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Quantum Simulation of Discretized Harmonic Oscillator on IBM Quantum Computer

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Here, we conduct a quantum simulation of a particle in a harmonic oscillator potential using a digital quantum simulator provided by IBM quantum experience platform. The simulation is carried out in two spatial dimensions and the algorithm used is generalized for n-spatial dimensions which can be used to simulate n-dimensional harmonic oscillator. We implement the unitary operator on an arbitrary quantum state to show that the probability amplitudes of position oscillate in time. We propose a quantum circuit to effectuate the unitary operator and design it on the simulator. The proposed circuit is then generalized for a n-qubit system that can be used to realize more meticulous simulations.

I. INTRODUCTION

The quantum harmonic oscillator[1] is one of the most significant and ubiquitous model studied rigorously in quantum mechanics. It is a quantum treatment applicable to any oscillating system with a typically discrete energy spectrum. Diatomic molecular vibrations are often imitated as 2-bodied quantum harmonic oscillator. Such treatments are conducted in three dimensions and include more realistic morse-potential for rotating and vibrating molecules[2]. The quantum mechanical harmonic chain of N identical atoms can be used to create simple quantum mechanical models of lattice. Various such models lead to the picture of free-quasi particles called 'phonons'[3]. In quantum chemistry, many helium like atoms can also be explained using Hook's method. This method can be used to measure population density of excited atoms[4]. A harmonic oscillator system customarily has a non-zero vacuum state giving rise to zero point energy when we quantify electric fields[5]. This gives rise to quantum fluctuations in free space which in turn gives rise to stimulated emissions which play a crucial role in the fields of quantum optics and lasers.

Feynman in 1982 drew the world's attention towards simulation of quantum systems. He proposed the idea that a computer can act as a quantum mechanical simulator[6]. Over the years there has been a rapidly growing interest in using quantum computation to study the time evolution of Hilbert spaces[7]. For large Hilbert spaces the standard computation techniques prove to be inadequate. Various instances of unattainable solutions have also shown up in simulating co-related quantum systems[8]. There are significant open problems in important areas, such as high temperature superconductivity, where progress is slow because we cannot adequately test our models or use them to make predictions. This exponential scaling of Hilbert space can only be matched by the increasing possible permutations which make a quantum system twice as memory-full with the addition of each qubit. Recent upsurge of quantum computation, information and quantum technologies aim to exploit these inherent properties of nature. Computational complexities pose restrictions on density functional theory[9] widely used in quantum mechanical modelling[10]. In this paper, we show how a system of total 14 qubits is well capable of observing the time evolution of a particle in a harmonic oscillator potential for two spacial dimensions.

The rest of the paper is organized as follows: Sec. II revisits the harmonic oscillator problem which is analytically solvable and discuss it's solution along with some of it's properties. In Sec. III, the discretization of the problem is discussed, explaining why finite elements and finite dimensional operators are important for computation. The aim of our simulation is to observe the time evolution of harmonic oscillator position eigenstates. Sec. IV deals with the simplification of the unitary operator along with a remarkable observation which allows us to generalize the simulation to arbitrarily higher dimensions along with a oversimplification of the quantum circuit. This section takes us from analytic matrices to realizable quantum gates. Sec. V is completely dedicated to simulation where the 2-qubit, 4-qubit and n-qubit algorithm is explained in detail. The quantum circuit required to implement the simulation has been generalized and discussed in Sec. VI. The detailed results for 2-qubit and 4-qubit simulation are provided in Sec. VII. We conclude in Sec. VIII with future directions.

II. THE HARMONIC OSCILLATOR PROBLEM

The well-known harmonic oscillator potential for two spatial dimensions is given by

$$V(x) = \frac{m\omega^2}{2}(x^2 + y^2)$$

where both $x, y \in (-\infty, \infty)$. The corresponding Hamiltonian is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}(x^2 + y^2) \tag{1}$$

The analytic solution to the time independent Schrodinger equation is given by[11] $\Psi(x, y, t)$

$$= \Sigma_{n_x=0}^{\infty}\Sigma_{n_y=0}^{\infty}(\frac{m\omega}{\pi\hbar})^{\frac{1}{2}}\frac{1}{2^n n!}H_{n_x}(\zeta)H_{n_y}(\beta)e^{-\zeta^2/2}e^{-\beta^2/2}U(t)$$

where $\zeta = \sqrt{\frac{m\omega}{\hbar}}x$ and $\beta = \sqrt{\frac{m\omega}{\hbar}}y$ respectively and H_n are the n-th order Hermite polynomials. The unitary operator of any system gives it's time evolution

$$U(t) = exp(\frac{-\iota E_n t}{\hbar}) \tag{2}$$

It can be observed that the unitary operator suggests the probability amplitude of the particle oscillation in time. An elegant simulation of this can be found in Ref.[12]. E_n are the 'allowed' energy values of the particle. It is only for these energy eigenvalues that the individual energy eigenstates are normalizable, therefore physically realizable. These energy eigenvalues are given by

$$E_n = (n_x + n_y + 1)\hbar\omega$$

. States corresponding to different energy eigenvalues are orthogonal to each other and satisfy

$$\int_{-\infty}^{\infty} \psi_j \ \psi_k \ dx_i = 0 \ ; \ \forall x_i$$

. A simplier way to solve this problem is by factoring the Hamiltonian into two non-commuting operators given by,

$$a_i^- = \frac{1}{\sqrt{2}}(\hat{x_i}^2 + \hat{p_i}^2) \ ; \ a_i^+ = \frac{1}{\sqrt{2}}(\hat{x_i}^2 - \hat{p_i}^2)$$

. Here we assume $\hbar$, m and ω to be unity for the sake of reducing mathematical clutter and i $\in [1, 2]$ co-respond to the spatial dimensions x and y. These operators are famously known as the annihilation and the creation operators which act as wonderful tools to realize states corresponding to unit energy lower or unit energy higher index in the given energy spectrum. The normalized expressions for these are given as

$$a^+\psi_j = \sqrt{j+1} \ \psi_{j+1} \ ; \ a^-\psi_j = \sqrt{j} \ \psi_{j-1}$$

. The time independent Schrodinger equation in terms of the annihilation and creation operators can be written as

$$\hbar\omega(a_1^+ a_1^- + a_2^+ a_2^- + 1)\psi = E\psi$$

.

Our interests however, lie in position eigenfunctions corresponding to 'discrete' position eigenvalues. The reason for discretization will be explained subsequently. These eigenfunctions of position can be found by solving the eigenvalue equation for position operator

$$\hat{x} \ \psi = x_0 \ \psi$$

, where $\hat{x}$ is the operator and x_0 is the eigenvalue. To satisfy this, we need a function which on multiplying with a variable gives the variable scaled by the number itself. One such function that satisfies this property is the Dirac delta function. To make an analogy with spectral decomposition theorem, we can expand any arbitrary function as a linear combination of Dirac-Delta functions corresponding to different eigenvalues. All we need to do is find the correct constants. We conclude therefore the position eigenfunctions are Dirac-delta function

$$f_x(x) = A \ \delta(x - x_0)$$

. For a discrete eigenspectrum the spectral decomposition will be given by,

$$\Psi(x) = \Sigma_0^N c_n \ \delta(x - x_0)$$

, where N is the total number of discrete elements taken into account. According to the expansion postulate $|c_n|^2$ gives the 'the probability of the state $\Psi(x)$ to collapse onto ψ_n upon a measurement. The coefficients can be calculated by exploiting the orthogonality of different states

$$c_n = \int_{\infty}^{-\infty} (\Sigma_0^N \ c_m \ \psi_m) \ \psi_n \ dx_i$$

$$= \int_{\infty}^{-\infty} (\Psi(x)) \ \psi_n \ dx_i$$

III. DISCRETIZATION OF THE PROBLEM

In order to do any computation, we need to work with finite number of elements which can yield results under realistic time scales. However, the Hamiltonian given in Eq. (1) allows for a continuous eigenspectrum of position. To tackle this problem, we need to 'discretize space'. This becomes the essence of the simulation. It implies that we have to account the probability amplitudes in elements of finite width rather than each and every space point. This creates a mesh in space which can be mapped over our potential 'bowl'. An intuitive picture can be grasped by Figs. 1 and 2.

The Hamiltonian for the 'discrete harmonic oscillator' can now be given by

$$\hat{H} = \frac{(\hat{p}^d)^2}{2} + \frac{((\hat{x}^d)^2 + (\hat{y}^d)^2)}{2} \tag{3}$$

where $\hat{p}^d$ is the discrete momentum operator and $\hat{x}^d, \hat{y}^d$ are the discrete position operators in x and y spatial coordinates respectively. If we consider N number of finite elements in a space of $x, y \in [-L, L]$ then a mesh of N^2 number of finite spatial elements can be created with each mesh point corresponding to a particular eigenvalue of x and y. Assuming the harmonic oscillator potential is centred at [0,0] we can create the position operator in the form of an N × N matrix with all the position eigenvalues lying along it's diagonal[13].

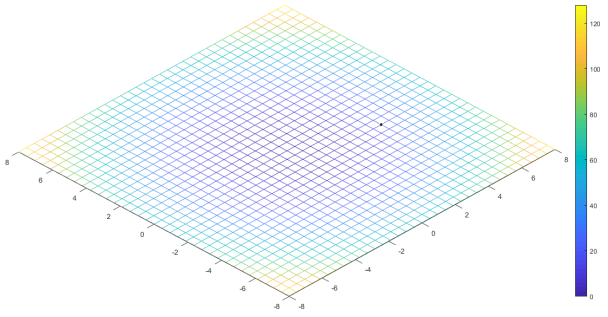

FIG. 1. Discrete two dimensional space. The colour bar indicates the amount of *stretch* required to map these points to harmonic oscillator potential.

$$\hat{x}^d = \sqrt{\frac{\pi}{2N}} \begin{pmatrix} -N/2 & 0 & 0 & . & . & 0 \\ 0 & (-N/2)+1 & 0 & . & & 0 \\ 0 & . & . & & & . \\ 0 & . & & . & & 0 \\ 0 & . & & & . & 0 \\ 0 & . & & . & 0 & (N/2)-1 \end{pmatrix} \tag{4}$$

All position operators act multiplicatively in Cartesian co-ordinate space. The operator for $(x^d)^2$ can also be calculated directly by multiplying x^d with itself. We can calculate the momentum operator in a similar manner. However, the momentum operators do not act multiplicatively. Also we have already expanded our total wavefunction in an eigenspectrum of position eigenfunctions. Calculating the momentum eigenvalues for each position eigenfunction can be a laborious task for large systems. A much more efficient approach needs to be taken to make a discrete quantum Fourier transform of the wave function. This takes the wave function to momentum space where the momentum operators act multiplicatively and the momentum eigenvalues will be the same as the position eigenvalues for respective discretized space points. An inverse discrete quantum Fourier transform can be done to bring back the function into Cartesian-space. The momentum operator can then be applied as a N × N matrix given by

$$p^d = (F^d)^{-1} \cdot x^d \cdot F^d \tag{5}$$

where F^d stands for standard discrete quantum Fourier transform matrix[14]. Each element of the matrix can be given by

$$[F^d]_{j,k} = \frac{exp(\iota 2\pi jk/N)}{\sqrt{N}}$$

. This approach is ideal as implementation of Q.F.T using quantum circuits is generalized for n-qubits and only gets more and more accurate for larger systems[13]. With both the position and momentum operators at hand we are now ready to simulate the unitary operator to study the time evolution of our system.

IV. UNITARY OPERATOR

From the Schrodinger's equation

$$\iota\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$$

implying

$$\Psi(t) = \Psi(0)exp(-\iota\hat{H}t)$$

. Therefore the unitary operator that we need to evaluate is $U(t) = exp(-\iota\hat{H}^d t)$ where $\hat{H}^d$ is the discretized Hamiltonian given in Eq. (3). The unitary operator is then given by

$$U(t) = exp(-\iota t[\frac{(\hat{p}^d)^2}{2} + \frac{(\hat{x}^d)^2 + (\hat{y}^d)^2}{2}])$$

$$U_x(t) = exp[\frac{-\iota t}{2}((F^d)^{-1} \cdot [x^d]^2 \cdot F^d) + [x^d]^2]$$

, where $U_x(t)$ is the unitary operator in x dimension. The position operator$[x^d]$ being a diagonal matrix can be expanded using the matrix exponential. Also having a finite number of elements it's expansion will be convergent

$$exp(\frac{-\iota t}{2}[A]) = \mathbb{I} + \Sigma_{m=1}^{\infty}(\frac{-\iota t}{2})^m \frac{[A]^m}{m!} \tag{6}$$

where A is the corresponding operator matrix. Using the matrix in this form, a time evolution can be performed for any arbitrary state. Such an evolution can be carried out using n-qubits in a quantum circuit. We generalize our simulation as well as the quantum circuit for n-qubits in the following section.

V. SIMULATION

Our simulation will be utilizing 4 qubits for each spatial dimension. For 4 qubits we are taking into account a $2^4 = 16$ dimentional Hilbert space. Each dimension of the Hilbert space corresponds to eigenfunction of a specific position eigenvalue. Each basis state of the 4 qubit system maps to an eigenfunction in the Hilbert space. **This is the essence of our simulation:** the probability distribution of each qubit state obtained after implementing the quantum circuit will correspond *one to one* with the probability distribution of each eigenfunction after the unitary operation. Allowing us to study the time evolution of the particle in terms of the time evolution of the qubit basis states. For two spatial dimensions our $x, y \in [-8, 8]$ space discretizes into 16 × 16 = 256 individual mesh point. Each point corresponds to

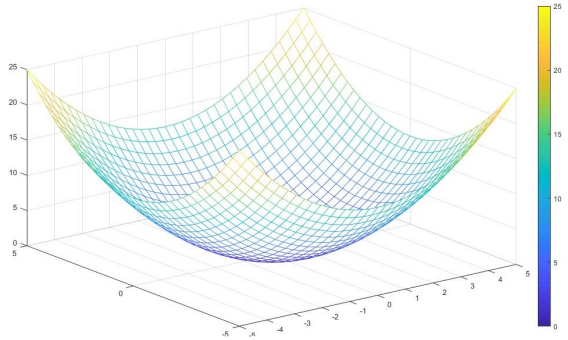

FIG. 2. Mapping the mesh of discrete space over that harmonic oscillator potential. This gives us an intuitive picture of the potential energy of the particle at particular space points.

different eigenvalues in x and y spatial dimensions. We can now evaluate the unitary operator in it's matrix form in order to construct quantum gates which can be later implemented in the quantum circuit. According to Eq. (4) the position operator is a diagonal matrix.

$$[x^d] = \sqrt{\frac{\pi}{32}} \begin{bmatrix} -8 & 0 & \dots & 0 \\ 0 & 7 & \ddots & \vdots \\ \vdots & \ddots & 6 & 0 \\ 0 & \dots & 0 & 7 \end{bmatrix}$$

Therefore the square of the operator will be a diagonal matrix with all eigenvalues squared. The kinetic energy operator will then be given by

$$[x^d]' = [x^d]^2 = \frac{\pi}{32} \begin{bmatrix} 64 & 0 & \dots & 0 \\ 0 & 49 & \ddots & \vdots \\ \vdots & \ddots & 36 & 0 \\ 0 & \dots & 0 & 49 \end{bmatrix}$$

From Eq. (6), we can write the unitary operator for potential energy part as

$$U_{\hat{x}}(t) = \mathbb{I} + (\frac{-\iota t}{2})\frac{[x^d]'}{1} + (\frac{-\iota t}{2})^2\frac{[x^d]'^2}{2!} + (\frac{-\iota t}{2})^3\frac{[x^d]'^3}{3!} + \dots.$$

A remarkable observation reveals each diagonal element of U(t) makes an exact Taylor series expansion of an exponential function with symmetry about the [8,8] element which will be unity

$U_{\hat{x}}[1,1]$	$1.0 + 3.14it - 4.963t^2 + 5.17it^3$	$exp(3.14\iota t)$
$U_{\hat{x}}[2,2]$	$1.0 - 2.4it - 2.89t^2 - 2.32it^3$	$exp(-2.4\iota t)$
$U_{\hat{x}}[3,3]$	$1.0 - 1.77it - 1.56t^2 + 0.92it^3$	$exp(-1.77\iota t)$
$\vdots$	$\vdots$	$\vdots$
$U_{\hat{x}}[15,15]$	$1.0 - 1.77it - 1.56t^2 + 0.92it^3$	$exp(-1.77\iota t)$
$U_{\hat{x}}[16,16]$	$1.0 - 2.4it - 2.89t^2 + 2.32it^3$	$exp(-2.4\iota t)$

(7)

$$U_{\hat{x}}(t) = \begin{bmatrix} e^{(\iota t * 3.14)} & 0 & \dots & \dots & 0 \\ 0 & e^{(-\iota t * 2.4)} & & & \vdots \\ . & \ddots & \ddots & \ddots & . \\ \vdots & & & e^{(-\iota t * 1.77)} & 0 \\ 0 & \dots & 0 & & e^{(-\iota t * 2.4)} \end{bmatrix}$$

We can now implement these different phases in a quantum circuit independently. Taking the [1,1] element a common multiple which will act as a global phase, we can write the unitary operator in the final form

$$U_{\hat{x}}(t) = e^{(\iota t * 3.14)} \begin{bmatrix} 1 & 0 & \dots & \dots & 0 \\ 0 & e^{(-\iota t * 5.54)} & & & \vdots \\ . & \ddots & \ddots & \ddots & . \\ \vdots & & & e^{(-\iota t * 4.91)} & 0 \\ 0 & \dots & 0 & & e^{(-\iota t * 5.54)} \end{bmatrix}$$

The benefit of this approach lies in the first element being unitary. The first basis of our four qubit system $|0000\rangle$ is incapable of picking up any phase term inadvertently. The rest of the diagonal terms will provide phase to the next 15 basis states in the sequence. The unitary operator for the kinetic energy can be formulated in a similar manner by making subsequent quantum Fourier transforms as explained in Eq. (5). The complete unitary transformation can be given by

$$U(t) = exp[(\frac{-\iota t}{2})(\hat{p_x}^2 + \hat{p_y}^2 + \hat{x}^2 + \hat{y}^2)] = U_{\hat{x}} \cdot U_{\hat{y}} \cdot U_{\hat{p_x} \cdot U_{\hat{p_y}}} \tag{8}$$

Both spatial dimensions being orthogonal to each other will follow the same mathematical structure independently. The position and momentum operators for orthogonal spacial dimensions commute. Hence we can generalize our algorithm to calculate the unitary operator for arbitrary spacial dimensions. The calculation of unitary operator for n qubits is given in the appendix below. We propose a generalized circuit to carry out the unitary operator for any arbitrary state using any arbitrary number of qubits, therefore making the approach complete.

VI. QUANTUM CIRCUIT

The complete unitary transformation given in Eq. (8) can be implemented by making a circuit for $U_{\hat{x}}(t)$ and $U_{\hat{p}}(t)$ in series. Since the $U_{\hat{x}}(t)$ only adds phase factors we will first implement the $U_{\hat{p}}(t)$. The quantum circuit for quantum Fourier transform can be executed using a series of Hadamard and control-phase rotation gates. An efficient circuit for 4-qubit system is given in Fig. 3,

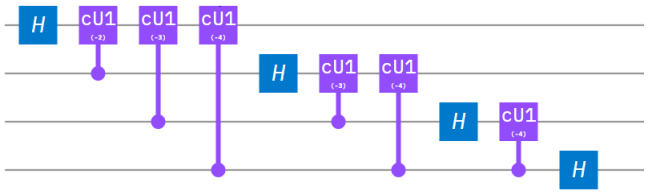

FIG. 3. An efficient quantum circuit for implementing the quantum Fourier transform.

where the phase of individual rotation gates can be calculated using

$$cU1_n = \frac{2\pi}{2^n}$$

The single qubit control-rotation gate would be matrices of the form

$$cU1_n = \begin{bmatrix} 1 & 0 \\ 0 & e^{2\pi\iota/2^n} \end{bmatrix} \tag{9}$$

For implementing the inverse quantum Fourier transform the mirror image of the direct Q.F.T circuit with conjugate phases at each c-rotation gate can be used (Fig. 4). In the middle of $[(F^d)]^{-1}$ and $[F^d)]$ lies the chief operator $[x^d]$ which can be implemented using a series of Toffolli and control-rotation gates. The crucial algorithm that can be executed is explained as follows: for each 4-qubit state we use a control gate for the qubit in $|1\rangle$ state and an anti-control for the qubit in the $|0\rangle$ state. Three ancilla qubits along with three cc-not gates are used to infer the states of all 4 qubits. This series of control and anti-control gates will simultaneously trigger only for a specific sequence of $|0\rangle$ and $|1\rangle$ states assuring a particular 4-qubit state has infiltrated. Now we can trigger the c-rotation gate calibrated to the phase corresponding to that particular 4-qubit state. This phase rotation can be performed at anyone of the qubits in $|1\rangle$ state. A mirror sequence of Toffolli gates after the c-rotation gate can be used to reverse all effects prior to our *filtering*. This makes the arbitrary 4-qubit state ready for the next series of Toffolli gates while the crucial phase information has also been imparted. Each set of filter prepares the state for the next set of filter and a series of 15 such filters can be used recursively to implement all 15 phase rotations to achieve complete $U_{\hat{x}}(t)$. A filter for the first state $|0001\rangle$ has been shown in Fig. 5.

A simpler circuit can be designed by realizing the same logic for a 2-qubit system. Analogues to the 4-qubit system the unitary matrix for a 2-qubit system will also have diagonal elements as the squared position eigenvalues. Without making any approximation, we observe the elements form a Taylor exponential series.

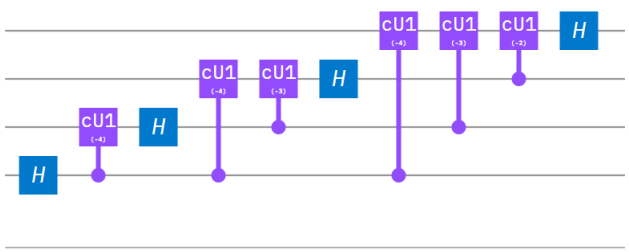

FIG. 4. The mirror image of Q.F.T circuit which conjugate phases to implement the inverse quantum Fourier transform.

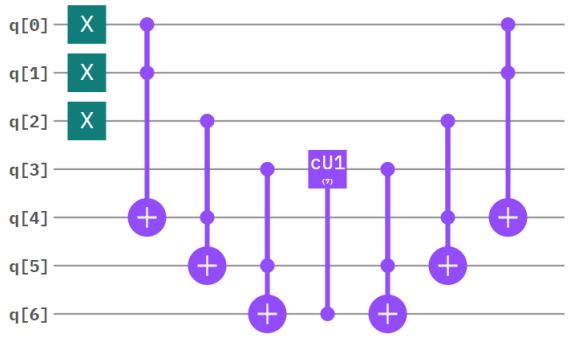

FIG. 5. A filter for the $|0001\rangle$ state which detects the state of all 4 qubits then performs a rotation on the 4^{th} qubit. The series of Toffolli gates after cU1 reverses all changes done to the initial state.

$$U^{[2]}_{\hat{x}}(t) = \begin{bmatrix} e^{-\iota t*0.785} & 0 & 0 & 0 \\ 0 & e^{-\iota t*0.196} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{-\iota t*0.196} \end{bmatrix} \tag{10}$$

We can take out the first element as a global phase. This will give us the first element as unity.

$$U^{[2]}_{\hat{x}}(t) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-\iota t*0.981} & 0 & 0 \\ 0 & 0 & e^{-\iota t*0.785} & 0 \\ 0 & 0 & 0 & e^{-\iota t*0.981} \end{bmatrix} \tag{11}$$

The quantum Fourier transform in 2 dimensions can be executed by two Hadamard and one control-rotation gate. The inverse Q.F.T can be executed by it's mirror image circuit with conjugate phase in the rotation gate. For two qubit system we will have 3 filters for $|01\rangle, |10\rangle$ and $|11\rangle$ respectively. A detailed figure is provided (Fig. 6) where two U3 gates can be used to initialize the system to any arbitrary state. We can use the same logic to propose a circuit which is generalized for n-qubits. Starting with the generalized circuit for the Fourier transform[15] for n qubits is given in Fig. 7. The inverse quantum Fourier transform can be given by the mirror image circuit and conjugate phases at the c-rotation gates. The position operator $[x^d]$ for n-qubits

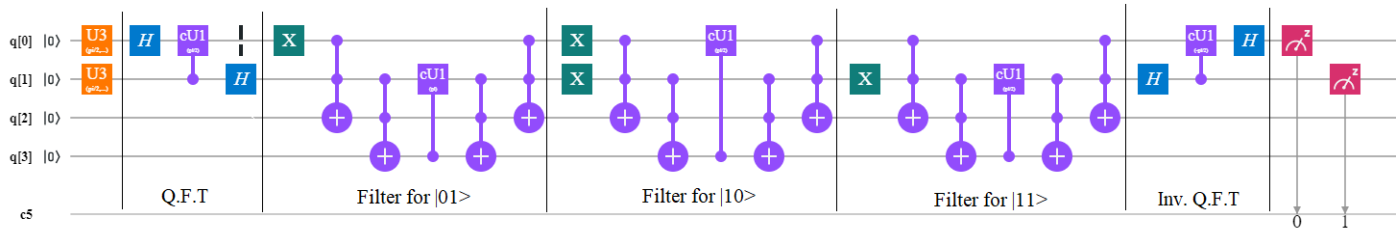

FIG. 6. Quantum circuit for implementing $U_{\hat{p}}(t)$ for a 2-qubit system.

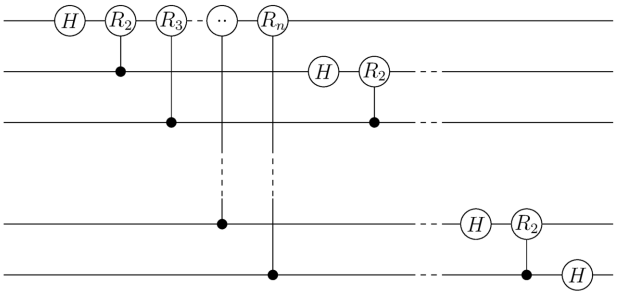

FIG. 7. A generalized quantum circuit for quantum Fourier transform of n-qubit system.

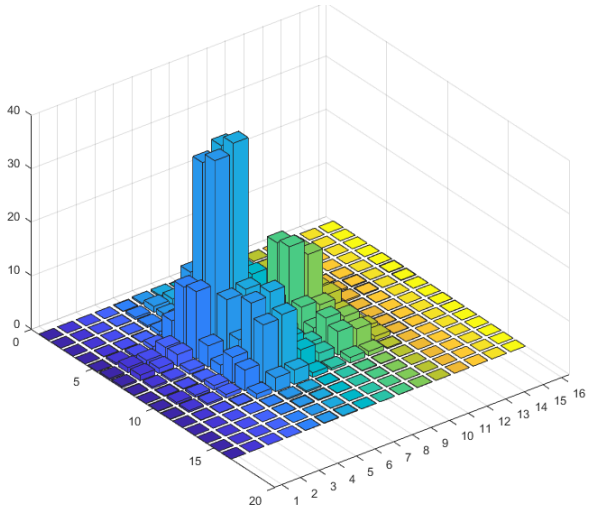

FIG. 8. A representation of cross multiplication of probability amplitudes at $t = \frac{T}{4}$, where T is total time period of oscillation.

will be a diagonal matrix with 2^n position eigen values each lying on the diagonal. The exponential expansion of the unitary operator gives a Taylor exponential series in each diagonal element. Inductively, each element will have a constant phase difference and therefore the system with n-parameters can be expressed using a single parameter. Hence, without any approximation we can create $[x^d]$ for a n-qubit system. The quantum circuit for n qubits can be implemented using the same algorithm proposed above; by placing control gates and anti-control gates on $|1\rangle$ and $|0\rangle$ respectively. Then sending the state information of n^{th} qubit to the $(n-1)^{th}$ ancilla in order to trigger the desired phase rotation gate on the required qubit only. This phase rotation will happen only for a particular state of n-qubits based on our filter configurations. A series of mirrored Toffolli gates can be used to undo all changes done by the filter. The qubits then can proceed to the next filter afresh. A series of (n-1) such filters are required to execute $U_{\hat{x}}^{[n]}$. Another series of (n-1) such filters when squeezed between the Q.F.T and inverse Q.F.T gates can be used to execute $U_{\hat{p}}^{[n]}$.

When we initialize our qubits to a particular state we provide large probability to a particular eigenvalue of the particle. According to our initialized state the position of the particle can be considerably pin-pointed to any of the corresponding mesh points. The quantum circuit then simulates the unitary operator to give time evolution of the particle in terms of time evolution of the probability amplitude for different eigenvalues. These eigenvalues probabilities map one to one with the corresponding probabilities of the qubit basis states. Multiple simulations with the variation of time parameter t are carried out until multiple identical oscillations of the particle are observed. Each individual simulation is carried out on *ibmq qasm simulator* with 8192 shots to give the best possible ensemble. In this simulation we divide the space of $x, y \in [-8, 8]$ $unit^2$ into 256 mesh points. A table of 4-qubit states and their corresponding mesh points are given in Eq. (12).

4-qubit state	Mesh point
$\|0000\rangle$	$x_i = -8$
$\|0001\rangle$	$x_i = -7$
$\|0010\rangle$	$x_i - 6$
$\vdots$	$\vdots$
$\|1111\rangle$	$x_i = 7$

(12)

VII. RESULTS

We are therefore capable of executing the unitary operation of a particle in a harmonic oscillator potential for any arbitrary number of qubits. The more number of qubits we take the denser is our spatial mesh resulting in further accuracy. We also become capable of performing the unitary operation for arbitrary spatial dimensions by executing 2n-1 qubit circuits in parallel for each dimension.
The results for a single oscillation of the particle for a 2-qubit and 4-qubit system are presented in Figs. 9, 10 and 11, 12 respectively where we initialize our state to $|0001\rangle$. A *cross multiplication* of both data sets presents an intuitive picture for the probability amplitudes in two spatial dimensions. One such representation is given in Fig. 8. The URL for a simple animation based on our data is cited below[16].

VIII. CONCLUSION

We infer from the experimental results that the probability amplitude of a particle in a harmonic oscillator potential oscillate in time mimicking the essence of a quantum harmonic oscillator. The probability amplitudes of two spatial dimensions are independent of each other which was expected for two non-commuting variables. The simulation helps us to understand the movement of a particle in such a potential intuitively. The change in probability amplitudes over time helps us comprehend the concept of velocity in the quantum realm. Ultimately, the simulation can be generalized for arbitrary spatial dimensions. The simulation can also be carried out using arbitrary number of qubits to make it more meticulous.

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[1] Quantum Harmonic Oscillator, en.wikipedia.org/wiki/Quantum_harmonic_oscillator#N-dimensional_harmonic_oscillator
[2] D. J. Kouri and C. A. Wells, Comparisons of Morse and harmonic oscillator models for vibration-rotation excitation of H_2 by Li^+, J. Chem. Phys. **60**, 2296 (1974).
[3] H. Bilz, Lattice Vibrations. In: S. Nudelman, S.S. Mitra (eds), Optical Properties of Solids, Optical Physics and Engineering, Springer (1969).
[4] T. Fujimoto, K. Miyazaki, and K. Fukuda, Measurement of population density of excited helium atoms by the hook method, J. Quant. Spectr. Rad. Trans. **14**, 377 (1974).
[5] M. Campisi, P. Hanggi, and P. Talkner, Colloquium. Quantum Fluctuation Relations: Foundations and Applications, Rev. Mod. Phys. **83**, 771 (2011).
[6] R. P. Feynman, Simulating Physics with Computers, Int. J. Theor. Phys. **21**, 467 (1982).
[7] D. Deutsch, Quantum theory, the Church-Turing principle and the universal quantum computer, Proc. R. Soc. Lond. A **400**, 1818 (1985).
[8] M. Troyer and U.-J. Wiese, Computational Complexity and Fundamental Limitations to Fermionic Quantum Monte Carlo Simulations, Phys. Rev. Lett. **94**, 170201 (2005).
[9] https://en.wikipedia.org/wiki/Density_functional_theory
[10] N. Schuch and F. Verstraete, Computational complexity of interacting electrons and fundamental limitations of density functional theory, Nat. Phys. **5**, 732 (2009).
[11] D. J. Griffiths, Introduction to Quantum Mechanics, Pearson Prentice Hall (2004).
[12] Harmonic Oscillator, URL:www.physics.weber.edu/schroeder/software/HarmonicOscillator.html
[13] R. D. Somma, Quantum simulations of one dimensional quantum systems, Quantum Inf. Comput. **16**, 1125 (2016).
[14] Quantum Fourier Transform, URL:https://en.wikipedia.org/wiki/Quantum$_$Fourier$_$transform
[15] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information, CAMBRIDGE UNIVERSITY PRESS, (2010).
[16] Dynamics of 2-qubit Harmonic Oscillator, URL:DOI:10.13140/RG.2.2.15777.15201
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APPENDIX

The Unitary operator for a n-qubit system can be calculated as follows;
The position operator for n-qubits will have $2^n = N$ dimensional Hilbert space. The operator is given by Eq. (4)

FIG. 9. Probability amplitudes over the first half of the Oscillation cycle for a 2-qubit simuation.

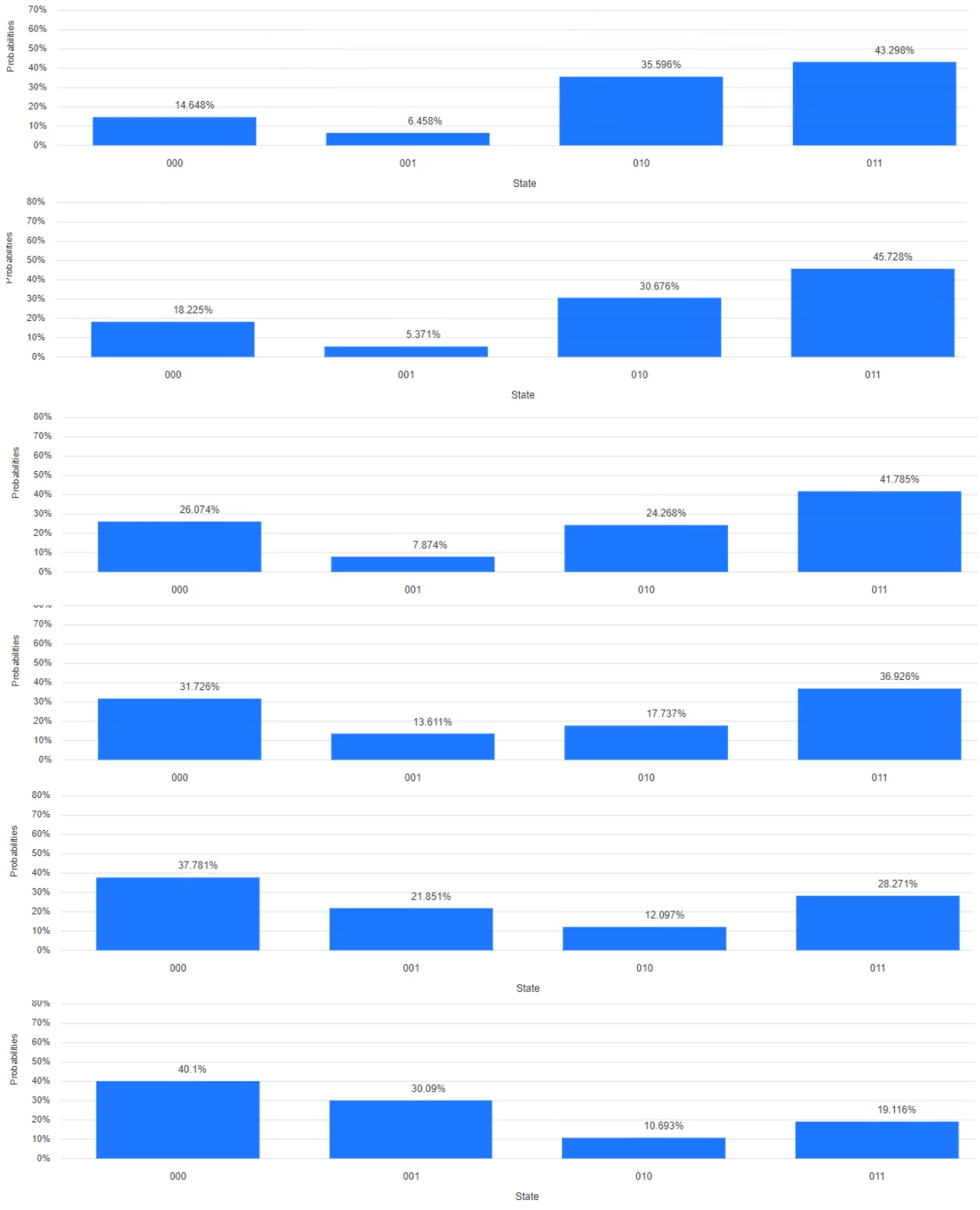

FIG. 10. Probability amplitudes over the second half of the Oscillation cycle for a 2-qubit simulation.

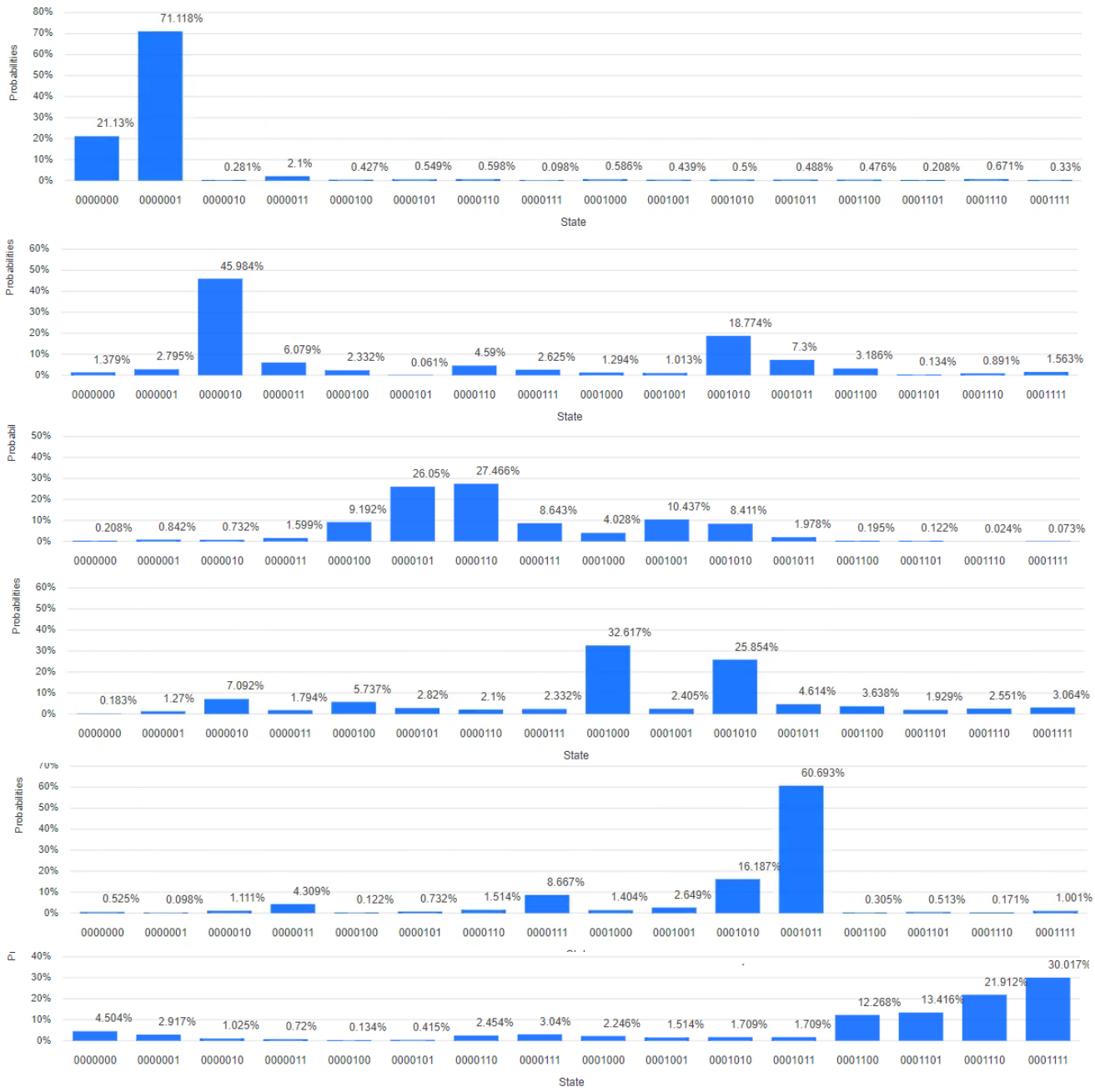

FIG. 11. Probability amplitudes over the second half of the Oscillation cycle for a 4-qubit simualtion.

$$\hat{x}^d = \sqrt{\frac{\pi}{2N}} \begin{pmatrix} -N/2 & 0 & 0 & . & . & 0 \\ 0 & (-N/2)+1 & 0 & . & & 0 \\ 0 & . & . & & & . \\ 0 & . & & . & & 0 \\ 0 & . & & & . & 0 \\ 0 & . & & . & 0 & (N/2)-1 \end{pmatrix} \tag{13}$$

$$[\hat{x}^d]' = \frac{\pi}{2N} \begin{pmatrix} (-N/2)^2 & 0 & 0 & . & . & 0 \\ 0 & ((-N/2)+1)^2 & 0 & . & & 0 \\ 0 & . & . & & & . \\ 0 & . & & . & & 0 \\ 0 & . & & & . & 0 \\ 0 & . & & . & 0 & ((N/2)-1)^2 \end{pmatrix} \tag{14}$$

The square of the operator will be given by

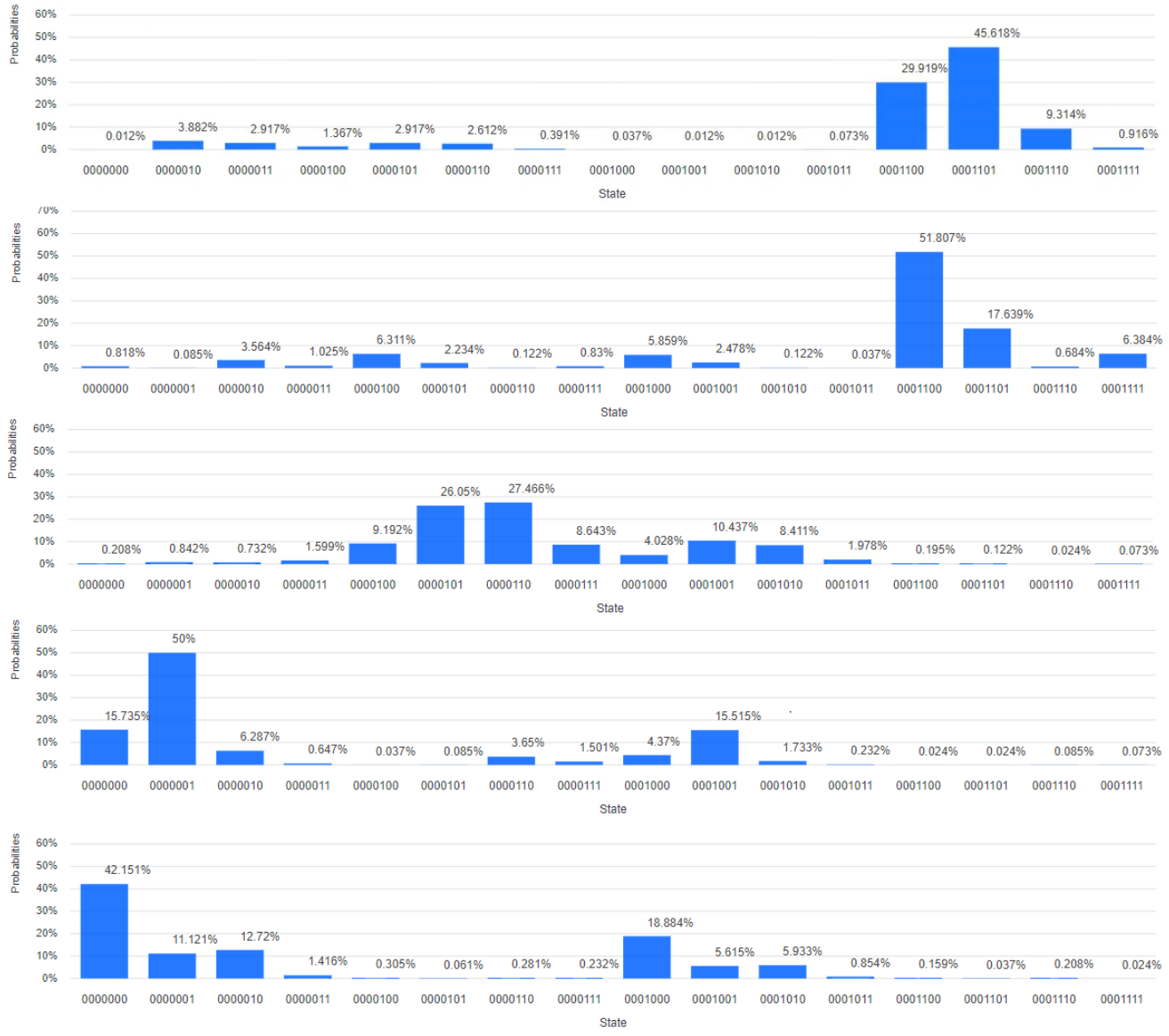

FIG. 12. Probability amplitudes over the second half of the Oscillation cycle for a 4-qubit simulation.

The Unitary operator will then be evaluated as

$$U_{\hat{x}}(t) = exp[\frac{-\iota[x^d]'^2 t}{2}]$$

Which can be expanded using (Eq. (6)) as

$$exp(\frac{-\iota t}{2}[x^d]') = \mathbb{I} + \Sigma_{m=1}^{\infty}(\frac{-\iota t}{2})^m \frac{[x^d]'^m}{m!} \tag{15}$$

After expanding we get

$$U_{\hat{x}}(t) = \mathbb{I} + (\frac{-\iota t}{2})\frac{[x^d]^2}{1} + (\frac{-\iota t}{2})^2\frac{[x^d]^4}{2!} + (\frac{-\iota t}{2})^3\frac{[x^d]^6}{3!} + ...$$

We ignore the $\frac{\pi}{2N}$ factor for reducing mathematical clutter and write the individual elements of the Unitary matrix in the table below

$U_{\hat{x}}[1,1]$	$1 - \frac{\iota t}{2}(\frac{-N}{2})^2 + \frac{\iota^2 t^2}{4}\frac{1}{2}(\frac{-N}{2})^4 - \frac{\iota^3 t^3}{8}\frac{1}{6}(\frac{-N}{2})^6 + ...$
$U_{\hat{x}}[2,2]$	$1 - \frac{\iota t}{2}(\frac{-N}{2}+1)^2 + \frac{\iota^2 t^2}{4}\frac{1}{2}(\frac{-N}{2}+1)^4 + ...$
$U_{\hat{x}}[3,3]$	$1 - \frac{\iota t}{2}(\frac{-N}{2}+2)^2 + \frac{\iota^2 t^2}{4}\frac{1}{2}(\frac{-N}{2}+2)^4 + ...$
$\vdots$	$\vdots$
$U_{\hat{x}}[N,N]$	$1 - \frac{\iota t}{2}(\frac{N}{2}-1)^2 + \frac{\iota^2 t^2}{4}\frac{1}{2}(\frac{N}{2}-1)^4 + ...$

Clearly, each element is a Taylor exponential expansion and the unitary matrix can be written as,

$$U_{\hat{x}}(t) = \begin{bmatrix} e^{(-\frac{\iota t}{2}(\frac{-N}{2})^2)} & 0 & \dots & 0 \\ 0 & e^{(-\frac{\iota t}{2}(\frac{-N}{2}+1)^2)} & & \vdots \\ . & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & e^{(-\frac{\iota t}{2}(\frac{-N}{2}-1)^2)} \end{bmatrix}.$$

We may now substitute the value of N=4 for 2-qubit system and N=16 for 4-qubit system to cross check the results. We can also take out the first element as a common multiplicative factor which acts as the global phase. This makes the first element unity as for N-dimensional system the first basis $|000....0\rangle$ is incapable of picking up any phase howbeit. We then observe a symmetry in the m^{th} and $(N-m+2)^{th}$ element. This is in accord with the calculations shown for 2-qubit and 4-qubit systems above.