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Quantum Computing Challenges for Transition Dynamics in Atomic and Molecular Systems

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Quantum computing (QC), based on principles of superposition, entanglement, and measurement of qubits, promises the advantage to surpass the performance of classical computing in cryptography, communication, and optimization problems, as well as in simulations of complex quantum system in physics and computation chemistry. Despite decades in development, fully coherent, fault-free universal quantum Turing machine with large number of qubits is not yet accessible. The decoherence and quantum noise in the so called near-term, noisy, intermediate-scale quantum (NISQ) computers impair the performance and accuracy of many applications [1]. This is partially mitigated by development of hybrid quantum-classical algorithms which reduce the depth of the quantum circuits, lessening sources of the noise [2].

We will present development of new family of quantum algorithms and relevant computational tools for simulating transition dynamics in time-dependent quantum systems on a quantum computer at NISQ era. These aim to answer two questions:
(1) How to simulate the transition dynamics, accurately and efficiently, between many states of an atomic system perturbed by strong time-dependent perturbation?
(2) How to compute the collisional S-matrix for the vibrational dynamics of the $+_2$ system, including dissociative processes?

To answer 1), a QC schemes were developed utilizing McLachlan variational principle in a hybrid quantum-classical algorithm, using both unary and qubit efficient encoding to accurately calculate the transition dynamics between excited states of a closed quantum system, an one electron atom, subject to a strong, attosecond laser pulses [3]. A systematic approach for optimal construction of a general N-state ansatz with unary N-qubit encoding is refined. The qubit efficient encoding reduces the number of qubits to $\log_2 N$, simultaneously diminishing depth of a quantum circuit.

Building an algorithm and a relevant system of quantum circuits [4] to calculate evolution operator in Trotter approximation for simulating the collisional $H + H_2$ system, answers question 2). The full S-matrix of the system is obtained, which describes transitions between all bound vibrational states and the discretized vibrational continuum of the ground electronic surface of H_3. Obtaining the cross sections for vibrational transitions coupled to the dissociative continuum paw a road for the QC description of the dynamic of the open quantum systems.

References:

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Primary author: KRSTIC, Predrag S. (Institute for Advanced Computational Science, Stony Brook University)

Presenter: KRSTIC, Predrag S. (Institute for Advanced Computational Science, Stony Brook University)

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