Simulation of Matrix Product State on a Quantum Computer

Amandeep Singh Bhatia* and Mandeep Kaur Saggi

Department of Computer Science, Thapar Institute of Engineering & Technology, India
E-mail: *amandeepbhatia.singh@gmail.com

(Dated: November 27, 2018)

The study of tensor network theory is an important field and promises a wide range of experimental and quantum information theoretical applications. Matrix product state is the most well-known example of tensor network states, which provides an effective and efficient representation of one-dimensional quantum systems. Indeed, it lies at the heart of density matrix renormalization group (DMRG), a most common method for simulation of one-dimensional strongly correlated quantum systems. It has got attention from several areas varying from solid-state systems to quantum computing and quantum simulators. We have considered maximally entangled matrix product states (GHZ and W). Here, we designed the quantum circuits for implementing the matrix product states. In this paper, we simulated the matrix product states in customized IBMs (2-qubit, 3-qubit and 4-qubit) quantum systems and determined the probability distribution among the quantum states.

I. INTRODUCTION AND MOTIVATION

Since, Feynman [1] proposed the idea of quantum computing and stated that quantum computers can simulate quantum mechanical systems exponentially faster, outstanding advancement has been made in simulation of quantum systems. In the last decade, the quantum simulation of closed and open systems has got overwhelming response among research communities. It promises powerful applications in the field of high energy physics, quantum chemistry and condensed matter, which are intractable on classical computers. The field of quantum computing is concern with the behavior and nature of energy at the quantum level to improve the efficiency of computations. The main aim of running quantum algorithms on quantum computers to solve the various computational tasks more efficiently and in less time as compared to existing classical ones. The quantum principle of superposition and entanglement is the backbone of quantum algorithms, which allows us to perform operations in large Hilbert spaces exponentially.

In the past few years, the research has been increased in simulating experiments on IBM (International Business Machines Corporation) Q Experience platform. IBM has given access to real quantum computers and simulators, which allows researchers to develop, test and implement their experiments [2]. Through IBM, we can examined the simulation results on classical computer and analysis on available quantum hardware to get a feel of the quantum system. It is becoming far more widespread and efficiently used to simulate several computational problems quickly [3]. Currently, the platform has been extensively used to implement several experiments such as quantum tunneling simulation [4], developing new algorithms for hard problems [5], Ising model simulation hard problems [6], quantum algorithms [7], quantum error correction [8–10], quantum machine learning [11], quantum games, benchmarking the quantum gates [12] to name a few.

Tensor network states are a new language for quantum many-body systems based on pure quantum mechanical phenomena ‘entanglement’ [13]. Tensor network states are classified on the basis of dimensions along which the tensors are crossed. Thus, it manages the exponentially growing Hilbert space by restricting the entanglement between two parts of the quantum system [14]. Although, the dimension of Hilbert space increases exponentially with the increase in size of the system, there exists some quantum many-body systems whose implementations are realizable by classical computers. A matrix product state (one-dimensional system) is an example of tractable quantum systems numerically. In MPS, low entangled states are efficiently represented, which is not with large dimensions tensor network states. It has some basic properties such as dense nature, finite correlation, translational invariance and one-dimensional area law [15].

Recently, matrix product state (MPS) provides a stepping stone to various advancements in field of condensed matter and quantum computational theory: unsupervised learning using MPS, quantum dynamics [16, 17], open source MPS simulation [18], lattice algorithm for inhomogeneous systems [19], simulating quantum computation [20], simulation of open quantum systems [21], quantum finite state machines of MPS [22], supervised learning [23] and neural network representation [24] and MPS based efficient, productive applications for high performance computers [25] and can be employed in various emerging technologies such as optical computing, quantum cryptography, image recognition and dynamic quantum clustering [26]. MPS provides an efficient approximation of realistic local Hamiltonians and can be generated by tensors sequentially. We focused on the maximum entangled MPS (GHZ and W states). In previous paper, we have efficiently simulated MPS with a broader quantum computational theory and investigated their relationship with quantum finite-state machine (QFSM) using unitary criteria [22]. In this paper, we have implemented simulation on customized real IBM quantum computer and simulator. Further, the probability distributions among
qubits is investigated. The paper is organized as follows: Section 2 is devoted to the family of matrix product state. In Section 3, simulation results are presented. Finally, Section 4 is the conclusion.

II. MATRIX PRODUCT STATE

Matrix product state is complete. Basically, it concede the extent of entanglement in bond dimensions. In fact, any pure quantum state can be described by substituting the coefficients e.g. rank-\(N\) tensor by \(N\)-rank 3 tensors and 2-rank by 2 tensors. In MPS, a pure quantum state \(|\phi\rangle\) is represented as:

\[
|\phi\rangle = \sum_{\sigma_1, \sigma_2, \ldots, \sigma_L} \text{Tr}[M_1^{\sigma_1}M_2^{\sigma_2} \cdots M_L^{\sigma_L}] |\sigma_1, \sigma_2, \ldots, \sigma_L\rangle
\]  

where \(M_i^{\sigma_i}\) are complex square matrices, \(d\) is dimension, \(\sigma_i\) represents the indices i.e. \(\{0, 1\}\) for qubits and \(\text{Tr}()\) denotes trace of matrices [27]. Figure 1 shows the MPS as one-dimensional array of tensors and an instance of finite system of 5 sites [15]. The GHZ state and W state can be represented using MPS:

- **GHZ state**: A Greenberger-Horne-Zeilinger (GHZ) [28] state of \(N\)-spins 1/2 is represented as

\[
|GHZ\rangle = \frac{1}{\sqrt{2}} (|0\rangle^\otimes N + |1\rangle^\otimes N)
\]  

It is defined as maximum entangled state, consisting some non-trivial entanglement features [29]. The 4-qubit GHZ state is represented as \(\frac{1}{\sqrt{2}} (|0000\rangle + |1111\rangle)\). Its matrix product state and unitary matrix (\(U_{GHZ}\)) are represented as:

\[
M^0 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad M^1 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad U_{GHZ} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}
\]

- **W state**: The \(n\)-qubit W state is represented as [27]:

\[
|W\rangle = \frac{1}{\sqrt{n}} (|100...0\rangle + |010...0\rangle + ... + |000...1\rangle)
\]  

The W state refers to the superposition of pure entangled states with same coefficients [29]. It is different from above GHZ state. It represents a multipartite entanglement, where one of the qubits is in up state \(|1\rangle\), while others are in down state \(|0\rangle\). The 4-qubit W state is represented as \(\frac{1}{\sqrt{4}} (|1000\rangle + |0100\rangle + |0010\rangle + |0001\rangle)\) [27]. The matrix representation is given as:

\[
A(1)^0 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad A(2)^0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad A(3)^0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad A(4)^0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}
\]

\[
A(1)^1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad A(2)^1 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad A(3)^1 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad A(4)^1 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}
\]
III. SIMULATION RESULTS

Before, we proceed to the simulation of matrix product state, it is useful to define the notion of some operators used over single qubit in quantum computation. The controlled NOT operator (CNOT) has two inputs as well as outputs [16]. The flip operation is performed over the target qubit when the first qubit is 1. The quantum circuit for CNOT operator is shown in Fig 3 and its matrix representation is given in Eq. (10). The other highly used quantum operators are flip operator (X): flips the qubit, identity operator (I): it does nothing i.e. outputs the qubit as it is, Hadamard operator (H): it generates superposition of states with equal probability in computational basis. Their matrices are given in Eq. (7-9) respectively. In quantum circuits, such operators can be represented using quantum gates. The universal set of quantum gates are shown in Fig 2.

\[ X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \]  
\[ X|0\rangle = |1\rangle \]  
\[ X|1\rangle = |0\rangle \]  

\[ I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \]  
\[ I|0\rangle = |0\rangle \]  
\[ I|1\rangle = |1\rangle \]  

\[ H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \]  
\[ H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \]  
\[ H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \]  

\[ CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \]

A. GHZ state

Experimentally, we utilized the IBM Quantum Experience (IBM-QE), a universal customized (2-qubit, 3-qubit and 4-qubit) quantum computer to perform our simulation. The following are the steps to test experiment on IBM-QE:

- Construct the quantum circuit for the computational problem through Python programming language and specify it using graphical interface.
Execute the quantum circuit on the IBM simulator and test whether it produces works correctly or not.

The implementation of the quantum circuit is performed on the hardware processor for given number of shots. During each shot, the specified quantum processor is assigned to implement the quantum circuit.

Finally, the measurement is performed and the probability of each process is calculated.

Here, we started with the maximally entangled 2-qubit GHZ state, which is represented as $|\text{GHZ}\rangle_2 = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. Initially, we have taken two quantum as well as classical registers. Both quantum registers are initialized to zero. The Hadamard gate and CNOT gate is used to create an entanglement between both qubits, followed by measurement of quantum state $q[0]$ and $q[1]$ to classical registers $c[0]$ and $c[1]$ respectively. Correspondingly, the quantum circuit for 2-qubit GHZ state is shown in Fig. 4. Further, the probability distribution is determined as 53.3906 % for state $|00\rangle$ and 49.6094 % for $|11\rangle$ respectively i.e. on summation it satisfies unitary property. The histogram of probability distribution for $|\text{GHZ}\rangle_2$ is shown in Fig. 5.

Next, we have considered 3-qubit GHZ state interpreted as $|\text{GHZ}\rangle_3 = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$. To simulate the $|\text{GHZ}\rangle_3$ on quantum computer, we have taken three quantum registers to carry out computation and three classical registers for measurement purpose at the end. The Hadamard and CNOT operation between first and second quantum qubit is similar to $|\text{GHZ}\rangle_2$. Then, the second CNOT operation is performed between second and third quantum qubit i.e. flips the $q[3]$ whenever the $q[2]$ is in excited state. The final results can be retrieved from classical registers. It creates the 3-qubit entangled GHZ state and its equivalent quantum circuit is given in Fig 6. Further, the probability distribution is calculated, which comes out to be same i.e. $\frac{1}{2}$ for both $|000\rangle$ and $|111\rangle$ respectively.

Further, the complex 4-qubit GHZ quantum state $|\text{GHZ}\rangle_4 = \frac{1}{\sqrt{2}}(|0000\rangle + |1111\rangle)$ is taken. A 4-qubit quantum circuit for $|\text{GHZ}\rangle_4$ is designed to check whether it is capable of showing quantum behavior on implementing repeatedly. Following the above procedure, the Hadamard gate and CNOT gate produces an entanglement between $q[3]$ and $q[4]$ as shown in Fig 8. Finally, the measurement is readout after one shot and yields the occurrence of state $|0000\rangle$ with
50.2930 % and $|1111\rangle$ with 49.7070 % respectively, shown in Fig 9. It can be easily checked that after every shot on quantum simulator, the summation of probabilities of occurrence of both quantum states is comes out to be 1. Thus, it confirms the probability distribution of four spins-1/2 GHZ state into single state i.e. highly entangled quantum state.
**B. W state**

The GHZ state and W state represent different types of entanglement, where W state is said to be less entangled as compared to GHZ. On measurement, GHZ state is collapse into mixture of other states. But, in case of W state, it leaves the bipartite entanglements on measuring one of its sub-systems.

In this subsection, we have considered 3 and 4-qubit W state and their equivalent quantum circuits are designed and tested on quantum simulator. The 3-qubit W state \( |W\rangle_3 = \frac{1}{\sqrt{3}} (|100\rangle + |010\rangle + |001\rangle) \) is considered. Here, we have used flip gate \((X)\) to flip the qubit and Pauli matrix \((R_y)\) to rotate the spin in \(y\)-direction with given theta \((\theta)\). After performing the flip operation over the third qubit, barrier is assigned between second \(q_1\) and third \(q_2\) to avoid the optimization of consecutive gates in a quantum circuit, as shown in Fig 10. Then, CNOT gate is applied successively between \(q_0, q_1\) and \(q_1, q_2\) to make one of qubits in excited state and other in ground state same time. Finally, the equivalent quantum circuit for \(|W\rangle_4\) is tested on IBM-QE and results are plotted in Fig. 11. The probability distribution of states is examined as approx 33 % for each \(|100\rangle\) and \(|010\rangle\), and 34 % for \(|001\rangle\). It agrees the superimposed 3-qubit W state into singlet state.

**FIG. 10:** Quantum circuit for 3-qubit W state

**FIG. 11:** Probability distribution for 3-qubit W state

Furthermore, we constructed the quantum circuit for complicated 4-qubit W state \(|W\rangle_4 = \frac{1}{\sqrt{4}} (|1000\rangle + |0100\rangle + |0010\rangle + |0001\rangle)\). Following the above computational procedure of \(|W\rangle_3\), we have used combination of Hadamard gates before and after the CNOT operation. Thus, it execute the CNOT operation in reverse direction using the Kronecker product \((H \otimes H)\) i.e. equal to \(\frac{1}{\sqrt{2}} \begin{bmatrix} H & H \\ H & -H \end{bmatrix} (4 \times 4)\) matrix. The constructed quantum circuit for \(|W\rangle_4\) is shown in Fig

**FIG. 12:** Quantum circuit for 4-qubit W state
Finally, after simulation, the measurement is retrieved from classical registers and the histogram of probability distribution among the states is plotted in Fig 13. It shows the occurrence of state $|1000\rangle$ and $|0010\rangle$ with approx 25% each, 24% of $|0100\rangle$ and state $|0001\rangle$ with 26% approximately.

### IV. CONCLUSION

In conclusion, we have demonstrated the two highly entangled matrix product states (GHZ and W). The main focus of this paper is towards the simulation on a quantum computer. We have designed quantum circuits for (2, 3 and 4-qubit) GHZ state and (3 and 4-qubit) W state. Further, the constructed quantum circuits have been simulated on a quantum computer and their probability distribution among the quantum states is investigated. To conclude, we have noticed that any matrix product state can be efficiently simulated on a quantum computer. This allows us to employ these circuits for efficient and productive quantum computational theoretical and experimental applications such as quantum machine learning, MPS based quantum algorithms and can be used in condensed matter physics for quantum state tomography in future.

### Acknowledgments

Amandeep Singh Bhatia was supported by Maulana Azad National Fellowship (MANF), funded by Ministry of Minority Affairs, Government of India.

---

[1] R. P. Feynman, Simulating physics with computers, International journal of theoretical physics 21 (6) (1982) 467–488.
[2] IBM Quantum Experience, https://www.research.ibm.com/ibm-q/. [Online; accessed 08-october-2018].
[3] Quantum computing gets an API and SDK, https://developer.ibm.com/dwblog/2017/quantumcomputing-api-sdk-david-lubensky/. [Online; accessed 08-october-2018].
[4] N. N. Hegade, B. K. Behera, P. K. Panigrahi, Experimental demonstration of quantum tunneling in ibm quantum computer (2017). {arXiv:1712.07326}.
[5] A. Dash, D. Sarmah, B. K. Behera, P. K. Panigrahi, Exact search algorithm to factorize large bprimers and a triprome on ibm quantum computer (2018). {arXiv:1805.10478}.
[6] A. Cervera-Lierta, Exact ising model simulation on a quantum computer (2018). [path](arXiv:1807.07112).
[7] P. J. Coles, S. Eidenbenz, S. Pakin, A. Adedoyin, J. Ambrosiano, P. Anisimov, W. Casper, G. Chennupati, C. Coffrin, H. Djidjev, et al., Quantum algorithm implementations for beginners (2018). {arXiv:1804.03719}.
[8] R. Harper, S. Flammia, Fault tolerance in the ibm q experience (2018). {arXiv:1806.02359}.
[9] D. Willsch, M. Nocon, F. Jin, H. De Raedt, K. Michielsen, Testing quantum fault tolerance on small systems (2018). {arXiv:1805.05227}.
[10] R. K. Singh, B. Panda, B. K. Behera, P. K. Panigrahi, Demonstration of a general fault-tolerant quantum error detection code for (2n + 1)-qubit entangled state on ibm 16-qubit quantum computer (2018). {arXiv:1807.02883}.  

FIG. 13: Probability distribution for 4-qubit W state
[11] Z. Zhao, A. Pozas-Kerstjens, P. Rebentrost, P. Wittek, Bayesian deep learning on a quantum computer (2014). \{arXiv: 1806.11463\}.

[12] K. Michielsen, M. Nocon, D. Willsch, F. Jin, T. Lippert, H. De Raedt, Benchmarking gate-based quantum computers, Computer Physics Communications 220 (2017) 44–55.

[13] S. R. White, Density-matrix algorithms for quantum renormalization groups, Physical Review B 48 (14) (1993) 10345.

[14] J. D. Biamonte, S. R. Clark, D. Jaksch, Categorical tensor network states, AIP Advances 1 (4) (2011) 042172.

[15] R. Orús, A practical introduction to tensor networks: Matrix product states and projected entangled pair states, Annals of Physics 349 (2014) 117–158.

[16] A. S. Bhatia, A. Kumar, Neurocomputing approach to matrix product state using quantum dynamics, Quantum Information Processing 17 (10) (2018) 278.

[17] W. W. Ho, S. Choi, H. Pichler, M. D. Lukin, Periodic orbits, entanglement and quantum many-body scars in constrained models: matrix product state approach (2018). \{arXiv:1807.01815\}.

[18] J. Johansson, P. Nation, F. Nori, QuTiP: An open-source python framework for the dynamics of open quantum systems, Computer Physics Communications 183 (8) (2012) 1760–1772.

[19] M. Ganahl, G. Vidal, Continuous matrix product states for non-relativistic quantum fields: a lattice algorithm for inhomogeneous systems (2018). \{arXiv:1801.02219\}.

[20] I. L. Markov, Y. Shi, Simulating quantum computation by contracting tensor networks, SIAM Journal on Computing 38 (3) (2008) 963–981.

[21] L. Bonnes, A. M. Läuchli, Superoperators vs. trajectories for matrix product state simulations of open quantum system: a case study (2014). \{arXiv:1411.4831\}.

[22] A. S. Bhatia, A. Kumar, Quantifying matrix product state, Quantum Information Processing 17 (3) (2018) 41.

[23] E. Miles Stoudenmire, D. J. Schwab, Supervised learning with quantum-inspired tensor networks (2016). \{arXiv:1605.05775\}.

[24] Y. Huang, J. E. Moore, Neural network representation of tensor network and chiral states (2017). \{arXiv:1701.06246\}.

[25] M. Dolfi, B. Bauer, S. Keller, A. Kosenkov, T. Ewart, A. Kantian, T. Giamarchi, M. Troyer, Matrix product state applications for the ALPS project, Computer Physics Communications 185 (12) (2014) 3430–3440.

[26] M. K. Saggi, S. Jain, A survey towards an integration of big data analytics to big insights for value-creation, Information Processing & Management 54 (5) (2018) 758–790.

[27] Matrix Product Formalism, http://www2.mpq.mpg.de/Therygroup/CIRAC/wiki/images/9/9f/Eckholt$_$Diplom.pdf/, [Online; accessed 25-Nov-2018].

[28] D. M. Greenberger, Ghz (greenbergerhornezeilinger) theorem and ghz states, in: Compendium of quantum physics, Springer, 2009, pp. 258–263.

[29] G. Uchida, Geometry of ghz type quantum states, Ph.D. thesis, Uniwien (2013).