Ground state estimation of Fermi Hubbard Hamiltonian using Matrix product states and variational quantum eigensolver

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Abstract : This documentation is a compilation of an attempt to estimate the ground state energy eigenvalue of Fermi Hubbard Hamiltonian for 2 sites, utilizing the Variational quantum eigensolver (VQE). The simulation is carried out using the suitable ansatz for this problem and Matrix product state (MPS) approach [8][6].

Contents

1 Practical Relevance of problem

In simpler words, the study of Fermi Hubbard model is important for understanding the interaction and correlation of fermions in an optical lattice [3]. This model provides an insight of many body quantum physics in condensed matter systems. The Hamiltonian of these systems is complex and does not provide an exact solution, that's where we realise the role of VQE. Implementing VQE for such systems may help us predict the properties [4] of the material.

2 Fermi Hubbard Hamiltonian

For simplicity, consider the Fermi Hubbard Hamiltonian [7] [9] for two nearest neighbours.

$$H = -t \sum_{\sigma} (\hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^{\dagger} \hat{c}_{i\sigma}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{1}$$

Here, $\sigma \in \left\{\frac{1}{2}, \frac{-1}{2}\right\}$ denotes the spin of electron, and the rest of the terms are as follows

- $\hat{c}_{i\sigma}^{\dagger}$ creates an electron on site/orbital i with spin σ
- $\hat{c}_{i\sigma}$ annihilates an electron on site/orbital i with spin σ
- $\hat{c}_{i\sigma}^{\dagger} \hat{c}_{i\sigma}$ counts weather there's an electron of spin σ on site i
- $\hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma}$ takes an electron with spin σ from site j and puts it on site i with the same spin σ
- $(\hat{c}_{i\sigma}^{\dagger})^2$ implies that it is not possible to create two electrons on the same site/orbital, as electron is a fermion hence obeys pauli exclusion principle.
- U takes into account the coulombic interaction of electrons and is a positive quantity. The energy of system increases if U increases.
- t corresponds to the kinetic energy and contributes negatively hence decreasing the energy of the system with increase in its magnitude.

3 Mapping the Hamiltonian

The Hamiltonian we have is a linear combination of ladder operators, these operators makes sense when taking about Quantum harmonic oscillators. Therefore, in order to simulate such a system, the first step is to transform it into a form that is executable by quantum circuits or a quantum computing platform. This is accomplished using Jordan-Wigner Transformations which is described in detail in the reference [2].

The Hopping term transforms to

$$H_{hop} = t\,[XXII + YYII + IIXX + IIYY] \tag{2}$$

Similarly, for interaction term

$$H_{int} = U\left[ZIIZ + IZZI + ZIII + IZII + IIZI + IIIZ\right] \tag{3}$$

Here, I, X, Y, Z represents the Pauli-spin matrices.

```
HoppingTerms = PauliList(['XXII','YYII','IIXX','IIYY'])


InteractionTerms = PauliList(['ZIIZ','IZZI','ZIII','IZII','IIZI','IIIZ'])
```

Figure 1: Creating a List of essential Pauli operators using Qiskit

```
t = -1.0 + 0.j # weight for the hopping terms
U = 0.5 + 0.j # weight for coulomb interaction term

# The hamiltonian is a linear combination of ladder operators
Hamilt = SparsePauliOp.from_list([('XXII', t), ('YYII', t), ('IIXX', t), ('IIYY',t),
                                  ('ZIIZ',U), ('IZZI',U),('ZIII',U),('IZII',U),('IIZI',U),('IIIZ',U)])
```

Figure 2: The Hamiltonian is defined using applicable weights for each Pauli matrix. The *SparsePauliOp* creates a linear sum of these matrices which is to be used as a Hamiltonian.

```
print(f"Number of qubits: {Hamilt.num_qubits}")

Number of qubits: 4
```

Figure 3: The number of qubits required to simulate the problem

4 MPS Ansatz

The matrix product states are of relevance when we talk about low entanglement [1]. It means that the interaction in quantum system is restricted to the nearest neighbours. Ansatz, on the other hand is an educated guess of how our trial wave-function should look like. I took the inspiration for MPS ansatz from the reference [5].

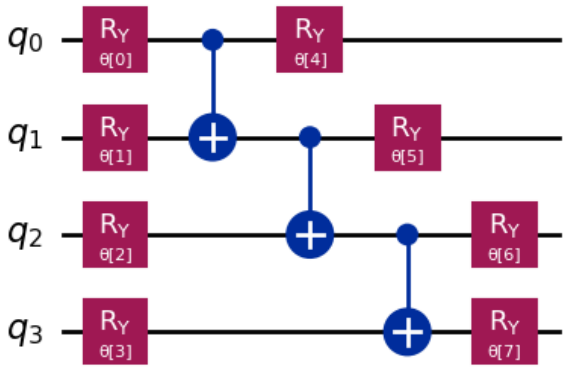

Figure 4: MPS ansatz for the mapped hamiltonian. The correlation is kept minimal by applying cx gates only to the nearest qubit, imitating the low entanglement of the system.

5 Coupling and Noise Modelling

A coupling map makes the simulation more realistic by mapping the qubits that can interact directly on the hardware platform. It helps us to incorporate the hardware limitations in our simulation.

```
# An arbitrary coupling map to simulate the problem with a more realistic approach

coupling_map = [(0, 1), (1, 2), (2, 3), (3, 4)]
device = GenericBackendV2(num_qubits=5, coupling_map=coupling_map, seed=54)

noise_model = NoiseModel.from_backend(device)

print(noise_model)
```

```
# Noise modelling with matrix product state method

noisy_estimator = AerEstimator(
    backend_options={
        "method": "matrix_product_state",
        "coupling_map": coupling_map,
        "noise_model": noise_model,
    },
    run_options={"seed": 54, "shots": 1024},
    transpile_options={"seed_transpiler": 54},
)
```

Figure 5: Coupling and Noise Modelling of the simulation

The noise modelling with MPS method is suitable in Qiskit when the entanglement is low.

6 Result Discussion

The minimum eigenvalue that was obtained for reference using NumpyMinimumEigensolver() is -4.12311. After noise modelling of the system, the minimum eigenvalue obtained is -3.98438, which is more than the estimated reference eigenvalue. This result reflects that the interaction of quantum systems with the environment contributes to the energy of the system. Note that this result is for the case when $|t| = 2U$. The results are different depending on how far apart U and t are in magnitude.

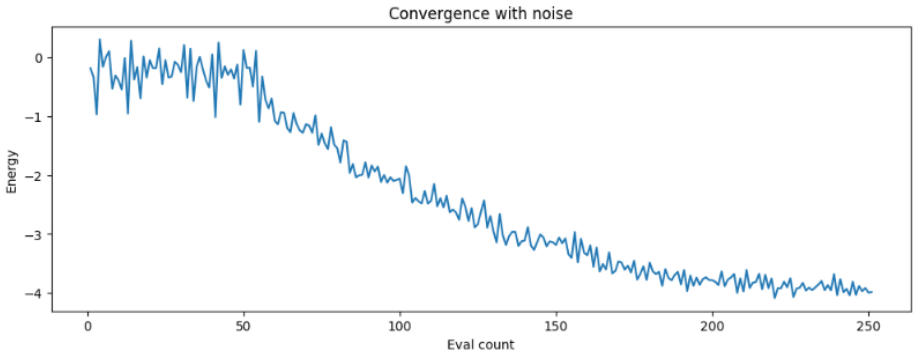

Figure 6: Evaluation of energy of the system under noise modelling, starting from the specified ansatz

7 Further Analysis

In this section I will discuss the ansatz whose results were not good enough as the one given in figure (4).

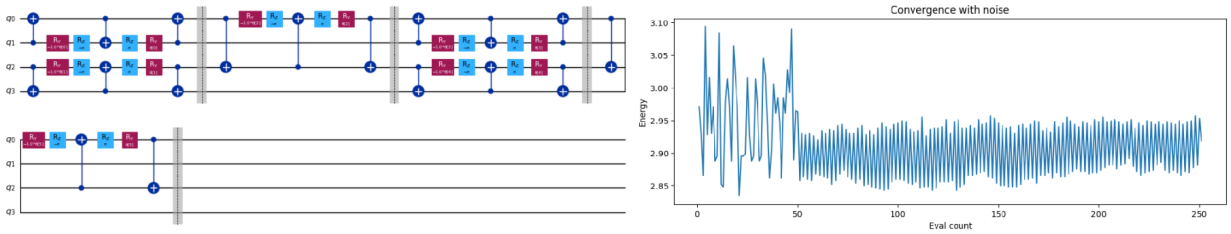

Figure 7: This ansatz is based on the problem specific ansatz given in the reference [2]. The eigenvalue obtained is way off the reference eigenvalue, hence this ansatz is not suitable.

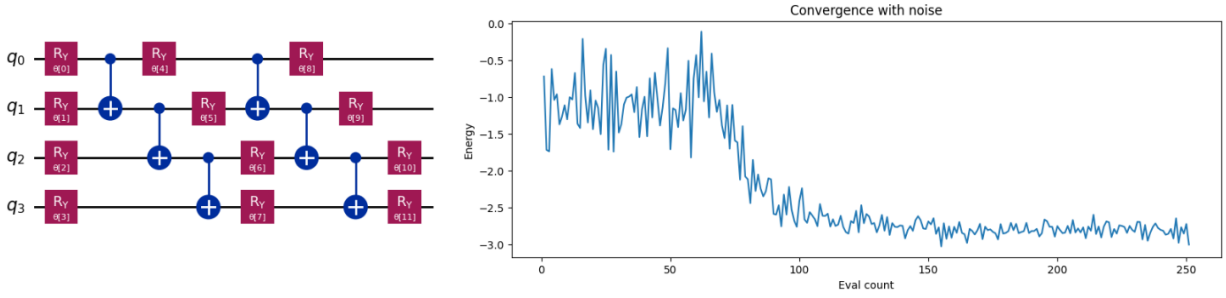

Figure 8: In this ansatz, the number of repetitions is double than that in circuit (4), the eigenvalue however is more but not too different.

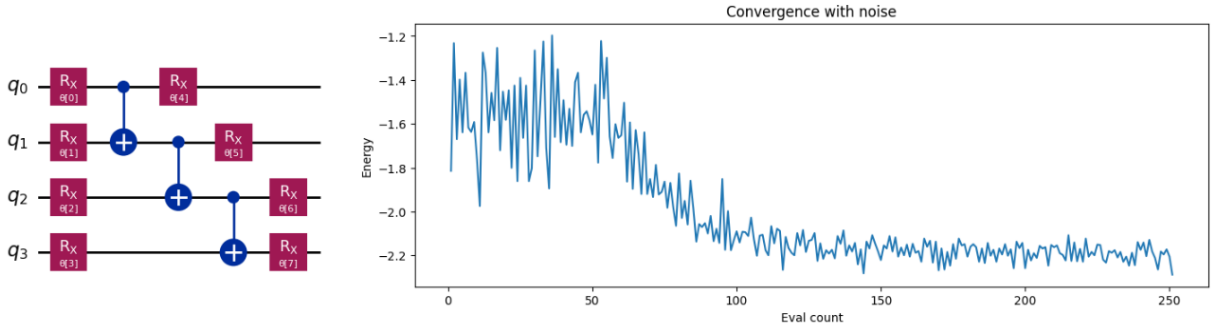

Figure 9: In this MPS ansatz, rx gate is used intead of ry, however, the lowest eigenvalue estimate is nearly -2.0, which is half the reference value. Hence, this ansatz is not suitable.

References

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