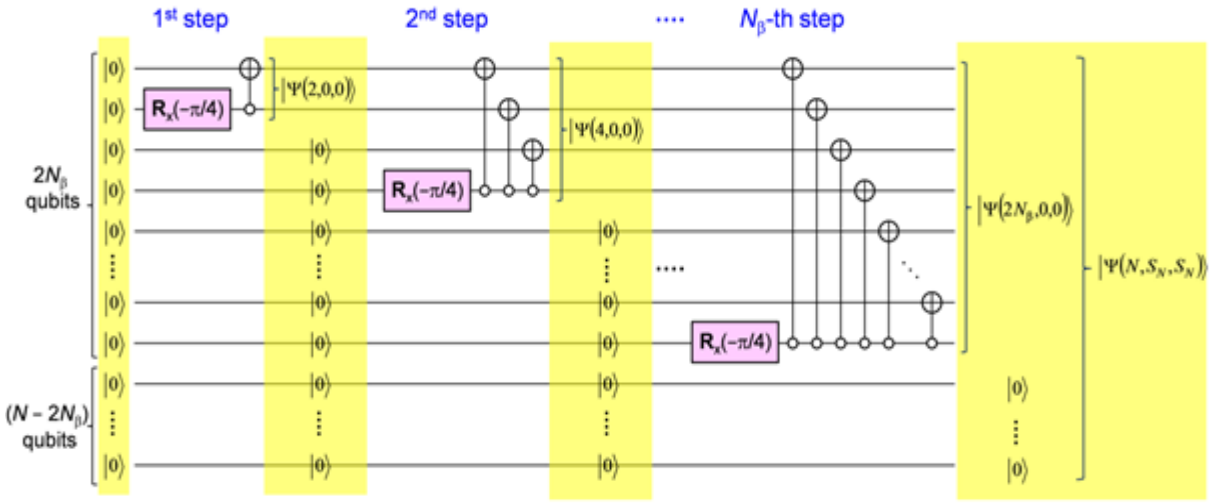

Figure. Quantum circuit implemented for the present quantum algorithm.

Further applications and perspectives:

The quantum algorithm discovered can be accommodated in quantum circuits of *any practical quantum computers*, and thus the algorithm is widely applicable to solving the Schrödinger equation in many fields including materials science, molecular biochemistry and protein structural science/technology, and contributes to progress in emerging relativistic quantum chemistry.

Journal/paper information:

Name of Journal: The Journal of Physical Chemistry A
Title of Paper: Quantum chemistry on quantum computers: A polynomial-time quantum algorithm for constructing the wavefunctions of open shell molecules
Names of Authors: *Kenji Sugisaki,* Satoru Yamamoto, Shigeaki Nakazawa, Kazuo Toyota, Kazunobu Sato,* Daisuke Shiomi, and Takeji Takui**
URL: http://pubsdc3.acs.org/doi/abs/10.1021/acs.jpca.6b04932

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