Quantum Simulation of Scattering Towards Computation Fusion Reaction

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Introduction

The collision processes and scattering physics of particles, atoms and molecules are crucial to our understanding of the fundamental structure of matter. Fusion is the quantum nuclear reaction that occurs when two light nuclei collide and fuse to create a single heavier nucleus with less mass than the two original nuclei. The leftover mass is converted to energy and is responsible for the generation of fusion energy. Harnessing practical fusion energy is identified as one of the Grand Challenges for Engineering in the 21st Century.

Current fusion devices focus on deuterium-tritium (D-T) reaction [Kikuchi10], with two branches:

$$D + T \rightarrow {}^{5}\mathrm{He}^{*} \rightarrow {}^{4}\mathrm{He}(3.5\ \mathrm{MeV}) + n(14.1\ \mathrm{MeV}),$$
$$D + T \rightarrow {}^{5}\mathrm{He}^{*} \rightarrow {}^{5}\mathrm{He}+\gamma(16.75\ \mathrm{MeV}).$$

The fusion power gain in a large fusion device such as the International Thermonuclear Experimental Reactor (ITER) or a Fusion Pilot Plant (FPP) is gauged by measuring neutron production. However, the γ to n branching ratio is very small, somewhere between $1\times10{-}5$ and $3\times10{-}4$ with an uncertainty of about 50% [Kim12].

Ab initio approaches, such as the no-core shell model with continuum (NCSMC), represents the state of the art for modeling D-T fusion [Hupin19]. To accurately model reactions, and in particular to get the correct absolute values, the NCSMC includes as many scattering and reaction channels as possible. Thus, not only is the relative motion of deuterium and tritium included, but also virtual excited states as well, requiring a fully five-body quantum-mechanical wave function.

Numerical simulation could serve to guide and accelerate the time to experimental discovery in quantum scattering. However, all known methods for classical simulation of fusion reaction, such as renormalization group, quantum Monte Carlo, and tensor network methods, suffer from issues of scalability, accuracy, and efficiency for quantum many-body systems, and introduce errors that are difficult to gauge. Thus, the fusion reaction problem is an ideal candidate for demonstrating early quantum advantage.

Quantum Algorithms

Quantum computation has the potential for the efficient simulation of many body quantum systems. This was demonstrated in polynomial time quantum algorithms, usually based on quantum phase estimation (QPE), to solve the ground state and low-energy excited states for certain families of quantum Hamiltonians with provable guarantees [Abrams99, Aspuru-Guzik05]. However, the QPE algorithm requires resources that are out of reach for near term quantum hardware and it is unclear when it will be achievable at scale. A variety of quantum algorithms for solving the ground state problem on near-term noisy and early fault-tolerant quantum hardware have been proposed, notably including the quantum metropolis algorithm, variational quantum eigensolver [Peruzzo14], and quantum imaginary time evolution (QITE) [Jouzdani22]. Below, we highlight recent demonstrations of quantum algorithms for the simulation of many body quantum Hamiltonians towards quantum scattering:

- Scattering in the Ising model with the Quantum Lanczos Algorithm [Yeter21].
- Simulating excited states of the Lipkin model on a quantum computer [Manqoba23].
- Nuclear shell-model simulation in digital quantum computers [Perez23].

Use Case Study

As a step towards applying quantum algorithms for the simulation of fusion reaction, we propose the case study of quantum simulation of scattering of low-energy states in a model many body quantum Hamiltonian. Such a study was performed for the Ising model on a 5-qubit IBM quantum computer [Yeter21].

In this study, participants will first select a model quantum many body Hamiltonian. For example,

- the Lipkin model [Manqoba23],
- a simple nuclear Hamiltonian for proton-neutron interaction [Jouzdani22],
- the anisotropic 1-D XXZ-Heisenberg [VanDyke21].

Next, participants will demonstrate scattering of low-energy states. For example, in the 1-D Heisenberg model in the ferromagnetic phase, low-energy excitations of an all up spin ground state have blocks of down spins of down spins on neighboring sites and are called magnon bound states. Scattering of magnon bound states have been shown to produce soliton-like behavior and have been studied classically using DMRG and Bethe ansatz methods. Participants will use quantum algorithms to determine physical quantities, such as scattering amplitudes, scattering phase, and block length displacements, that describe the outcomes of scattering processes [Francis20]. For example, a scattering amplitude, or transition probability, between an initial and final state may be computed by

$$A(t) = \langle \psi_{fin} | \psi_{in}(t) \rangle \qquad \text{where} \qquad |\psi(t)\rangle = e^{-iHt}|\psi\rangle$$

Various methods can be used when performing scattering calculations such as a Green's function approach through the Schwinger-Lipmann equation [Baker21] or dynamic approach with time-evolved two-point correlation functions [Yeter21].

References

[Abrams99] D. S. Abrams and S. Lloyd. *Quantum algorithm providing exponential speed increase for finding eigenvalues and eigenvectors*. Physical Review Letters **83**(24), 5162 (1999)

[Aspuru-Guzik05] A. Aspuru-Guzik, A. D. Dutoi, P. J. Love, and M. Head-Gordon. *Simulated quantum computation of molecular energies*. Science **309**(5741), 1704–1707 (2005)

[Baker21] T. E. Baker. Lanczos recursion on a quantum computer for the green's function and ground state. Physical Review A 103(3), 032404 (2021)

[Hupin19] G. Hupin, S. Quaglioni, and P. Navrátil. *Ab initio predictions for polarized deuterium- tritium thermonuclear fusion*. Nature communications 10(1), 1–8 (2019)

[Francis20] A. Francis, J. K. Freericks, and A. F. Kemper. *Quantum computation of magnon spectra*. Phys. Rev. B 101, 014411 (2020)

[Jouzdani22] P. Jouzdani, C. W. Johnson, E. R. Mucciolo, and I. Stetcu. *Alternative approach to quantum imaginary time evolution*. Phys. Rev. A 106, 062435 (2022)

[Kikuchi10] M. Kikuchi, *A Review of Fusion and Tokamak Research Towards Steady-State Operation: A JAEA Contribution*. Energies 3, no. 11: 1741-1789 (2010)

[Kim12] Y. Kim, J. Mack, H. Herrmann, C. Young, G. Hale, S. Caldwell, N. Hoffman, S. Evans, T. Sedillo, A. McEvoy et al. *Determination of the deuterium-tritium branching ratio based on inertial confinement fusion implosions*. Physical Review C 85(6), 061601 (2012)

[Manqoba23] M. Q. Hlatshwayo, Y. Zhang, H. Wibowo, R. LaRose, D. Lacroix, and E. Litvinova. *Simulating excited states of the Lipkin model on a quantum computer*. Phys. Rev. C 106, 024319 (2023)

[Perez23] A. Pérez-Obiol, A. M. Romero, J. Menéndez, A. Rios, A. García-Sáez, and B. Juliá-Díaz. *Nuclear shell-model simulation in digital quantum computers*. Sci Rep 13, 12291 (2023).

[Peruzzo14] A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru- Guzik, and J. L. O'brien. A variational eigenvalue solver on a photonic quantum processor. Nature communications 5(1), 1–7 (2014)

[VanDyke21] J. S. Van Dyke, E. Barnes, S. E. Economou, and R. I. Nepomechie. *Preparing exact eigenstates of the open XXZ chain on a quantum computer*. Phys. A: Math. Theor. 55 055301 (2021)

[Yeter21] K. Yeter-Aydeniz, G. Siopsis, and R. C. Pooser. Scattering in the Ising model with the quantum lanczos algorithm. New Journal of Physics 23(4), 043033 (2021)