EPJ Web of Conferences **302**, 17002 (2024) https://doi.org/10.1051/epjconf/202430217002
SNA + MC 2024

Variational Quantum Simulation of Deuteron Ground State Energy at Higher Order Expansion

Changyuan Liu[1,*]

[1]New Compute Laboratory, No. 89, Jianguo Road, Beijing, China

Abstract. Recent development of quantum computing has been extended to nuclear physics. Researchers have demonstrated that the quantum simulation of deuteron ground state energy using the variational quantum eigenvalue solver. In this existing work, only 2 and 3 qubits are used. In this work, the theory of higher order expansion of the deuteron ground state Hamiltonian has been established. On a classical quantum simulator, the convergence of the ground state energy as the number of qubits increases has been verified up to 22 qubits.

1 Introduction

The noisy intermediate-scale quantum computers (NISQ) are the most practical quantum computers. Because of the noise in the quantum operations, the depth of the quantum circuit is limited to be a few tens to hundreds, beyond which the information readout might be fully corrupted, so that hardly any useful information can be obtained.

For NISQ quantum computers, the variational quantum eigenvalue solver (VQE) algorithm has demonstrated to be effective in the calculation of ground state energy of chemical molecules [1]. Finding the ground state energy of chemical molecules consumes enormous computing power that grows exponentially with the molecular mass. Quantum computers are believed to tackle this hard problem. As a result, the precise structure of caffeine and Nitrogenase may be understood. Understanding the Nitrogenase will help us chemically reappear an important process in the synthesis of protein. Later, Dumitrescu has successfully applied the VQE algorithm to find the ground state energy of deuteron [2]. This seminal work opens doors for using NISQ quantum computer to understand nuclear physics. However, limited by the capability of quantum computers by then, only 2 and 3 qubits have been experimented.

Besides the VQE algorithm, McArdle [3] has also applied quantum annealing approach common in the analog quantum computers has been applied to study the Deuteron ground state energy. In quantum annealing, an initial Hamiltonian with quantum states prepared at the ground state already known has been gradually evolving to the target Hamiltonian. This evolution of Hamiltonian is in the imaginary time.

In this work, we extend the problem with higher order expansion, and the contributions are listed as followed:

- Extend the Hamiltonian for deuteron to arbitrary order of expansion
- Verification of convergence of deuteron ground state energy with classical quantum simulator up to 22 qubits

*e-mail: changyuan_liu@163.com

2 Deuteron Ground State Energy and Hamiltonian

2.1 Derivation of Hamiltonian

In quantum mechanics, the wave function of deuteron can be described by an Hamiltonian. According to Dumitrescu [2], the Deuteron Hamiltonian for ${}^3S_1$ wave equation with angular momentum $l = 0$ is written as

$$H_N = \sum_{n=0}^{N-1}\sum_{n'=0}^{N-1}\langle n'|(T+V)|n\rangle\, a_{n'}^\dagger a_n, \tag{1}$$

where $|n\rangle$ is the wave function of s-wave harmonic oscillator, and T is the kinetic energy operator, and V is the potential energy operator, $a_n^\dagger$ and a_n are the creator and annihilator of state $|n\rangle$. The expectation value of kinetic energy is expanded as

$$\langle n'|T|n\rangle = \frac{\hbar\omega}{2}\left[\left(2n+\frac{3}{2}\right)\delta_{n,n'} - \sqrt{n\left(n+\frac{1}{2}\right)}\delta_{n,n'+1} - \sqrt{(n+1)\left(n+\frac{3}{2}\right)}\delta_{n,n'-1}\right], \tag{2}$$

and the potential energy is expanded as

$$\langle n'|V|n\rangle = V_0\delta_{n,0}\delta_{n,n'}, \tag{3}$$

where $\delta_{n,n'}$ is the Kronecker's delta function, $V_0 = -5.686\,581\,11$ MeV, and ω is the harmonic oscillator angular frequency. $\hbar\omega$ is set to be -7 MeV. For case $N = 2$, the Hamiltonian is

$$H_2 = \left(\frac{3}{4}\hbar\omega + V_0\right)a_0^\dagger a_0 - \frac{\hbar\omega}{2}\sqrt{\frac{3}{2}}\left(a_0^\dagger a_1 + a_1^\dagger a_0\right) + \frac{7}{4}\hbar\omega\, a_1^\dagger a_1. \tag{4}$$

For $N = 3$,

$$H_3 = H_2 - \frac{\hbar\omega}{2}\sqrt{5}\left(a_1^\dagger a_2 + a_2^\dagger a_1\right) + \frac{11}{4}\hbar\omega\, a_2^\dagger a_2. \tag{5}$$

In general, for $N \geq 2$

$$H_N = H_{N-1} - \frac{\hbar\omega}{2}\sqrt{\frac{(N-1)(2N-1)}{2}}\left(a_{N-2}^\dagger a_{N-1} + a_{N-1}^\dagger a_{N-2}\right) + \frac{4N-1}{4}\hbar\omega\, a_{N-1}^\dagger a_{N-1}. \tag{6}$$

The Hamiltonians are hermitian. Solving Hamiltonian H_N for the lowest eigenvalue leads to the ground state energy for deuteron.

2.2 Qubit Encoding

To encode the quantum state on qubits, the Jordan Wigner transformation is used. For Hamiltonian H_N, N qubits are used. With the Jordan Wigner transformation, the Hamiltonian H_N can be transformed into sum of products of Pauli operations X, Y, and Z, which are defined as followed.

$$\text{(Pauli) } X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{7}$$

$$\text{(Pauli) } Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \tag{8}$$

$$\text{(Pauli) } Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{9}$$

Besides, the identity matrix is defined as followed.

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{10}$$

As an example, the 2 qubit Hamiltonian H_2 after Jordan Wigner transformation leads to the following.

$$\begin{aligned} H_2 &= \left(\frac{5}{4}\hbar\omega + \frac{1}{2}V_0\right) I \otimes I - \left(\frac{3}{8}\hbar\omega + \frac{1}{2}V_0\right) Z \otimes I - \frac{7}{8}\hbar\omega\, I \otimes Z \\ &\quad -\frac{1}{4}\sqrt{\frac{3}{2}}\,\hbar\omega\,(X \otimes X + Y \otimes Y), \end{aligned} \tag{11}$$

where $\otimes$ is the tensor product. The tensor product of two 2×2 matrices is a 4×4 matrix. Take the example of $\hbar\omega = 7$ MeV and $V_0 = -5.686\,581\,11$ MeV, the Hamiltonian H_2 is given as followed.

$$H_2 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 12.25 & -4.28661 & 0 \\ 0 & -4.28661 & -0.436581 & 0 \\ 0 & 0 & 0 & 11.8134 \end{bmatrix}. \tag{12}$$

The minimum eigenvalue of H_2 is -1.749 159 876 321 530 MeV.

In addition, Matteo [4] has proposed an alternative encoding using Gray code, where H_N uses $\lceil \log_2 N \rceil$ qubits instead of N qubits for method discussed above, while the number of Pauli terms in H_N is in the order of $O(N \log N)$ instead of $O(N)$ qubits for method discussed above. Although the number of Pauli terms in the Hamiltonian has a higher complexity, Matteo has shown that using Gray code produces less variance and error in the eigenvalue for N from 2 to 16 on the IBM qiskit classical quantum simulator with noise.

3 Variational Quantum Eigenvalue Solver (VQE)

3.1 UCC Ansatz

The unitary coupled clustered (UCC) ansatz has been used to quantum simulate ground state energy of molecules in quantum chemistry [1]. It defines a parameterized unitary

$$U(\vec{\theta}) = e^{T(\vec{\theta}) - T^\dagger(\vec{\theta})}, \tag{13}$$

where $T(\vec{\theta})$ are sum of anti-hermitian cluster operators

$$T(\vec{\theta}) = \sum_{k=1} T_k(\vec{\theta}), \tag{14}$$

and $T^\dagger(\vec{\theta})$ is the Hamiltonian conjugate to $T(\vec{\theta})$. In quantum chemistry, the use of singlet term $T_1(\vec{\theta})$ and doublet term $T_2(\vec{\theta})$ are common. Its form is

$$T_1(\vec{\theta}) = \sum_{\substack{i \in \text{occupied orbitals} \\ a \in \text{virtual orbitals}}} \theta_{i,a}\, a_a^\dagger a_i, \tag{15}$$

and

$$T_2(\vec{\theta}) = \sum_{\substack{i > j \in \text{occupied orbitals} \\ a > b \in \text{virtual orbitals}}} \theta_{i,j,a,b}\, a_a^\dagger a_b^\dagger a_i a_j. \tag{16}$$

The Ansatz is defined in fermion operators. So a transform into qubits operator is necessary. A Trotter-Suzuki decomposition may be used for calculating the unitary $U(\vec{\theta})$. Experience has shown that the Jordan Wigner transform of $-i(T(\vec{\theta}) - T^{\dagger}(\vec{\theta}))$ is a sum of Pauli Hamiltonians with real coefficients.

We turns to UCC ansatz define in Eq. (13), only the singlet term $T_1(\vec{\theta})$ is used, see Eq. (15). The initial quantum state is the 'Hartree-Fock' state, where $|1\rangle$ is prepared for all occupied orbitals under Jordan-Wigner transform, and $|1\rangle$ is prepared for all virtual orbitals. For deuteron, only one orbital is occupied, so for $N = 2$,

$$T_1(\vec{\theta}) = \theta_{1,0}\, a_0^{\dagger} a_1, \text{ initial state } |10\rangle \text{ (in Jordan Wigner).} \tag{17}$$

For $N = 3$,

$$T_1(\vec{\theta}) = \theta_{1,0}\, a_0^{\dagger} a_1 + \theta_{2,0}\, a_0^{\dagger} a_2, \text{ initial state } |100\rangle \text{ (in Jordan Wigner).} \tag{18}$$

For $N = 4$,

$$T_1(\vec{\theta}) = \theta_{1,0}\, a_0^{\dagger} a_1 + \theta_{2,0}\, a_0^{\dagger} a_2 + \theta_{3,0}\, a_0^{\dagger} a_3, \text{ initial state } |1000\rangle \text{ (in Jordan Wigner).} \tag{19}$$

3.2 Numerical Calculation of Ground State Energy with VQE

To find the ground state energy, we use the VQE solver with the UCC ansatz. Both the energy Hamiltonian and the Ansatz are transformed to qubits Hamiltonian with Jordan-Wigner transform. The model is simulated for expansion order $N = 2 \ldots 22$, as in Eq. (1). The qubits Hamiltonian statistics are listed in Table 1. For expansion order N, it needs N qubits, and there are $3N - 1$ Pauli terms in the Jordan-Wigner transformed energy Hamiltonian, and $N - 1$ parameters are needed for the ansatz.

Table 1: Quantum circuit complexity for energy Hamiltonian H_N and ansatz

Expansion order N	Qubits count	Pauli terms in H_N (Including identity)	Ansatz parameters count
2	2	5	1
3	3	8	2
4	4	11	3
5	5	14	4
N	N	$3N - 1$	$N - 1$

The convergence of ground state energy as function of expansion order N has been shown in Fig. 1. The reference energy of deuteron is about $E \approx -2.22$ MeV. For expansion $N \geq 7$, the model has a ground state energy within 0.01 MeV from this reference. Fig. 1 shows the exact lowest eigenvalue from direct numerical calculation from the Hamiltonian matrix expression, where Eq. (12) provides an example of the 2-qubit case. The quantum simulated values agree with these exact values as well. For $N = 2$ and 3 in the previous work [2], the ground state energy is larger than 3% from convergence.

Both the Nelder-Mead and L-BFGS minimization algorithms have been tested, and the number of functions (i.e. bundles of quantum circuits to calculate energy) evaluated have been shown in Fig. 2. The L-BFGS minimization algorithm requires much less number of function evaluations than the Nelder-Mead algorithm.

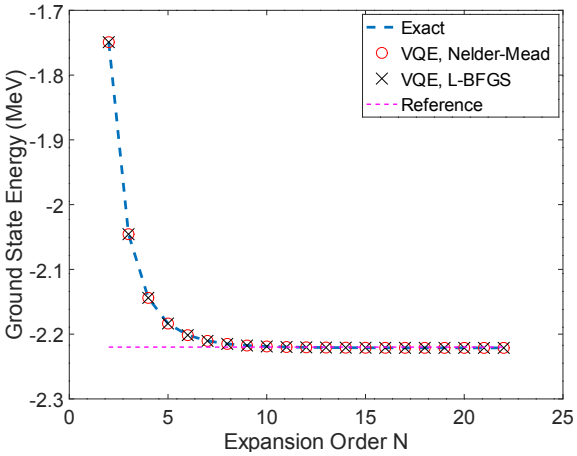

Figure 1: Convergence of ground state energy as expansion order increases

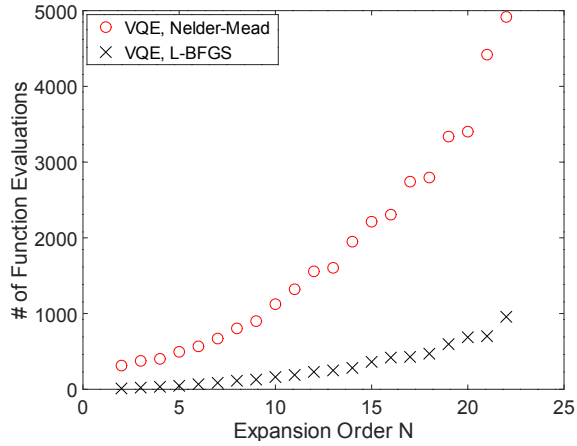

Figure 2: Number of function evaluations in VQE minimization

Finding the minimum eigenvalue using VQE is a non-linear optimization problem, Table 2 compares some optimization algorithms. For the two methods Nelder-Mead and L-BFGS adopted, Nelder-Mead does not requires the calculation of either gradient and Hessian, while L-BFGS requires the calculation of gradient but not Hessian.

3.3 Discussion about the Choice of Potential V_0

Table 3 compares the VQE eigenvalues and the exact eigenvalues from direct numerical calculation from the Hamiltonian matrix expression. The potential V_0 is also varied to be 6, 7, or 8 MeV. The good agreement of eigenvalues in about 15 digits shows that the L-BFGS optimization algorithm converges to the minimal eigenvalue.

Table 2: Comparison of Minimization Algorithms

Algorithm	Needs Gradiant	Needs Hessian
Nelder-Mead	No	No
BFGS	Yes	No
CG	Yes	No
Steepest Descent	Yes	No
L-BFGS	Yes	No
Newton	Yes	Yes

Table 3: Comparison of VQE eigenvalues and the exact eigenvalues from direct numerical calculation from the Hamiltonian matrix expression

Expansion Order	V_0 (MeV)	Exact (MeV)	VQE L-BFGS (MeV)
2	6	-2.245757107628286	-2.2457571076282985
2	7	-1.7491598763215308	-1.749159876321545
2	8	-1.2593838066311984	-1.2593838066312122
3	6	-2.4615677478547062	-2.461567747854758
3	7	-2.045670898406442	-2.0456708984064984
3	8	-1.644076509718204	-1.6440765097182664
8	6	-2.5665794719119464	-2.5665794719127972
8	7	-2.2150378722677115	-2.215037872269007
8	8	-1.8939834859045488	-1.8939834859056361
16	6	-2.5688912688365813	-2.5688912688427283
16	7	-2.2210588667158047	-2.2210588667222035
16	8	-1.9069786313183714	-1.9069786313120276

As the expansion order N increases, the converged eigenvalues for potential $V_0 = 6, 7, 8$ MeV are about -2.56, -2.22, -1.91 MeV. Since the experimental Deuteron ground state energy is about 2.225 MeV [5], the choice of $V_0 = 7$ MeV is the judged.

3.4 Discussion about Noise on Quantum Computers

Note that we use a classical quantum simulator, so the expectation value can be calculated by directly accessing the quantum states without sampling.

However, on real NISQ quantum computers, the noisy in the quantum operations will lead to sub-optimal eigenvalues [2]. According to Table 2, the L-BFGS method requires the calculation of gradient, the noisy in the quantum computer will lead to discontinuity in the values of expectation of circuits, so the gradient will be subjected to oscillatory noises to void the optimization process.

To tackle the problem of too much error in gradient, McArdle [3] has adopted an alternative approach, which has demonstrated to effectively suppress the noise in the eigenvalue, compared to the optimization approach with gradient decent optimization algorithm. Notice

that, in gradient decent method (steepest decent method in Table 2), the gradient has also to be computed.

4 Conclusions

In this work, the Hamiltonian to find the deuteron ground state energy has first been established at arbitrary expansion orders. Second, the UCC ansatz and the VQE algorithm have been reviewed. Finally, classical simulation of the VQE algorithms for Hamiltonian up to 22 qubits has been performed. The ground state energies converge to the reference as the expansion order increases. Beyond expansion order 7, the difference between calculated eigenvalue and the reference is less than 0.01 MeV. Using the L-BFGS minimization algorithm costs much less function evaluations than the Nelder-Mead algorithm.

References

[1] A. Kandala, A. Mezzacapo, K. Temme, M. Takita, J. M. Chow, and J. M. Gambetta, Nature **549**, 242 (2017)

[2] E. F. Dumitrescu,A. J. McCaskey, G. Hagen, G. R. Jansen, T. D. Morris, T. Papenbrock, R. C. Pooser, D. J. Dean, and P. Lougovski, Physics Review Letters **120**, 210501 (2018)

[3] S. McArdle, T. Jones, S. Endo, Y. Li, S. C. Benjamin and X. Yuan, npj Quantum Information**5**, 75 (2019)

[4] O. D. Matteo, A. McCoy, P. Gysbers, T. Miyagi, R. M. Woloshyn, and P. Navrátil, Physics Review A **103**, 042405 (2021)

[5] S. Binder, A. Ekström, G. Hagen, T. Papenbrock, and K. A. Wendt, Physics Review C **93**, 044332 (2016)