Exploring algorithms for quantum computing of atomic nuclei

Aman Gupta[1],* Pooja Siwach[2], and P. Arumugam[1]
[1]*Department of Physics, Indian Institute of Technology Roorkee, Roorkee-247667, Uttarakhand, India and*
[2]*Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, USA*

Introduction

Quantum computers can mimic any quantum system upto a limit that is offered by the hardware. Therefore the quantum simulators allow the study of quantum systems which are very difficult to study in traditional laboratories and impossible to model complex ones. The field of quantum computing is introduced only recently and its most obvious application in the field of quantum chemistry has been growing rapidly ever since. Many atoms and molecules have already been successfully simulated on a quantum computer with a higher accuracy & very much improvement in computation speed. The simulation of LiH molecule has already been done on a quantum computer by IBM in just 9 hours [1].

The most popular methods to simulate atoms and molecules are Variational Quantum EigenSolver(VQE) and Quantum Phase Estimation(QPE). The idea is to apply these methods to simulate a nucleus(to understand complex nuclear structures), compare between the methods and propose a hybrid of VQE and QPE algorithms.

Methods

VQE

To demonstrate the method, we use an example of a simple nucleus i.e. deuteron. The two body Hamiltonian (therefore, 2 qubits are required) for deuteron in the form of weighted Pauli operators is given by [2, 3]:

$$H_2 = \omega_1 I + \omega_2 Z_0 + \omega_3 Z_1 + \omega_4 (X_0 X_1 + Y_0 Y_1) \quad (1)$$

and three body Hamiltonian(3 qubits) as:

$$H_3 = H_2 + \omega_5 (I - Z_2) + \omega_6 (X_1 X_2 + Y_1 Y_2) \quad (2)$$

Now the aim is to find the lowest value for the observables $\langle\psi|H_2|\psi\rangle = \epsilon_2$ and $\langle\psi|H_3|\psi\rangle = \epsilon_3$ using a classical gradient descent methods and the obtained value is expected to be the ground state energy, and the corresponding wave functions as the ground state of the nucleus. To obtain the observable, we use variational approach: guess a wave function(ansatz) with a parameter (say θ), obtain the value of the observables and minimise this with respect to θ to get optimal value of θ, hence value of optimal value for ϵ_2 and ϵ_3.[4]

QPE

The idea of quantum phase estimation is to implant the Hamiltonian as a phase onto the qubits. Using the same two body and three body Hamiltonians(H_2 and H_3, from eq. 1 and 2 respectively) , we prepare the state of the system as one of the eigen vectors of the Hamiltonians, although a random input state can also work; and then do the time evolution of the state as :

$$|\psi\rangle_f = e^{-iHt}|\psi\rangle \quad (3)$$

to obtain a new state. Now according to phase estimation algorithm, we except to observe the state to be:

$$|\psi\rangle_f = e^{i2^n\theta}|\psi\rangle \quad (4)$$

after measurement. Therefore, the measurement of θ technically gives us the time evolution of the system . By setting the value of time we can also get the ground state energy of the deuteron.

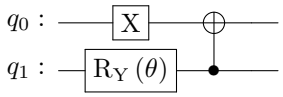
*Electronic address: a_gupta@ph.iitr.ac.in

VQE + QPE hybrid

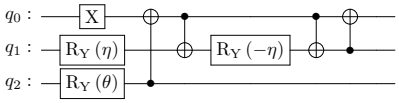
As we know it is not always possible to get eigenvectors and eigenvalues of an arbitrary Hamiltonian. Therefore, a very better and efficient method with less error would be to obtain the initial state (stationary state) of the system using VQE and then using it as an initial state for QPE method to study its time evolution.

Results and Discussions

For ground state eigenvalue, we use the mentioned two body and three body Hamiltonians with $\omega_1 = 5.906709$,$\omega_2 = 0.218291$,$\omega_3 = -6.125$,$\omega_4 = -2.143304, \omega_5 = 9.625, \omega_6 = -3.913119$. In case of VQE, we use 2 qubit ansatz: For 3 qubit



case, we use the following ansatz: For



QPE algorithm, we use different time steps of $t = \frac{1}{20}, \frac{1}{3}, \frac{1}{2}, 1$. The number of work qubits (control) is 7 and simulation qubits(target) is equal to the number of required qubits (2,3).

TABLE I: A comparison between different methods for 2 body and 3 body deutron hamiltonian

Method	**Eigen value (ϵ)**	**Evaluation Time**
VQE(2 qubit)	-1.74916	0.708
QPE(2 qubit)	-1.6198	17.9814
VQE(3 qubit)	-2.04567	1.15
QPE(3 qubit)	-1.3744	17.929
Hybrid(2 qubit)	-1.7369	42.32
Hybrid(3 qubit)	-1.9083	43.67

From very preliminary results, we observe several interesting features. First, for a simple Hamiltonian, VQE clearly performs better in all aspects. But this method uses classical gradient descent for optimization. Hence, it is vulnerable to local minima and can also not account for system evolution and interactions. Second, while QPE can model time evolution and its result can only get better with more iterations, it uses a lot of resources. Furthermore, we see the hybrid algorithm as a trade-off middle ground between the two, where we get better results than QPE and can also model evolution and interactions. But it uses more resources than both.

References

[1] F. Ismael *et al.*, IBM Quantum , (2021), `https://research.ibm.com/blog/120x-quantum-speedup`.
[2] P. Siwach and P. Arumugam, Phys. Rev. C **104**, 034301 (2021).
[3] E. Dumitrescu, *et al.*, Phys. Rev. Lett. **120**, 0210501 (2018).
[4] A. Peruzzo *et al.*, Nat. Commun. **5**, 4213 (2014)