Quantum computation of Hubbard Model using IBM Q

December 12, 2019

Abstract

In this work are described the steps and the calculation results of the Hubbard Model evolution using simulations and real runs on IBM Quantum processors. The Hubbard Model has been approached considering hopping and interaction terms calculated separately, then the quantum circuit has beed developed to simulate all Hamiltonian terms leveraging on IBM Quantum Experience.

I. Introduction

Hubbard Model is an approximate model that can be used to described interactive particles into a lattice, for example electrons interacting on a chain of atoms of a conductor or semiconductor. The Hamiltonian describing the temporal evolution of this system is quite simple, as it is composed by a kinetic (or hopping) term, describing the particle jumps between chain sites, and by a potential (or interaction) term, describing the particle interactions on the same site.

In general, particles described by Hubbard Model can be either bosons or fermions: in this paper are considered the electrons running on a chain of atoms, thus the particles considered are fermions.

The complete Hubbard Hamiltonian for electrons with spin interacting on a chain of atoms is an interesting model that can be mapped into a quantum processor: the aim of this work is to map the complete Hubbard Hamiltonian on IBM Q quantum simulator and real processors, considering spin interaction and dynamic of the system.

II. The Hubbard Model

The Hubbard Model temporal evolution is described by the following Hamiltonian:

$$\mathcal{H} = -t \sum_{<i,j>}^{N} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i) + V \sum_{i}^{N} (\hat{n}_{i\uparrow} \hat{n}_{i\downarrow}) \quad (1)$$

with $\hat{n}_{i\uparrow} = (\hat{b}_i^\dagger \hat{b}_i)_\uparrow$ and $\hat{n}_{i\downarrow} = (\hat{b}_i^\dagger \hat{b}_i)_\downarrow$, and where $\hat{b}_i^\dagger$ and $\hat{b}_j$ are respectively the fermionic creation operator in site i and the fermionic annihilation operator in site j, with N the total sites number.

The $< i, j >$ means that just the neighbour nearest are selected, and t and V are respectively the hopping parameter and the spin interaction potential.

In case of 2 sites:

$$\begin{aligned}\mathcal{H} = &-t(\hat{b}_{1\uparrow}^\dagger \hat{b}_{2\uparrow} + \hat{b}_{2\uparrow}^\dagger \hat{b}_{1\uparrow} + \hat{b}_{1\downarrow}^\dagger \hat{b}_{2\downarrow} + \hat{b}_{2\downarrow}^\dagger \hat{b}_{1\downarrow}) \\ &+ V(\hat{b}_{1\uparrow}^\dagger \hat{b}_{1\uparrow} \hat{b}_{1\downarrow}^\dagger \hat{b}_{1\downarrow} + \hat{b}_{2\uparrow}^\dagger \hat{b}_{2\uparrow} \hat{b}_{2\downarrow}^\dagger \hat{b}_{2\downarrow})\end{aligned} \quad (2)$$

Using a more compact notation:

$$\begin{aligned}\mathcal{H} = &[-t \sum_{\sigma} (\hat{b}_{1,\sigma}^\dagger \hat{b}_{2,\sigma} + \hat{b}_{2,\sigma}^\dagger \hat{b}_{1,\sigma})] + \\ &+ [V \sum_{i}^{2} (\hat{n}_{i\downarrow} \hat{n}_{i\uparrow} + \hat{n}_{i\uparrow} \hat{n}_{i\downarrow})]\end{aligned} \quad (3)$$

The Hubbard Model Hamiltonian can be expressed highlighting the hopping and the interaction terms:

$$\mathcal{H} = \mathcal{H}_{hop} + \mathcal{H}_{int} \quad (4)$$

In general, the hopping term is related to the movement of the particles through the atom chain, from site 1 to site 2, while the interaction term defines the interaction of two particles with opposite spin into the same site.

III. Hubbard Hamiltonian in spin notation

In the next sections are performed the calculations of hopping and interaction terms of Hubbard Model Hamiltonian. In general, the following notation will be applied to define lattice sites and electron spins:

$$\begin{aligned} ① &\rightarrow Site\ 1,\ spin\ \uparrow \\ ② &\rightarrow Site\ 1,\ spin\ \downarrow \\ ③ &\rightarrow Site\ 2,\ spin\ \uparrow \\ ④ &\rightarrow Site\ 2,\ spin\ \downarrow \end{aligned} \tag{5}$$

i. Hopping term

Consider the hopping Hamiltonian, it is possible to calculate the analytical expression:

$$\mathcal{H}_{hop} = -t \sum_{i,\sigma}^{N} (\hat{b}^{\dagger}_{i,\sigma} \hat{b}_{i+1,\sigma} + h.c.) \tag{6}$$

we can perform a *Fourier Transform* to find the Energy eigenvalues:

$$\hat{b}_j = \sum_{k=1}^{\infty} e^{-ikj} \hat{b}_k$$

$$\hat{b}_{j+1} = \sum_{k=1}^{\infty} e^{-ik(j+1)} \hat{b}_k = \sum_{k=1}^{\infty} e^{-ikj+k} \hat{b}_k$$

$$\begin{aligned} \mathcal{H}_{hop} = t \sum_{i,\sigma}^{N} \sum_{k} (\hat{b}^{\dagger}_{k,\sigma} \hat{b}_{k',\sigma} e^{-i(k-k')j+k'} + \\ + \hat{b}^{\dagger}_{k+1,\sigma} \hat{b}_{k',\sigma} e^{-(-k+k')j+k}) \end{aligned} \tag{7}$$

Considering that $\sum_j e^{-i(k-k')j} = \delta(k-k')$ and applying the Eulero Identity, it is possible to obtain the hopping term analytical expression:

$$\mathcal{H}_{hop} = 2t \sum_{i,\sigma}^{N} cos(k)\, \hat{b}^{\dagger}_{k,\sigma} \hat{b}_{k,\sigma}$$

Now, starting from 3 it is possible to apply the *Jordan-Wigner Transform* to express the hopping term using spin notation. In general, the *Jordan-Wigner Transform* maps the fermionic operators $\hat{b}_i$ using spin states S, in particular with the notation $\hat{b}^{k}_{i} \rightarrow S^{+} e^{i\alpha_j}$ with $\alpha = \sum_i (\hat{n}_i)\pi$.

Thus, the spin creation operator in site 2 and the spin annihilation operator in site 1 are defined as:

$$\begin{aligned} S^{+}_{2} &= \mathbb{1} \otimes S^{+} \\ S^{-}_{1} &= S^{-} \otimes \mathbb{1} \end{aligned} \tag{8}$$

as the particle is moving from site 1 to site 2, so it annihilates in site 1 and recreates in site 2.

In order to proceed with Hamiltonian expression, it's needed to discuss the commutation of some quantities:

$$\begin{aligned} \{\hat{b}^{\dagger}_{i}, \hat{b}_j\} &= \delta_{i,j} \\ \{\hat{b}^{\dagger}_{i}, \hat{b}_i\} &= \{S^{+}_{i}, S^{-}_{i}\} = \mathbb{1} \\ \{S^{+}_{2}, S^{-}_{1}\} &= \{\mathbb{1}, S^{-}\} \otimes \{S^{-}, \mathbb{1}\} \\ \{\sigma_z, S^{+}\} &= 0 \end{aligned} \tag{9}$$

from which can be obtained:

$$S^{+}_{2} = \prod_{i=0}^{n_i \neq 0} \sigma_z S^{+}_{i} \tag{10}$$

and

$$\hat{b}^{\dagger} = \prod_{j=0}^{i-1} \sigma_z \cdots \sigma^{+}_{j} \prod_{j=i+1}^{n} \mathbb{1} \tag{11}$$

Using the described quantities, the terms of the equation 6 can be written as:

$$\begin{aligned} \hat{b}^{\dagger}_{1} \hat{b}_2 &= (\sigma^{+} \otimes \mathbb{1}) \otimes (\sigma_z \otimes \sigma_z) = \\ &= -\sigma^{-} \otimes \sigma^{-} \end{aligned} \tag{12}$$

$$\begin{aligned} \hat{b}^{\dagger}_{2} \hat{b}_1 &= (\sigma_z \otimes \sigma^{+}) \otimes (\sigma^{-} \otimes \mathbb{1}) = \\ &= \sigma^{+} \otimes \sigma^{+} \end{aligned} \tag{13}$$

where $\sigma^{+} = \frac{\sigma_x + i\sigma_y}{2}$ and $\sigma^{-} = \frac{\sigma_x - i\sigma_y}{2}$. Considering the relationships below

$$\begin{aligned} \sigma^+ + \sigma^+ &= \sigma_x \\ \sigma^+ - \sigma^+ &= i\sigma_y \end{aligned} \tag{14}$$

the hopping term of the Hubbard Model Hamiltonian can be written using spin notation in this way:

$$\mathcal{H}_{hop} = -\frac{t}{2}(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y) \tag{15}$$

Generalizing the t parameter and applying the reference notation 5, it is possible to obtain the hopping term:

$$\begin{aligned} \mathcal{H}_{hop} = t[&(\sigma^x \otimes \mathbb{1} \otimes \sigma^x \otimes \mathbb{1}) \\ &+ (\sigma^y \otimes \mathbb{1} \otimes \sigma^y \otimes \mathbb{1}) + \\ &+ (\mathbb{1} \otimes \sigma^x \otimes \mathbb{1} \otimes \sigma^x) + \\ &+ (\mathbb{1} \otimes \sigma^y \otimes \mathbb{1} \otimes \sigma^y)] \end{aligned} \tag{16}$$

ii. Interaction term

The calculation of the interaction term of Hubbard Model Hamiltonian follows an approach similar to the hopping term. Starting from the interaction term

$$\mathcal{H}_{int} = V n_{i,\uparrow} n_{i,\downarrow} = V(\hat{b}^\dagger_{i,\uparrow}\hat{b}_{i,\uparrow})(\hat{b}^\dagger_{i,\downarrow}\hat{b}_{i,\downarrow}) \tag{17}$$

and applying the notation 5 to get the structure of the interation in the position j, it is possible to obtain a compact notation for the fermionic operators using pauli matrices:

$$\begin{aligned} \hat{b}^\dagger_{①} &\to \hat{b}^\dagger_{1,\uparrow} = \sigma^+ \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \\ \hat{b}^\dagger_{②} &\to \hat{b}^\dagger_{1,\downarrow} = \sigma^z \otimes \sigma^+ \otimes \mathbb{1} \otimes \mathbb{1} \\ \hat{b}^\dagger_{③} &\to \hat{b}^\dagger_{2,\uparrow} = \sigma^z \otimes \sigma^z \otimes \sigma^+ \otimes \mathbb{1} \\ \hat{b}^\dagger_{④} &\to \hat{b}^\dagger_{2,\downarrow} = \sigma^z \otimes \sigma^z \otimes \sigma^z \otimes \sigma^+ \end{aligned} \tag{18}$$

$$\begin{aligned} \hat{b}_{①} &\to \hat{b}^\dagger_{1,\uparrow} = \sigma^- \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \\ \hat{b}_{②} &\to \hat{b}^\dagger_{1,\downarrow} = \sigma^z \otimes \sigma^- \otimes \mathbb{1} \otimes \mathbb{1} \\ \hat{b}_{③} &\to \hat{b}^\dagger_{2,\uparrow} = \sigma^z \otimes \sigma^z \otimes \sigma^- \otimes \mathbb{1} \\ \hat{b}_{④} &\to \hat{b}^\dagger_{2,\downarrow} = \sigma^z \otimes \sigma^z \otimes \sigma^z \otimes \sigma^- \end{aligned} \tag{19}$$

Applying 18 and 19 to the terms of 17, it is possible to obtain:

$$\begin{aligned} \hat{b}^\dagger_{①}\hat{b}_{①} &= \frac{(\mathbb{1} + \sigma^z)}{2} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \\ \hat{b}^\dagger_{②}\hat{b}_{②} &= \mathbb{1} \otimes \frac{(\mathbb{1} + \sigma^z)}{2} \otimes \mathbb{1} \otimes \mathbb{1} \\ \hat{b}^\dagger_{③}\hat{b}_{③} &= \mathbb{1} \otimes \mathbb{1} \otimes \frac{(\mathbb{1} + \sigma^z)}{2} \otimes \mathbb{1} \\ \hat{b}^\dagger_{④}\hat{b}_{④} &= \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \frac{(\mathbb{1} + \sigma^z)}{2} \end{aligned} \tag{20}$$

Considering the above formulas, the interaction term of Hubbard Model Hamiltonian can be written as:

$$\mathcal{H}_{int} = V(\hat{b}^\dagger_{①}\hat{b}_{①})(\hat{b}^\dagger_{②}\hat{b}_{②})(\hat{b}^\dagger_{③}\hat{b}_{③})(\hat{b}^\dagger_{④}\hat{b}_{④})$$

$$\begin{aligned} \mathcal{H}_{int} = V[&\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} + \\ &+ \sigma_z \otimes \sigma_z \otimes \mathbb{1} \otimes \mathbb{1} + \\ &+ \mathbb{1} \otimes \mathbb{1} \otimes \sigma_z \otimes \sigma_z + \\ &+ \sigma_z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} + \\ &+ \mathbb{1} \otimes \sigma_z \otimes \mathbb{1} \otimes \mathbb{1} + \\ &+ \mathbb{1} \otimes \mathbb{1} \otimes \sigma_z \otimes \mathbb{1} + \\ &+ \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \sigma_z + \\ &+ \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1}] \end{aligned} \tag{21}$$

iii. Full spin Hamiltonian

Combining the hopping term 16 and the interaction term 21 it is possible to write the full Hubbard Model Hamiltonian.

$$\begin{aligned} \mathcal{H} = \mathcal{H}_{hop} + \mathcal{H}_{int} = \\ = t[&(\sigma^x \otimes \sigma^z \otimes \sigma^x \otimes \mathbb{1}) + (\sigma^y \otimes \sigma^z \otimes \sigma^y \otimes \mathbb{1}) + \\ &+ (\mathbb{1} \otimes \sigma^x \otimes \sigma^z \otimes \sigma^x) + (\mathbb{1} \otimes \sigma^y \otimes \sigma^z \otimes \sigma^y)] + \\ &+ V[(\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1}) + (\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1}) + \\ &+ (\sigma^z \otimes \sigma^z \otimes \mathbb{1} \otimes \mathbb{1}) + (\mathbb{1} \otimes \mathbb{1} \otimes \sigma^z \otimes \sigma^z) + \\ &+ (\sigma^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1}) + (\mathbb{1} \otimes \sigma^z \otimes \mathbb{1} \otimes \mathbb{1}) + \\ &+ (\mathbb{1} \otimes \mathbb{1} \otimes \sigma^z \otimes \mathbb{1}) + (\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \sigma^z)] \end{aligned} \tag{22}$$

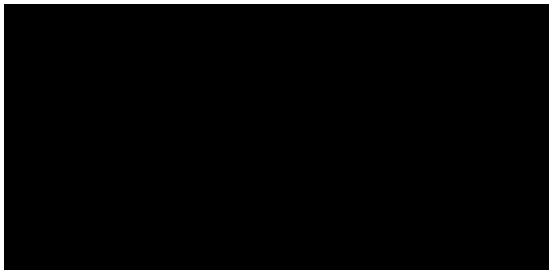

Figure 1: *Hopping and interaction terms.*

Optimized (no 3 body component)

$$\begin{aligned}\mathcal{H} &= \mathcal{H}_{hop} + \mathcal{H}_{int} = \\ &= t[(\sigma^x \otimes \mathbb{1} \otimes \sigma^x \otimes \mathbb{1}) + (\sigma^y \otimes \mathbb{1} \otimes \sigma^y \otimes \mathbb{1}) + \\ &+ (\mathbb{1} \otimes \sigma^x \otimes \mathbb{1} \otimes \sigma^x) + (\mathbb{1} \otimes \sigma^y \otimes \mathbb{1} \otimes \sigma^y)] + \\ &+ V[(\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1}) + (\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1}) + \\ &+ (\sigma^z \otimes \sigma^z \otimes \mathbb{1} \otimes \mathbb{1}) + (\mathbb{1} \otimes \mathbb{1} \otimes \sigma^z \otimes \sigma^z) + \\ &+ (\sigma^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1}) + (\mathbb{1} \otimes \sigma^z \otimes \mathbb{1} \otimes \mathbb{1}) + \\ &+ (\mathbb{1} \otimes \mathbb{1} \otimes \sigma^z \otimes \mathbb{1}) + (\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \sigma^z)]\end{aligned} \tag{23}$$

Optimized (mapping 2)

$$\begin{aligned}\mathcal{H} &= \mathcal{H}_{hop} + \mathcal{H}_{int} = \\ &= t[(\sigma^x \otimes \sigma^x \otimes \mathbb{1} \otimes \mathbb{1}) + (\sigma^y \otimes \sigma^y \otimes \mathbb{1} \otimes \mathbb{1}) + \\ &+ (\mathbb{1} \otimes \mathbb{1} \otimes \sigma^x \otimes \sigma^x) + (\mathbb{1} \otimes \mathbb{1} \otimes \sigma^y \otimes \sigma^y)] + \\ &+ V[(\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1}) + (\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1}) + \\ &+ (\sigma^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \sigma^z) + (\mathbb{1} \otimes \sigma^z \otimes \sigma^z \otimes \mathbb{1}) + \\ &+ (\sigma^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1}) + (\mathbb{1} \otimes \sigma^z \otimes \mathbb{1} \otimes \mathbb{1}) + \\ &+ (\mathbb{1} \otimes \mathbb{1} \otimes \sigma^z \otimes \mathbb{1}) + (\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \sigma^z)]\end{aligned} \tag{24}$$

IV. Benchmark with analytical solution

In order to check if the Hubbard Hamiltonian has been correctly expressed in spin notation, it is necessary to proceed with a benchmark: this is performed expressing the time evolution (expressed with the notation $e^{-i\mathcal{H}t}$) of the system using both the exact analytical solution and the trotterized analytical solution. In the first case, it is possible to perform a classical analytical calculation of time evolution of a system of two sites, using the notation expressed in figure 1. In the second case, the same calculation can be performed considering the trotterization of the Hubbard Hamiltonian.

In the following figures is reported the benchmark results.

After verification of the spin translation of the Hubbard Hamiltonian 27 using the performed benchmarks, the Hamiltonian expression 27 can be translated into a quantum circuit leveraging on 4 qubits, as the operators are mainly the basic IBM Q quantum gates. In the next section is described the quantum algorithm creation.

V. Hubbard quantum circuit

In this section is reported the complete Hubbard hamiltonian to be implemented on the quantum processor. The first needed operation is to map the notation expressed in 5 on qubits, as the following relations:

$$\begin{aligned} Qubit\ 0 &\rightarrow ① \rightarrow Site\ 1,\ spin\ \uparrow \\ Qubit\ 1 &\rightarrow ② \rightarrow Site\ 1,\ spin\ \downarrow \\ Qubit\ 2 &\rightarrow ③ \rightarrow Site\ 2,\ spin\ \uparrow \\ Qubit\ 3 &\rightarrow ④ \rightarrow Site\ 2,\ spin\ \downarrow \end{aligned} \tag{25}$$

The best form of Hubbard hamiltonian ready to be implemented on quantum processor is built from relation 24: here are not considered the trivial $\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1}$ terms, and are specified the qubit involved on each operation, following the mapping 25:

$$
\begin{aligned}
\mathcal{H} &= \mathcal{H}_{hop} + \mathcal{H}_{int} = \\
&= \frac{t}{2}[\sigma^x_{①} \otimes \sigma^x_{③} + \sigma^y_{①} \otimes \sigma^y_{③}] + \\
&+ \frac{t}{2}[\sigma^x_{②} \otimes \sigma^x_{④} + \sigma^y_{②} \otimes \sigma^y_{④}] + \\
&+ V[\sigma^z_{①} \otimes \sigma^z_{②} \otimes \mathbb{1}_{③} \otimes \mathbb{1}_{④}] + \\
&+ V[\mathbb{1}_{①} \otimes \mathbb{1}_{②} \otimes \sigma^z_{③} \otimes \sigma^z_{④}] + \\
&+ V[\sigma^z_{①} \otimes \mathbb{1}_{②} \otimes \mathbb{1}_{③} \otimes \mathbb{1}_{④}] + \\
&+ V[\mathbb{1}_{①} \otimes \sigma^z_{②} \otimes \mathbb{1}_{③} \otimes \mathbb{1}_{④}] + \\
&+ V[\mathbb{1}_{①} \otimes \mathbb{1}_{②} \otimes \sigma^z_{③} \otimes \mathbb{1}_{④}] + \\
&+ V[\mathbb{1}_{①} \otimes \mathbb{1}_{②} \otimes \mathbb{1}_{③} \otimes \sigma^z_{④}]
\end{aligned}
\tag{26}
$$

The relationship 26 can be expressed in a more compact view, excluding the trivial $\mathbb{1}_{①}$ terms:

$$
\begin{aligned}
\mathcal{H} &= \mathcal{H}_{hop} + \mathcal{H}_{int} = \\
&= \frac{t}{2}[\sigma^x_{①} \otimes \sigma^x_{③} + \sigma^y_{①} \otimes \sigma^y_{③}] + \\
&+ \frac{t}{2}[\sigma^x_{②} \otimes \sigma^x_{④} + \sigma^y_{②} \otimes \sigma^y_{④}] + \\
&+ V[\sigma^z_{①} \otimes \sigma^z_{②} + \sigma^z_{③} \otimes \sigma^z_{④}] + \\
&+ V[\sigma^z_{①} + \sigma^z_{②} + \sigma^z_{③} + \sigma^z_{④}]
\end{aligned}
\tag{27}
$$

While a single σ^z can be easily implemented on a quantum computer using a standard rotation among z-axis, the implementation of $\sigma^x \otimes \sigma^x$, $\sigma^y \otimes \sigma^y$ and $\sigma^z \otimes \sigma^z$ require the application of a transformation of the reference coordinate system. In particular, the relationships used are the following:

$$
\begin{aligned}
\hat{X} &\rightarrow [R_y(-\frac{\pi}{2})\ Z\ R_y(\frac{\pi}{2})] \\
\hat{Y} &\rightarrow [R_x(-\frac{\pi}{2})\ Z\ R_x(\frac{\pi}{2})] \\
\hat{Z}\hat{Z} &\rightarrow [CNOT\ R_z(2\delta)\ CNOT]
\end{aligned}
\tag{28}
$$

where the parameter δ is the angle related to the temporal evolution of the system. Using the "building blocks" reported in 28, a quantum circuit describing the Hubbard Model hamiltonian has been created, following the compact notation 27 with the qubit numbers in which to apply the quantum gates:

References