Simulation of Excitation Energy Transfer Using a Quantum Computer

Shin Sun and Yuan-Chung Cheng*

*Department of Chemistry, National Taiwan University, Taipei City, Taiwan

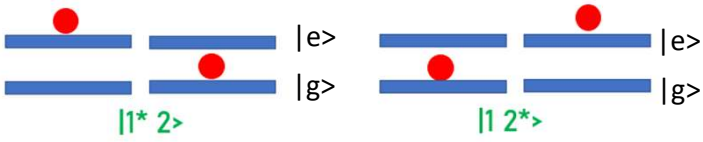
National Taiwan University

Abstract

Quantum computers promise to revolutionize computations in several areas highly related to chemistry using their the exponential large state space, quantum parallelism, and the power of entanglement. Several quantum algorithms for chemical problems have been proposed. For example, the Quantum Phase Estimation Algorithm (PEA) for calculating ground state energy for molecules has proven to be exponentially more efficient than classical Full Configuration Interaction (FCI) methods, which could enable in- silico design of new catalysts, pharmaceuticals, and materials. However, contemporary quantum computers suffer from severe errors, termed as Noisy Intermediate-Scale Quantum (NISQ), which render long quantum circuit useless for practical purposes. To make use of near term NISQ computers, we must find suitable problems and design efficient quantum algorithms. Hence, in my research, I intend to characterize the intrinsic noises in current quantum computers and try to utilize the noises to simulate energy transfer process in a dissipative environment, which could provide more insight into the dynamics of open quantum systems, non-equilibrium statistical mechanics in general, and help develop better devices.

Encoding the Hamiltonian

Start with the site-based exciton Hamiltonian in the second quantized form. We can map the number-preserved excitation operator to corresponding Pauli operators acting on the qubit Hilbert space. We use a simple symmetric dimer model to demonstrate the concept.



The model system Hamiltonian in site basis:

$$H = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad H = a_1^+ a_2 + a_1 a_2^+$$

By employing a Jordan-Wigner-like transformation, the corresponding qubit Pauli operators for creation and annihilation operators can be deduced.

$$a_n^+ = \frac{1}{2}(X_n - iY_n) \qquad a_n = \frac{1}{2}(X_n + iY_n)$$

Hence, the system can be mapped to a two-qubit system with qubit Hamiltonian.

$$\tilde{H} = \frac{1}{2}(X_1X_2 + Y_1Y_2)$$

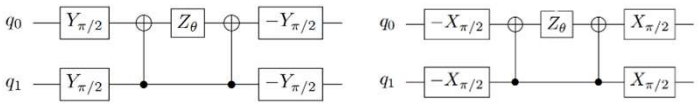
Trotterization and Quantum Evolution Circuit

For a qubit Hamiltonian written as sum of local terms (local Hamiltonian), the propagator can be easily cast into quantum circuit using only local quantum gates by the Trotter formula. In our simulation, we use trotter expansion to propagate the dynamics.

$$e^{i(A+B)t} = \lim_{n\to\infty}(e^{iAt/n}e^{iBt/n})^n$$

$$|\Psi(t+\delta t)> \approx e^{-iA\delta t}e^{-iB\delta t}|\Psi(t)>$$

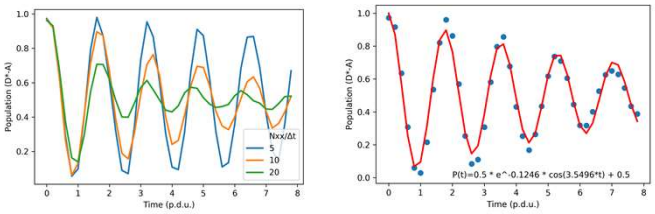
Quantum circuits for time evolution:



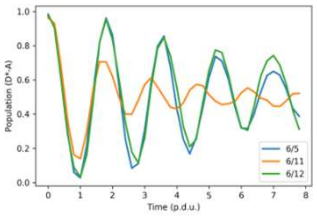
XX YY

Population Dynamics of the Dimer Model

We have designed quantum programs to extract the population dynamics for our dimer model and carried out the simulation on IBM Q system. The damping effects are achieved by inserting XX gates proportional to the simulation time, which deliberately amplify the noises.



Temporal Inconsistency



During our experiments, we also observed that the current IBM-Q platform does not offer enough stability for consistent and quantitative simulation of dissipative quantum dynamics in molecular systems

Conclusions

- We have reproduced simple proof-of-concept experiments for dimer model population dynamics on real quantum devices.
- Intrinsic noises on QC can produce clear damping effect in the dimer model simulation.
- The damping strength could be controlled by the number of XX gates. Further quantitative analysis and calibration will be necessary.
- In conclusion, our model and algorithms successfully reproduce the expected dynamics for an coherent-to-incoherent transition for a excitation energy transfer process qualitatively. We will explore better calibration of the NISQ devices, pulse-level control for optimized consistency, and quantitative analysis of based on transfer tensor network algorithms in order to improve the results.
- We hope that by carefully introduce and control noises on NISQ, we can turn NISQ into a efficient platform for open quantum system simulation, which might be another application with quantum advantage.

References

1. Nielson, M.; Chuang, I. Quantum Computation and Quantum Information, 1st ed.; Cambridge University Press: Cambridge, 2000
2. Kassal, I.; Whitfield, J.; Perdomo-Ortiz, A.; Yung M. H.; Aspuru-Guzik, A. Annu. Rev. Phys. Chem. 2011, 62, 185-207.
3. P. J. J. O'Malley et al. Phys. Rev. X 6, 031007, 2016