Quantum Simulation of Pairing Hamiltonian in Superconductivity

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Developments in the field of Quantum Computing had achieved remarkable success in recent years. Although a universal quantum computer is still far from reach, the tremendous advances in controllable quantum devices, in particular with solid-state systems, make it possible to physically implement "quantum simulators". Quantum simulators are physical setups able to simulate other quantum systems efficiently that are intractable on classical computers. Based on solid state qubit systems with various types of nearest-neighbor interactions, we propose a complete set of algorithms for simulating pairing Hamiltonian in superconductivity. We realize four different interaction Hamiltonian through IBM superconducting qubit quantum computer for three qubit systems. We studied the fidelity vs iterations in Trotter decomposition. We also analyze the complexity analysis and comparison of tunable and constant interactions. Our simulation might be feasible with state-of-the-art technology in solid-state quantum devices.

Keywords: Superconductivity, Pairing Hamiltonians, Quantum simulation, IBM quantum experience

I. INTRODUCTION

Classical computers fail to effectively simulate quantum systems with complex many-body interactions due to the exponential growth of variables for characterizing these systems [1]. Simulating quantum mechanical systems face a great computational problem, especially when dealing with large systems. This difficulty was overcome in 1980's when quantum simulation was proposed to solve such an exponential explosion problem using a controllable quantum system [2]. It was shown in 1996, that a quantum computer only containing few particle interactions can be used to efficiently simulate many body quantum Hamiltonians [4]. Quantum simulation has applications in the study of a variety of problems in a plethora of domains like- starting from condensed-matter physics to high-energy physics [5], quantum chemistry [6] aimed at quantum information processing and quantum gravity [7]. A large number of quantum systems like- neutral atoms [8], ions [9], polar molecules [10], electrons in semiconductors, nuclear spins [9] and photons have been proposed as quantum simulators. Recently, quantum simulators using trapped ions cold atoms [12] and photons have already been experimentally demonstrated to some extent.

Feynman proposed solution to this problem and coined a term with his new concept-quantum computer [3]. In fact, it has made clear over the past three decades, a quantum computer ensured to do much more than simulating quantum mechanics, and therefore in the present world, quantum computation and quantum information theory are very active research fields [16, 17]. Feynman realized at the time that a quantum machine would itself experience an exponential explosion, but with good consequences. The machine would have the capacity to contain an exponentially large amount of information without using an exponentially large amount of physical resources, thus making it a natural tool to perform quantum simulation [13].

In recent years, the interest in quantum simulation has been elevating, and the reason for this is twofold. First, there are a large number of potential applications of quantum simulation in physics [13], chemistry [18] and even biology [19]. Second, the technologies required for the coherent control of quantum systems have matured enough to allow for the physical implementation of practical quantum simulation in the very near future [14]. A great number research groups are now actively focusing at the experimental realization of quantum simulators with tens of qubits, which would be the first practical applications in which quantum computers outperform their classical counterparts [15]. Quantum simulators are classified into analog and digital ones. An analog quantum simulator is a control labile quantum system mimicking the behaviors of the target quantum system whose evolution can be effectively mapped onto the simulator, while a digital quantum simulator normally imitates the time evolution operator of the target system through the implementation of a series of elementary quantum gates. Practically, these two approaches are often used together.

Pairing Hamiltonians, e.g., BCS Hamiltonian [20] in conventional superconductors, feature long-range many-body interactions which are generally intractable on classical computers. Nevertheless, large-scale numerical calculations based on pairing Hamiltonians are of great importance, for instance in mesoscopic condensed matter, ultrasmall metallic grains and heavy nuclei [21]. To tackle this problem, a polynomial time quantum algorithm based on a nuclear magnetic resonance (NMR) [22]

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quantum computer was proposed, however liquid NMR has several constrains that make NMR quantum computer not scalable. Thus, large-scale implementation of the NMR-based quantum algorithm is unlikely in accordance with the state-of-the-art technology [22]. Superconducting quantum circuits [23] has rapidly progressed in the past decades, thus enabling them to be one of the most promising candidates towards practical quantum information processing. The unique flexibility on design and fabrication of superconducting circuits enables wide tunability in extensive Hamiltonian parameter ranges and the techniques for scaling up are compatible with those for modern integrated circuits. Moreover, the research on other solid-state qubit devices, e.g., quantum dot in semiconductors [24] and defect systems have also made significant progress in the past years.

In the past few decades, awareness has grown in the scientific world that quantum computation may be a more natural and desirable method of computation than the classical one, and the fundamental results may be more easily revealed through the ideas of quantum computation. Feynman's 1982 paper on quantum computing was motivated by the observation that quantum systems seem difficult to simulate on conventional classical computers [16]. The visible difficulty of solving a problem of quantum many-body physics of fermions (and bosons) on a classical computer is the requirement of an exponentially large basis set [25]. Lloyd (1996) showed that a quantum computer [26] can be made of ensembles of qubits $|0\rangle$ and $|1\rangle$ on which quantum gates can act, which can be regarded as a universal quantum simulator [26]. The simulation of an operator requires a platform that is given by IBM Q. With the use of proper analogous quantum gates, most of the operators can be simulated on IBM Q [27, 28]. The IBMQ experience platform provides the general public access to IBM's prototype quantum processors via the cloud. Exploiting the benefits of it, a large number of experiments have been designed to date related to quantum information [37, 38], quantum simulation [39–43], quantum key distribution [44], quantum teleportation [45], quantum cryptography [46, 47], quantum currency [48], quantum devices [49, 50] to name a few. In this paper, we have simulated the many-body pairing models using various Hamiltonians existed in superconductivity. The simulations and the models are suitable for a wide range of models especially superconducting quantum circuits and semiconducting qubit systems. We have computed the quantum state tomography and calculated the fidelity vs. iterations using the Suzuki-Trotter decomposition with graphs for 3 qubits system. We determined the complexity analysis, and studied the time evolution of the system by tuning interaction parameters.

II. MODEL

A. Pairing Hamiltonian in Superconductivity

The BCS pairing Hamiltonian has been widely used in different fields- condensed matter physics, nuclear physics etc. The Hamiltonian is typically expressed in terms of fermionic or bosonic creation (annihilation) operators- $c^\dagger_{\pm m}$ and $c_{\pm l}$ and $n^F_{\pm m} = c^\dagger_{\pm m} c_{\pm m}$ are fermionic number operators.

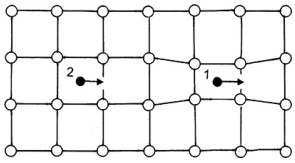


FIG. 1: Pictorial representation of the BCS Pairing Theory . Picture courtesy: Electrons in Solids, Dunlap, Richard A, 2019

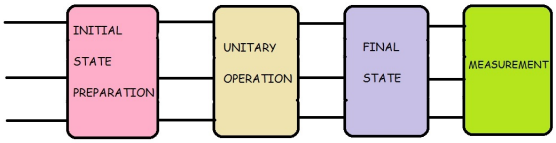


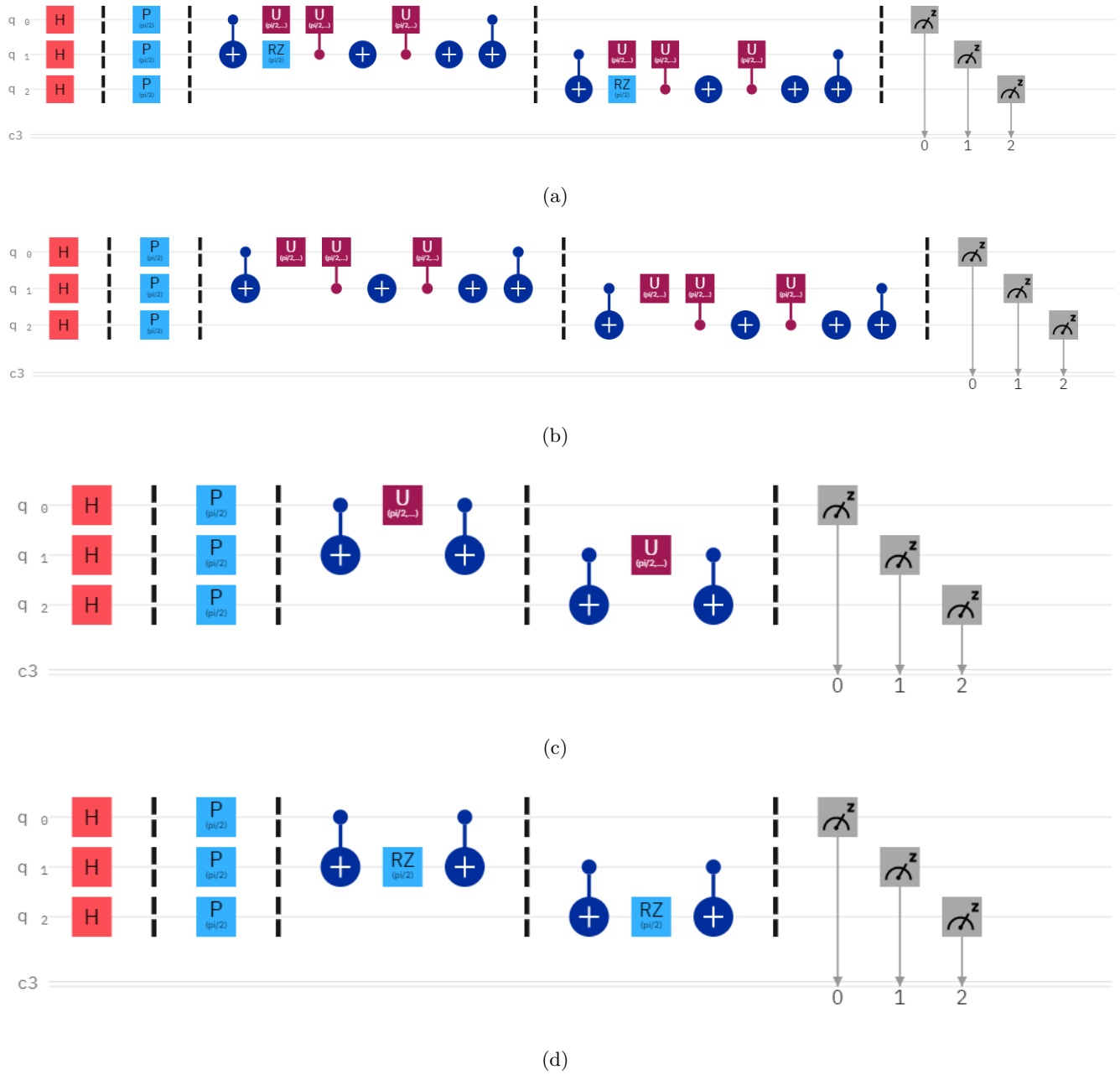
FIG. 2: Schematic diagram of the method of simulation of the 3-qubits pairing Hamiltonian.

The pairing hamitonian is given by-

$$H_{BCS} = \sum_{m=1}^{N} \frac{\epsilon_m}{2}(n^F_m + n^F_{-m}) + \sum_{l=1}^{N}\sum_{m=1}^{N} V_{ml} c^\dagger_m c^\dagger_{-m} c_{-l} c_l \tag{1}$$

where, the matrix elements $V^+_{ml} \equiv \langle m, -m|V|l, -l\rangle$ are real and can be estimated or calculated,e.g.,for superconductors, in terms of Coloumb force and the electron phonon interaction. Pairs of fermions are labeled by the quantum numbers m and $-m$, according to the Cooper pair situation where paired electrons have equal energies but opposite momenta and spins: $m = (\mathbf{p}, \uparrow)$ and $-m = (\mathbf{-p}, \downarrow)$. These are time-reversed and degenerate partners whose energies are considered to be phenomenological parameters.

To convert the concept of BCS hamiltonian to quantum circuits we have to map the fermionic or bosonic operators to qubit operators. As has been analyzed by....the Hamiltonian is mapped into qubit space based on the isomorphic algebras of spin-fermion connection. The fermionic pair operators can be mapped onto qubit operators $\sigma^x_m, \sigma^y_m, \sigma^z_m$ through transformation $\{\sigma^x_m, \sigma^y_m, \sigma^z_m\}$ $= \{c^\dagger_m c^\dagger_{-m} + c_{-m} c_m, ic_{-m} c_m - ic^\dagger_m c^\dagger_{-m}, n^F_m + n^F_{-m} - 1\}$.



(a)

(b)

(c)

(d)

FIG. 3: (a) Circuit representation of the Heisenberg Nearest-Neighbour Hamiltonian. (b) Circuit representation of the XY Nearest-Neighbour Hamiltonian.(c) Circuit representation of the Transverse Ising Nearest-Neighbour Hamiltonian.(d)Circuit representation of the Longitudinal Ising Nearest-Neighbour Hamiltonian.

The Hamiltonian in Eq.(1) can be re-written int the qubit form as-

$$H_p = \sum_{m=1}^{N} \frac{\varepsilon_m}{2}\sigma_m^z + \sum_{m<l} \frac{V_{ml}}{2}(\sigma_m^x\sigma_l^x + \sigma_m^y\sigma_l^y), \tag{2}$$

with $\varepsilon_m = \epsilon_m + V_{mm}$.

B. Nearest Neighbour Coupling Interactions in Superconductivity

Coupling of qubits can be achieved through various type of interactions. For Superconducting Qubits the coupling can be done through many ways such as through inductance, capacitance or Josephson junctions. The interaction models can be classified into four categories- XY Model, Heisenberg Model, Transverse Ising Model and Longitudinal Ising Model. These four type of Hamil-

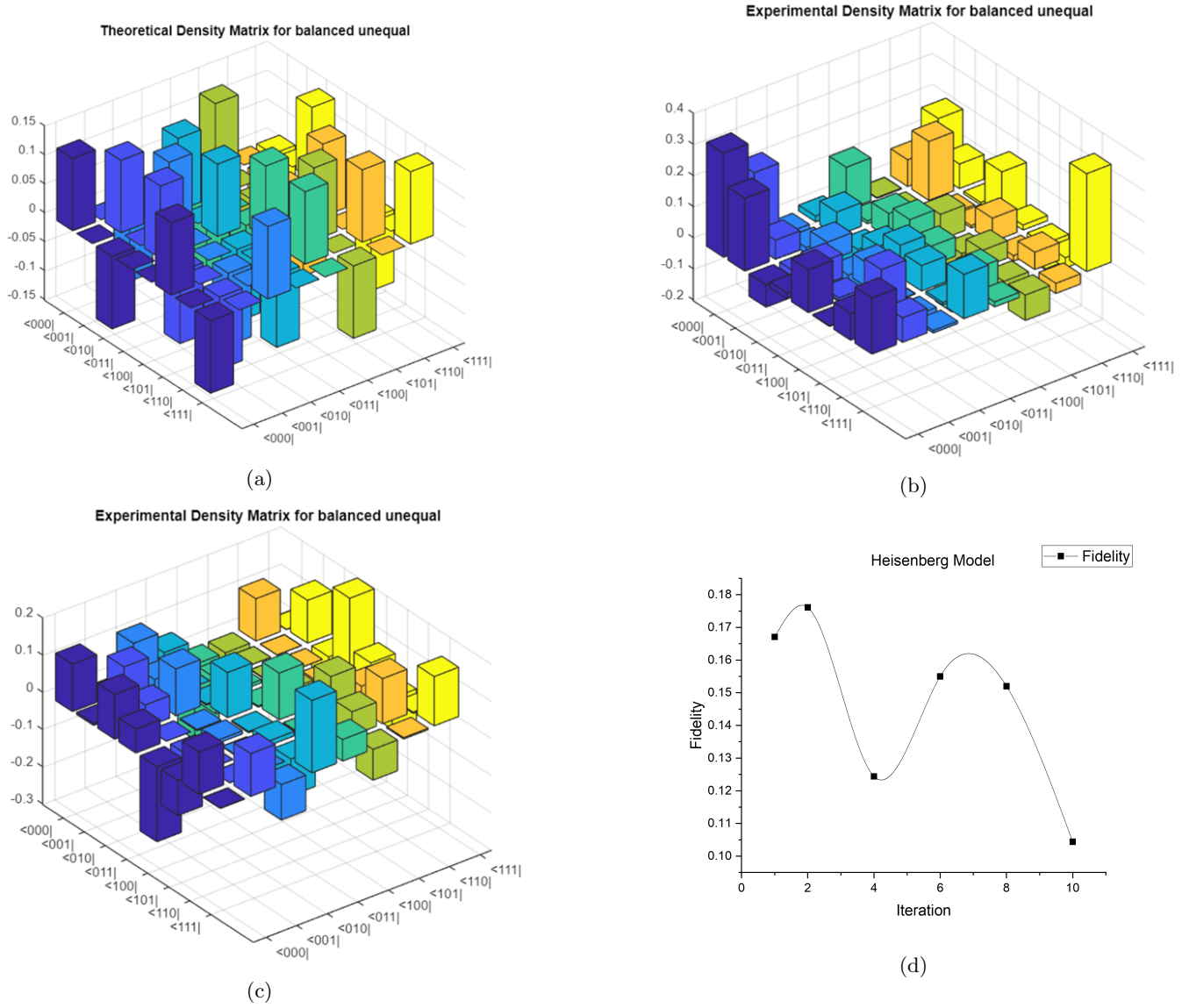


FIG. 4: (a) Theoretical Density Matrix for Heisenberg Model. (b) Experimental Density Matrix for 2 Iteration.(c) Experimental Density Matrix for 10 Iteration.(d) Fidelity vs Iteration for iteration ranging from 2 to 10.

TABLE I: Interaction Hamiltonians for the four different models

Interaction Models	**Interactions Hamiltonians**
XY model	$H_{XY} = H_0 + \sum_{i=x,y} \sum_{l=1}^{N-1} J_l \sigma_l^i \sigma_{l+1}^i$
Heisenberg model	$H_H = H_0 + \sum_{i=x,y,z} \sum_{l=1}^{N-1} J_l^i \sigma_l^i \sigma_{l+1}^i$
Transverse Ising model	$H_{Ising,T} = H_0 + \sum_{l=1}^{N-1} J_l \sigma_l^x \sigma_{l+1}^x$
Longitudinal Ising model	$H_{Ising,L} = H_0 + \sum_{l=1}^{N-1} J_l \sigma_l^z \sigma_{l+1}^z$

tonian can be written together as-

$$H = H_0 + H_I \tag{3}$$

with H_0 denoting the single-qubit Hamiltonian.

$$H_0 = \sum_{l=1}^{N} \frac{1}{2} \omega_l \sigma_l^z \tag{4}$$

and H_I denoting the interation Hamiltonian

$$H_I = \sum_{l=1}^{N-1} (J_l^x \sigma_l^x \sigma_{l+1}^x + J_l^y \sigma_l^y \sigma_{l+1}^y + J_l^z \sigma_l^z \sigma_{l+1}^z) \tag{5}$$

Here $\sigma_l^x, \sigma_l^y, \sigma_l^z$ are Pauli matrices in the basic of σ_l^z and l denotes the lth qubit. The coupling strength between the lth and the $(l+1)$th qubits is denoted by $J_l (l = 1, ..., N-1)$.

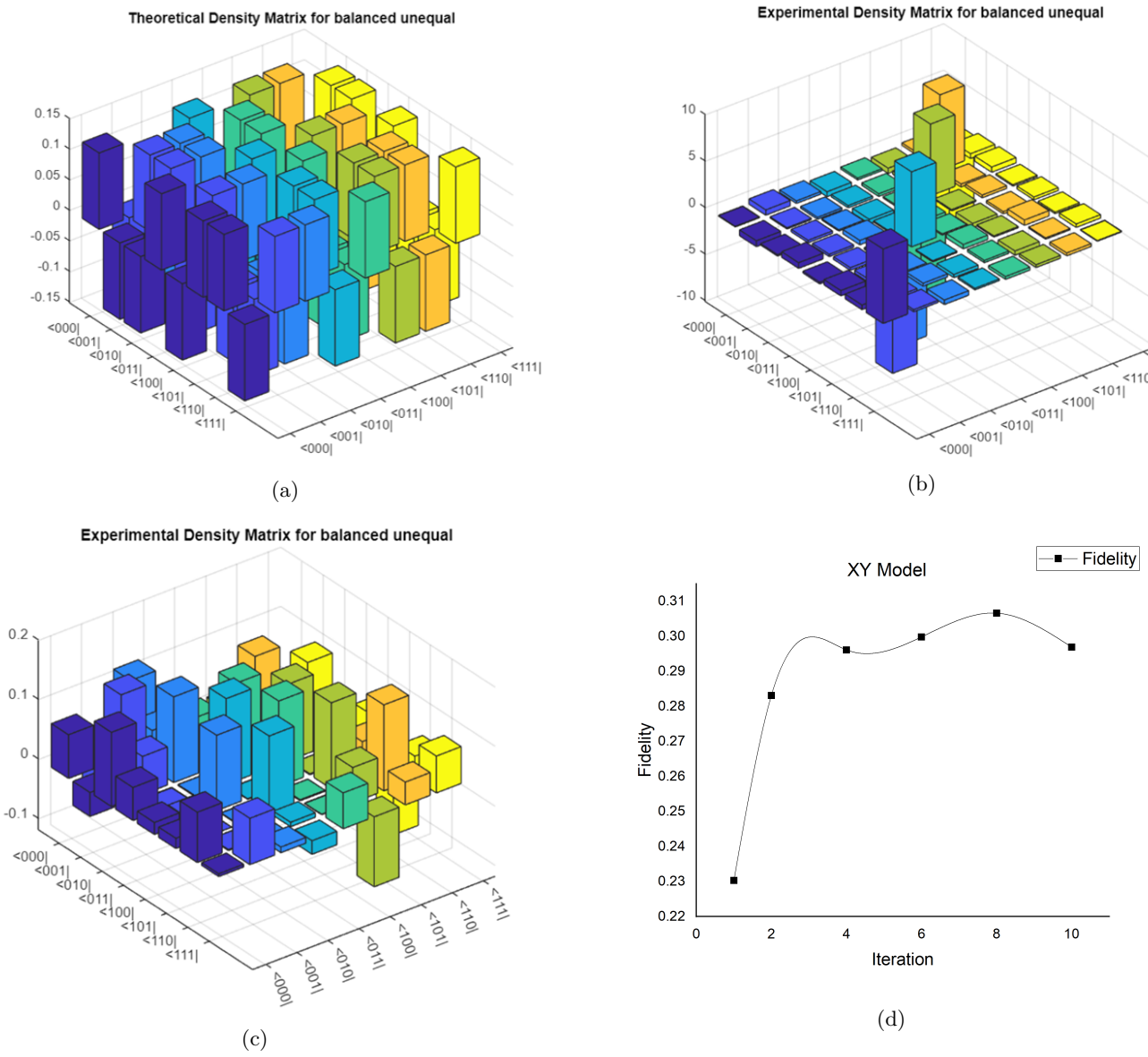


FIG. 5: (a) Theoretical Density Matrix for XY Model. (b) Experimental Density Matrix for 2 Iteration.(c) Experimental Density Matrix for 10 Iteration.(d) Fidelity vs Iteration for iteration ranging from 2 to 10.

The parameters of the previous two equations are chosen to get the Hamiltonian of four different models and J_l is fixed accordingly. It can be seen that the pairing models in Eq.(2) does not follow the form of the Hamiltonians of Eq.(3). Thus it is imperative to design algorithms to simulate these pairing Hamiltonians using the four types of interaction Hamiltonian.

For the operators $\sigma_m^x, \sigma_m^y, \sigma_m^z$ it should be taken care when simulating in the Suzuki-Trotter decoposition as the operators may not commute.We note that the tunability of parameters $\omega_l (l = 1, ..., N)$ and $J_l^x (i = x, y, z; l = 1, ..., N-1)$ affects the efficiency of the algorithms.

III. SIMULATION OF HAMILTONIAN OPERATOR

Given the initial state at time t=0, we can solve it to obtain the state at any later instant [55]. If $\hat{H}$ is independent of time, then

$$|\psi(x,t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle \tag{6}$$

Where $U(t) = e^{-i\hat{H}t}$, is the time evolution operator. U(t) is a unitary operator, i.e., $U^\dagger U = 1$. For our case we have to simulate four different Hamiltonian thus finding the corresponding unitary operations to build the quantum circuit. In general if we try to find the matrices for

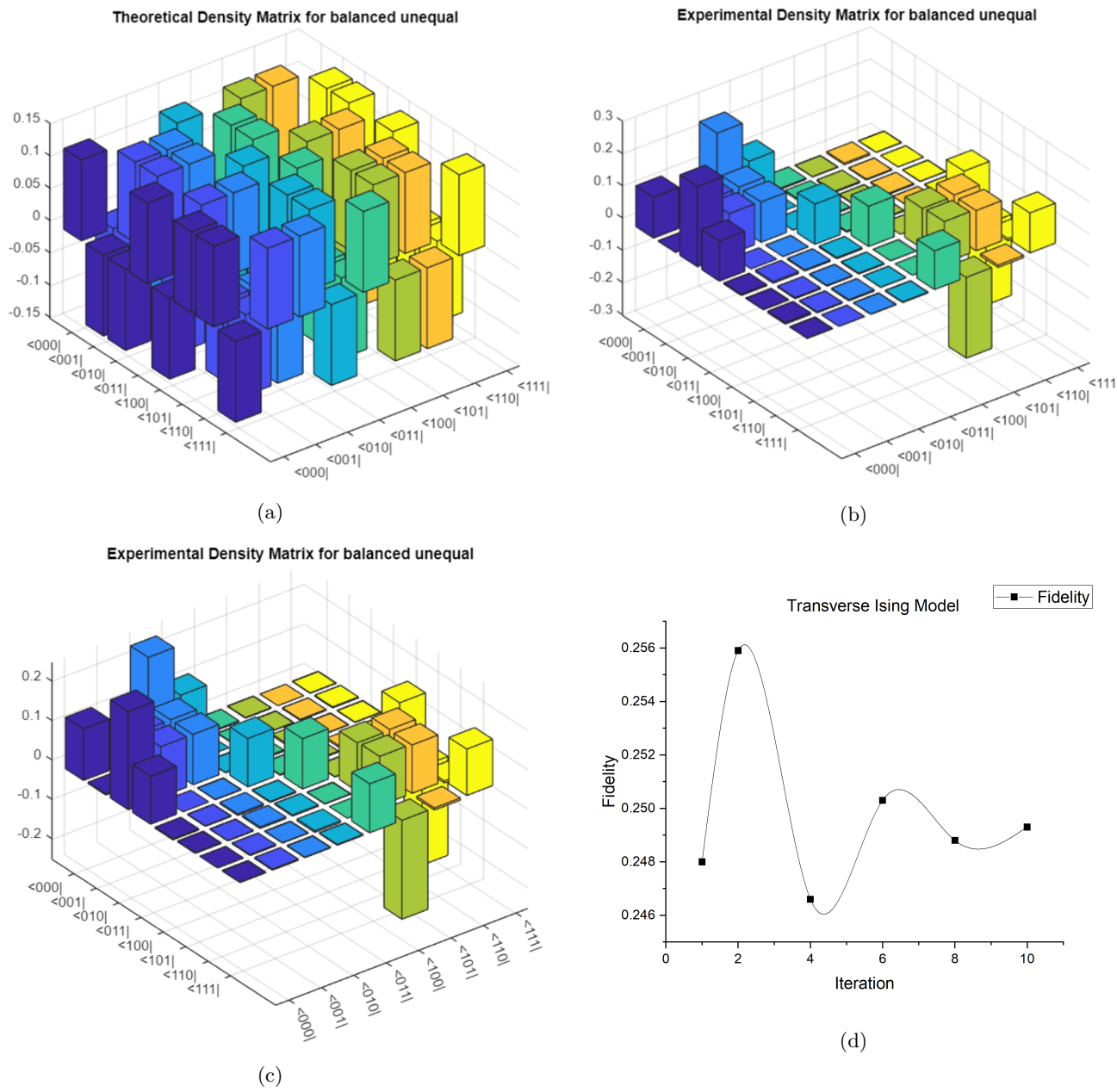


FIG. 6: (a) Theoretical Density Matrix for Transverse Ising Model. (b) Experimental Density Matrix for 2 Iteration.(c) Experimental Density Matrix for 10 Iteration.(d) Fidelity vs Iteration for iteration ranging from 2 to 10.

the time evolution operator we will have to find how the terms $\hat{\sigma}^x, \hat{\sigma}^y, \hat{\sigma}^z, \hat{\sigma}^x\hat{\sigma}^x, \hat{\sigma}^y\hat{\sigma}^y$ and $\hat{\sigma}^z\hat{\sigma}^z$ look like.

We can write separate terms for x, y and z as $\hat{\sigma}^x\hat{\sigma}^x$, $\hat{\sigma}^y\hat{\sigma}^y$ and $\hat{\sigma}^z\hat{\sigma}^z$ commute with each other.

The Hamiltonian of our choice is-

$$H = \sum_{l=1}^{N} \frac{1}{2}\omega_l \sigma_l^z + \sum_{l=1}^{N-1} (J_l^x \sigma_l^x \sigma_{l+1}^x + J_l^y \sigma_l^y \sigma_{l+1}^y + J_l^z \sigma_l^z \sigma_{l+1}^z) \tag{7}$$

The corresponding time evolution operator is given by-

$$U(t) = e^{-i(\sum_{l=1}^{N} \frac{1}{2}\omega_l \sigma_l^z)t} e^{-i\sum_{l=1}^{N-1}(J_l^x \sigma_l^x \sigma_{l+1}^x + J_l^y \sigma_l^y \sigma_{l+1}^y + J_l^z \sigma_l^z \sigma_{l+1}^z)t} \tag{8}$$

Here, $\hat{\sigma}^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $\hat{\sigma}^y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$, and $\hat{\sigma}^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

We can write the first part of the operator as per the value of pauli matrix($\hat{\sigma}^z$) shown.

The term $e^{-iJ_l\hat{\sigma}^x\hat{\sigma}^x t}$ in the second part of the operator, can be written as,

$\mathbb{I} cos\ J_1 t - \hat{\sigma}^x \bigotimes \hat{\sigma}^x isin\ J_1 t$

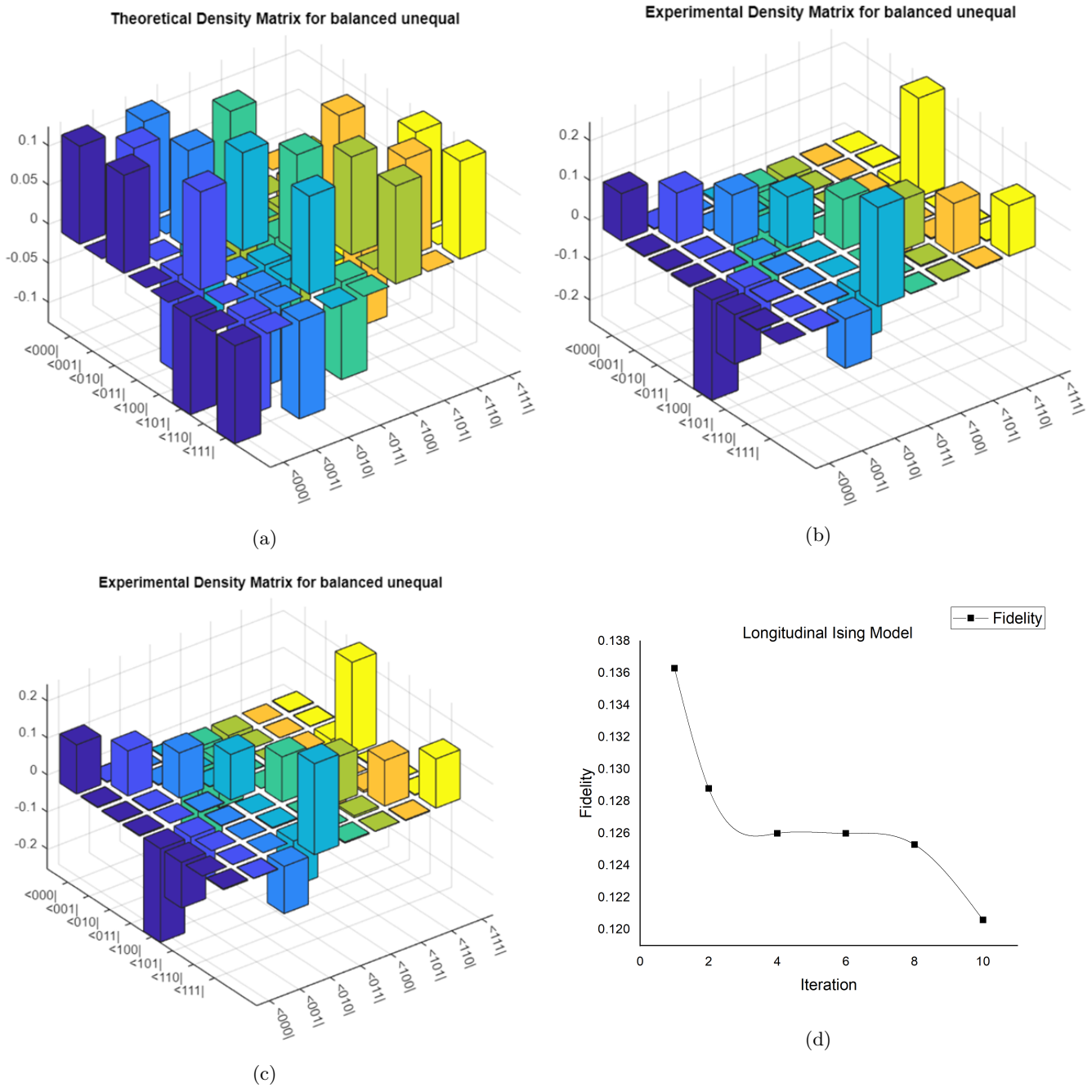


FIG. 7: (a) Theoretical Density Matrix for Longitudinal Ising Model. (b) Experimental Density Matrix for 2 Iteration.(c) Experimental Density Matrix for 10 Iteration.(d) Fidelity vs Iteration for iteration ranging from 2 to 10.

$$= \begin{bmatrix} cos(J_l t) & 0 & 0 & -isin(J_l t) \\ 0 & cos(J_l t) & -isin(J_l t) & 0 \\ 0 & -isin(J_l t) & cos(J_l t) & 0 \\ -isin(J_l t) & 0 & 0 & cos(J_l t) \end{bmatrix} \tag{9}$$

The term $e^{-iJ_l\hat{\sigma}^y\hat{\sigma}^y t}$in the second part of the operator can be written as,

$\mathbb{I}cos\ J_l t - \hat{\sigma}^y \bigotimes \hat{\sigma}^y isin\ J_l t$

$$= \begin{bmatrix} cos(J_l t) & 0 & 0 & isin(J_l t) \\ 0 & cos(J_l t) & -isin(J_l t) & 0 \\ 0 & -isin(J_l t) & cos(J_l t) & 0 \\ isin(J_l t) & 0 & 0 & cos(J_l t) \end{bmatrix} \tag{10}$$

The term $e^{-iJ_l\hat{\sigma}^z\hat{\sigma}^z t}$ in the second part of the operator can be written as,

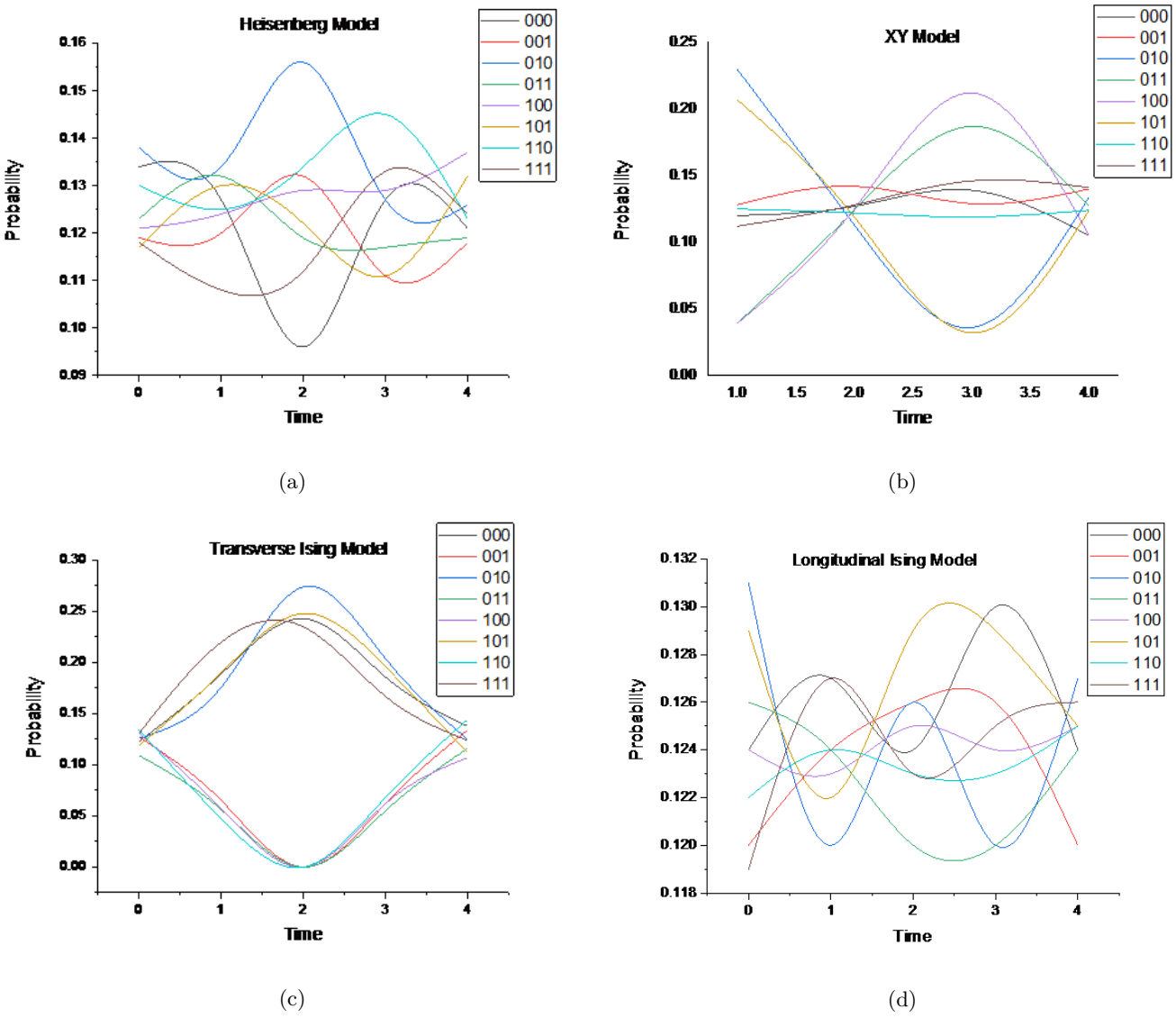


FIG. 8: Time Evolution of different Models at $\omega = \frac{\pi}{4}$ -(a)Heisenberg Model. (b) XY Model. (c) Transverse Ising Model. (d) Longitudinal Ising Model.

$$\mathbb{I} cos\ J_l t - \hat{\sigma}^z \bigotimes \hat{\sigma}^z isin\ J_l t$$

$$= \begin{bmatrix} e^{-iJ_l t} & 0 & 0 & 0 \\ 0 & e^{iJ_l t} & 0 & 0 \\ 0 & 0 & e^{iJ_l t} & 0 \\ 0 & 0 & 0 & e^{-iJ_l t} \end{bmatrix} \quad (11)$$

Now, referring to the four hamiltonians, we can write the time evaluation operator and thus proceed to implement. Each of these four types of Hamiltonians is a special case of Eq. (**??**)(8) with parameters being properly chosen.The Hamiltonian can be thus reduced to (i) longitudinal Ising Hamiltonian for parameters $J_l^x = J_l^y = 0$ and $J_l^z = J_l$; (ii)the transverse Ising Hamiltonian for parameters $J_l^y = J_l^z = 0$ and $J_l^x = J_l$;(iii)the XY Hamiltonian for parameters $J_l^z = 0$ and $J_l^x = J_l^y = J_l$; (iv) the Heisenberg Hamiltonian for parameters$J_l^x = J_l^y = J_l^z = J_l$. For 3 qubit system, the parameter l will range 1 to 3 to account for the coupling between qubits. The following step is to implement the unitary operator as obtained from the previous calculations in an order to the initial superposed state and obtain the time evolution of the Hamiltonian.

IV. IMPLEMENTATION ON IBM QUANTUM EXPERIENCE

A. Initial state preparation and unitary operation

The initial state is prepared by superposing the states of all the three qubits required to define the hamiltonian as per the superconducting pairing models.

This is done by putting a Hadamard gate on each qubit. This will provide contribution of all the qubits to the measurement.The unitary operators obtained in the previous section corresponding to the XX, YY, and ZZ type of interaction are then converted into quantum gates [17] and applied to form a circuit.

- For XX type of interaction:

  Comparing with the standard U_3 gate i.e,

$$U3(\theta,\phi,\lambda) = \begin{bmatrix} cos\theta/2 & -e^{i\lambda}sin\theta/2 \\ e^{i\phi}sin\theta/2 & e^{i(\phi+\lambda)}cos\theta/2 \end{bmatrix} \quad (12)$$

  We find the parameters for the gate to be used as:

  $\theta = 2J_l t$, $\phi = -\pi/2$ and $\lambda = \pi/2$.

- For YY type of interaction:

  Parameters obtained for $U3$ gate:

  $\theta = 2J_l t$, $\phi = -\pi/2$ and $\lambda = \pi/2$.

  Parameters obtained for $U3^\dagger$ gate:

  $\theta = 2J_l t$, $\phi = \pi/2$ and $\lambda = -\pi/2$.

- For ZZ type of interaction: Comparing with the standard $U1$ gate, i.e.,

$$U1(\lambda) = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{bmatrix} \quad (13)$$

  we get the parameter $\lambda = 2J_l t$.

B. Using Quantum State Tomography for Suzuki-Trotter Decomposition of Quantum Circuit

In this section, we take a look at use of Suzuki-Trotter decomposition to count the fidelity vs. the number of iterations of the quantum circuit. The circuit was iterated for $n = 2, 4, 6, 8, 10$. We have used Quantum State Tomography [59] to get the theoretical and experimental density matrices, thus calculating the fidelity of the circuit.

The general form of Quantum State Tomography is given by-

$$\rho = \frac{1}{2^N} \sum_{l=i_1,i_2,...,i_N=0}^{3} T_{i_1,i_2,...,i_N} \sigma_{i_1} \otimes \sigma_{i_2} \otimes ...\sigma_{i_N} \quad (14)$$

The experimental matrices of the circuits were computed through the density matrix as shown above. The experimental density matrix and the theoretical density matrix were compared and the fidelity of the quantum circuits were thus calculated.

V. MEASUREMENTS AND RESULTS

Probabilistic simulations and related calculations of quantum systems are usually carried out using the Monte Carlo method on a classical computer [25]. Such methods were devised to overcome the setback offered by exponentially growing phase spaces. Whereas, a quantum simulator [58] is usually very much under control of the experimenter. It is capable of simulating the dynamical behaviours of the physical model under inspection. Irrespective of the degree of internal correlations or entanglement between the degrees of freedom of the model, it can perform its job efficiently [57]. In this Section, the results corresponding to the different circuits designed during our attempt of quantum simulation of the Pairing Hamiltonian in Superconductivity are provided.

Fig.4 shows the theoretical density matrix and the experimental density matrix of Heisenberg Model .The fidelity vs. iteration of the circuit is also plotted. The matrices and the graphs are also plotted for XY Model, Transverse Ising Model, Longitudinal Model in Fig.5,Fig.6,Fig.7 respectively.

It can be seen in Fig.4,that for the Heisenberg Model the experimental density matrix deviates clearly from the theoretical density matrix. There can be changes which can be seen in the experimental density matrix also as the number of iteration is increased. The fidelity thus found is seen to show a sort of periodic nature with with fidelity decreasing from 2 iteration to 4, again increasing for 6 and 8 iteration and again decreasing for 10 iteration.

In Fig.5, for XY model it was seen that the experimental density matrix was similar for 2,4,6,8 iteration, but, was different for 10 iteration. As per the fidelity vs. iteration plot, the fidelity was increasing as the iteration increases from 2-8 but falls rapidly for 10 iteration.

For Transverse Ising Model(Fig.6) it was seen the experimental density matrix had similar figures for 2,4,6,8,10 iteration. The fidelity of the circuit decreased rapidly from 2 iteration to 4 iteration but after that gradually increased from 6-10 iteration.

Lastly for Longitudinal Ising Model(Fig.7) the experimental density matrix showed similar figures for all the iteration from 2-10. But the fidelity of the circuit decreased from 2-4 iteration, slightly increased for 6 iteration and again decreased for 8-10 iteration.

Fig.8 shows the variation of probability of possible states with respect to different values at $\omega = \frac{\pi}{4}$ and the time varies for t=0,..,4.

VI. CONCLUSION

In summary, we have studied algorithms and circuits for simulating the pairing Hamiltonians based on various nearest-neighbor interactions, e.g., Heisenberg Hamiltonian, longitudinal Ising Hamiltonian, XY Hamiltonian and transverse Ising Hamiltonian, which are available in the solid-state quantum devices. The Hamiltonians

are all been implemented on IBM superconducting qubit quantum computer. We have analyzed the probability change for time evolution and also found out the Quantum State Tomography for the different Hamiltonian thus finding the fidelity vs. iterations of the different circuits using Suzuki-Trotter decomposition.

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