Quantum Simulation of N Harmonic Oscillators via gray code and one hot encoding

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Abstract

A Quantum computer is a specialized computer that uses quantum bits instead of normal bits. This makes a quantum computer a natural tool to carry out simulation of quantum system as this problem is too difficult to solve on a classical computer. In this report, we establish two schemes to simulate bosonic systems like the quantum harmonic oscillator on a quantum computer. We will also be looking at an algorithm to map the exponential of a Hamiltonian, which is a linear combination of Pauli operators to single qubit and two qubit gates. And finally, we will simulate a system of coupled oscillators and analyze the results of the simulation by plotting expectation values of observables such as position, momentum, and energy.

1 Introduction

To simulate any system, one needs to understand how the system changes over time. In quantum mechanics, we are interested in analyzing the time evolution of the initial state of the system. The time evolution operator is given by $e^{i\hat{H}t/\hbar}$, and its action on a state is as follows:

$$|\psi(t)\rangle = e^{i\hat{H}t/\hbar}|\psi(0)\rangle \tag{1}$$

Once $|\psi(t)\rangle$ is obtained, expectation values of required observables can be computed to know how they are varying with time as follows:

$$\langle\hat{H}\rangle = \langle\psi(t)|\hat{H}|\psi(t)\rangle \tag{2}$$

So in all these steps, computing the matrix representation of the time evolution operator $e^{iHt/\hbar}$ is very challenging because, in general, H is comprised of the sum of multiple operators and as these operators usually don't commute, we can't write the exponential of the sum as the product of exponentials. Another challenge is computing the exponential of these individual operators, which can be represented as matrices, we can use quantum computing to compute this exponential quickly if the Hamiltonian is in a linear combination of Pauli terms. We will discuss the algorithm used by OpFlow module of qiskit to compute the same. For the specific case of Quantum Harmonic Oscillator (QHO), we will be providing two schemes to map the Hamiltonian and its eigenstates onto the qubit Hamiltonian which is in terms of Pauli matrices whose exponential can be simulated efficiently. The first scheme is mapping the occupation number basis to its corresponding one-hot encoding in the Z basis that is, $|0\rangle$, $|1\rangle$, $|2\rangle$ and $|3\rangle$ are mapped to $|1000\rangle$, $|0100\rangle$, $|0010\rangle$ and $|0001\rangle$. The second scheme is the same but the occupation number basis is mapped to its corresponding gray code that is, $|0\rangle$, $|1\rangle$, $|2\rangle$ and $|3\rangle$ are mapped to $|00\rangle$, $|01\rangle$, $|11\rangle$ and $|10\rangle$. We will be discussing the simulation for both of these mappings in detail and we will be looking at the results of the simulation by plotting the expectation values of the observables such as position, momentum, and energy. And finally we will also be looking at N-coupled oscillators.

2 Analytical solution of the Quantum Harmonic oscillator

In this section, we will demonstrate an elegant solution[1] to the quantum harmonic oscillator with which we can calculate the energy eigenvalues without calculating the corresponding eigenvectors. The

Hamiltonian of SHO is given by:

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \tag{3}$$

which can we re-written in terms of $\hat{p}$ and $\hat{x}$ operators as:

$$\hat{H} = \frac{1}{2m}(\hat{p}^2 + (m\omega\hat{x})^2) \tag{4}$$

Inspired from the following property of numbers,

$$u^2 + v^2 = (iu + v)(-iu + v)$$

we define two non-hermitian operators called *annihilation* and *creation* operators $\hat{a}$ and $\hat{a}^\dagger$ as (note that hats will be dropped from operators wherever there is no ambiguity):

$$\hat{a} = \sqrt{\frac{m\omega}{2A}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right), \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2h}}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right) \tag{5}$$

Commutator of both the operators is given by

$$\left[a, a^\dagger\right] = \left(\frac{1}{2h}\right)(-i[x,p] + i[p,x]) = 1 \tag{6}$$

a hermitian operator called *number* operator can be defined as

$$a^\dagger a = N \tag{7}$$

then,

$$\begin{aligned} a^\dagger a &= \left(\frac{m\omega}{2\hbar}\right)\left(x^2 + \frac{p^2}{m^2\omega^2}\right) + \left(\frac{i}{2\hbar}\right)[x,p] \\ &= \frac{H}{\hbar\omega} - \frac{1}{2} \end{aligned} \tag{8}$$

from this, it can be noted that the number operator and Hamiltonian have simultaneous eigenstates so, Hamiltonian in can be represented in terms of number operator as

$$H = \hbar\omega\left(N + \frac{1}{2}\right) \tag{9}$$

say eigenvalue of N is n, and we can represent the corresponding eigenstate (which is also energy eigenstate) as $|\psi_n\rangle$ then,

$$N|\psi_n\rangle = n|\psi_n\rangle \tag{10}$$

this implies that

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{11}$$

now all that remains is to find the range of n, to do this we will analyse the action of a, $a^\dagger$ operators on the energy eigenstate $|\psi_n\rangle$ for that, consider the following commutator

$$[N, a] = \left[a^\dagger a, a\right] = a^\dagger[a, a] + \left[a^\dagger, a\right]a = -a \tag{12}$$

similarly,

$$[N, a^\dagger] = a^\dagger \tag{13}$$

now consider the action of N on the states $a^\dagger|\psi_n\rangle$ and $a|\psi_n\rangle$

$$\begin{aligned} Na^\dagger|\psi_n\rangle &= \left(\left[N, a^\dagger\right] + a^\dagger N\right)|\psi_n\rangle \\ &= (n+1)a^\dagger|\psi_n\rangle \end{aligned} \tag{14}$$

and

$$\begin{aligned} Na|\psi_n\rangle &= ([N, a] + aN)|\psi_n\rangle \\ &= (n-1)a|\psi_n\rangle. \end{aligned} \tag{15}$$

the Eqn. (14) and Eqn. (15) show that $a^\dagger|\psi_n\rangle$ and $a|\psi_n\rangle$ are eigenstates of N but with eigenvalues decreased and increased by one respectively, this is why $a^\dagger$ and a are called creation and annihilation operators respectively, they increase and decrease decrease the energy of system respectively. These are also called as the *ladder* operators of the same reason, this implies

$$a|\psi_n\rangle = c|\psi_{n-1}\rangle \tag{16}$$

where c is the normalisation constant and can be computed as follows

$$\langle\psi_n|a^\dagger a|\psi_n\rangle = |c|^2\langle\psi_{n-1}|\psi_{n-1}\rangle \tag{17}$$

as the eigenstates can be assumed to be orthonormal and from Eqn. (10), we can rewrite the above equation as

$$\langle\psi_n|N|\psi_n\rangle = |c|^2 \Rightarrow n = |c|^2 \tag{18}$$

therefore,

$$a|\psi_n\rangle = \sqrt{n}|\psi_{n-1}\rangle \tag{19}$$

similarly, it can be shown that

$$a^\dagger|\psi_n\rangle = \sqrt{n+1}|\psi_{n+1}\rangle \tag{20}$$

successive action of a and $a^\dagger$ on an eigenstate will bring it back to same state but multiplied with a constant n, from this it can be understood that the number operator $N = a^\dagger a$ just gives the index of energy eigenstate $|\psi_n\rangle$

$$N|\psi_n\rangle = a^\dagger a|\psi_n\rangle = \sqrt{n}a^\dagger|\psi_{n-1}\rangle = n|\psi_n\rangle$$

so, all possible values that n can take depends on possible values of energy, to analyse that, we can consider the action of a on $|\psi_0\rangle$, it is easy to see that

$$a|\psi_0\rangle = 0 \tag{21}$$

this implies that for $n = 0$ the energy is minimum so, $|\psi_0\rangle$ is the groundstate of SHO, similarly $|\psi_1\rangle$ is the first excited state, $|\psi_2\rangle$ is the second excited state and so on, so the $n = 0, 1, 2...\infty$. So, from Eqn.

(11) the energy of SHO is given by,

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, n = 0, 1, 2...\infty \tag{22}$$

2.1 Matrix Representation of Operators

In this section, we will be representing all the relevant operators in matrix form in the occupation number basis. We can represent the eigenvectors of the Number operator as unit vectors. The first few are written:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}.$$

All the eigenkets are of infinite dimension and that they are orthonormal. The Hamiltonian has the unit vectors as the eigenstate. Therefore, Hamiltonian must be diagonal with eigenvalues on the main diagonal:

$$\hat{H} = \hbar\omega \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 3/2 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 5/2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 7/2 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 9/2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

By using Eqn.(19) and Eqn.(20) we can find the matrix representation of the annihilation and creation operator,

$$\hat{a} = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\hat{a}^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Since we have the representation for $\hat{a}$ and $\hat{a}^\dagger$, the matrix representation of $\hat{x}$ and $\hat{p}$ are trivial to calculate. Using Eqns.(5),

$$\hat{x} = \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(a + a^\dagger\right), \hat{p} = i\left(\frac{\hbar m\omega}{2}\right)^{1/2}\left(a - a^\dagger\right) \tag{23}$$

Using above equation we can get matrix representation of $\hat{x}$ and $\hat{p}$,

$$\hat{x} = \left(\frac{\hbar}{2m\omega}\right)^{1/2} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \hat{p} = i\left(\frac{m\omega\hbar}{2}\right)^{1/2} \begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & -\sqrt{4} & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

3 Baker–Campbell–Hausdorff formula

For time evolution of a state, we act a time dependent unitary operator on the initial state of the system(at t = to),

$$|\psi(t)\rangle = \hat{U}(t)|\psi(to)]\rangle, \tag{24}$$

where $|\psi(to)\rangle$ is the state at the initial time(to). $\hat{U}(t)$ for a time independent Hamiltonian is defined by,

$$\hat{U}(t) = e^{-i\hbar\hat{H}t} \tag{25}$$

where $\hat{H}$ is in general sum of two non-commuting operator as evident in the Eq.(3) and hence it can not be expressed in the form $e^{A+B} = e^A e^B$(A and B are two operators) and so we use the BCH formula for the product of the exponentials of two operators A and B,

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}([A,[A,B]]+[B,[B,A]])+\ldots} \tag{26}$$

where the ... represents terms that are at least cubic in A and B and involve nested commutators of A and B. The derivation of the formula won't be stated as it has already been done in the presentation but two important intermediate formulas will be given,

$$e^A B e^{-A} = B + [A,B] + \frac{1}{2}[A,[A,B]] + \ldots \frac{1}{n!}[\overbrace{A,[A,\ldots[A}^{nA's},B]..] + \ldots. \tag{27}$$

$$e^{-A}\frac{d}{dx}e^A = \int_0^1 dy e^{-yA}\frac{dA}{dx}e^{yA} = A' + \frac{1}{2}[A',A] + \frac{1}{3!}[[A',A],A] + \ldots \tag{28}$$

where $A' = dA/dx$.
BCH equation is quite useful as in some cases where the commutator $[A,B]$ is a number, the infinite series truncates. Even in other cases, we can still truncate the series and add an error term as follows:

$$e^{i\hat{A}t+i\hat{B}t} = e^{i\hat{A}t}e^{i\hat{B}t} + O(t^2) \tag{29}$$

This is the first order trotter expansion. As the error grows as t^2, we can take small time steps to eliminate error term.

$$e^{i\hat{A}t+i\hat{B}t} = e^{\frac{n(i\hat{A}t+i\hat{B}t)}{n}} = (e^{\frac{i\hat{A}t}{n}}e^{\frac{i\hat{B}t}{n}})^n + O\left(\frac{t^2}{n}\right) \tag{30}$$

If we set n to some very large number, the error goes to zero. With this we can evaluate exponental of sum of operators as:

$$e^{i\hat{A}t+i\hat{B}t} = \lim_{n\to\infty}(e^{\frac{i\hat{A}t}{n}}e^{\frac{i\hat{B}t}{n}})^n \tag{31}$$

it is evident that this formula is very important for us as the $e^{(\hat{A}+\hat{B})t}$ is similar to $\hat{U}(t)$ given in Eq(25).

4 Coherent States

We also briefly discussed about Coherent States[2] which are basically the eigenstates of the annhilation operator, with eigen value α

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \tag{32}$$

Since $\hat{a}$ is a non-hermitian operator the phase $\alpha = |\alpha|e^{i\phi} \in C$ is a complex number. We can easily see that $|0\rangle$ is a coherent state with $\alpha = 0$
We will now define the displacement operator $D(\alpha)$ which is defined by,

$$D(\alpha) = e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}} \tag{33}$$

The displacement operator is an unitary operator, i.e. $D^\dagger D = 1$ and we can also rewrite it using Eq. (26).We therefore start by calculating the commutator of A and B

$$[A, B] = [\alpha\hat{a}^\dagger, \alpha^*\hat{a}] = \alpha\alpha^*[\hat{a}^\dagger, \hat{a}] = -|\alpha|^2$$

Since A, B commutator is a number so commutators. [[A , B] , A] and [[A , B] , B] vanish. Hence we can use Eq.(26) and rewrite Eq(33) as

$$D(\alpha) = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha\hat{a}^\dagger} e^{\alpha^*\hat{a}} \tag{34}$$

The coherent states $|\alpha\rangle$ is generated from the ground state $|0\rangle$ by the displacement operator $D(\alpha)$

$$|\alpha\rangle = D(\alpha)|0\rangle \tag{35}$$

We will be using the above definition to derive the Eq.(4.1):

$$\begin{aligned} D(\alpha)D^\dagger(\alpha)\hat{a}|\alpha\rangle = D(\alpha)D^\dagger(\alpha)\hat{a}D(\alpha)|0\rangle = D(\alpha)(\hat{a}|0\rangle + \alpha|0\rangle) \\ = \alpha D(\alpha)|0\rangle = \alpha|\alpha\rangle \\ \implies \hat{a}|\alpha\rangle = \alpha|\alpha\rangle \end{aligned}$$

In the above justification we have used two properties of the displacement operator, $D^\dagger D = 1$ which implies that displacement operator is unitary and $D^\dagger(\alpha)\hat{a}D(\alpha) = \hat{a} + \alpha$ which can be easily be shown using Eq.(27).
We can use the definition defined in Eq.(35) to get coherent states as below,

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle \tag{36}$$

For eigenstates of $\hat{a}^\dagger$, let an arbitraty state be

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n|n\rangle$$

Now applying the raising operator

$$\hat{a}^\dagger|\psi\rangle = \hat{a}^\dagger \sum_{n=0}^{\infty} c_n|n\rangle = \sum_{n=0}^{\infty} c_n\sqrt{n+1}|n+1\rangle$$

$$= \sum_{n=1}^{\infty} c_{n-1}\sqrt{n}|n\rangle$$

If $|\psi\rangle$ is an eigenstate of $\hat{a}^\dagger$ with eigenvalue α then we have

$$\sum_{n=0}^{\infty} c_n|n\rangle = \sum_{n=1}^{\infty} c_{n-1}\sqrt{n}|n\rangle$$

the only solution to this equation is $c_n = 0$ for all n. Therefore, there is no eigenstate of $\hat{a}^\dagger$.

5 Approach to circuit construction for Hamiltonian simulation

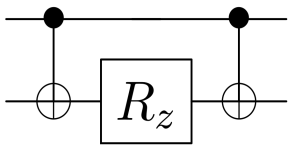
In this section, we will be discussing the approach to circuit construction for Hamiltonian simulation[3] followed by Qiskit's Opflow module, which we have used in the simulation of the quantum Harmonic Oscillator shown in further sections.
Any Hermitian (Hamiltonian) matrix H can be decomposed by the sum of Pauli products with real coefficients. The unitary operator responsible for time evolution for time-independent Hamiltonian $\hat{H}$ is defined by $e^{-i\hbar\hat{H}t}$ as given in eq.(24). Hence we have to create a circuit for $e^{i\hat{H}t}$ via trotter decomposition

$$e^{iHt} \approx \big(\prod_k e^{ic_k P_k t/N}\big)^N$$

t is a parameter that can have either positive or negative values, P_k are the Pauli terms, c_k are the coefficients of the corresponding P_ks, $H = \sum_k c_k P_k$, N is the Trotter number. By increasing N it is possible to decrease the error of the Trotter decomposition as much as desired. If all P_k Pauli terms are commuting to each other, then we can take $N = 1$ (no Trotter decomposition is needed). For this simulation, we need to know how to simulate individual Pauli products $e^{iP_k t}$. Let's start with the simplest one $e^{i\sigma_z\otimes\sigma_z\otimes\cdots\otimes\sigma_z t}$. Firstly, we can see that RZ(-2t) = $e^{i\sigma_z t}$ where RZ represents the operator the single qubit rotation around Z-axis

$$R_z(\lambda) = \exp\left(-i\frac{\lambda}{2}Z\right) = \begin{pmatrix} e^{-i\frac{\lambda}{2}} & 0 \\ 0 & e^{i\frac{\lambda}{2}} \end{pmatrix}$$

Now the circuit for $e^{i\sigma_z\otimes\sigma_z t}$ is given by



Before showing why this is true, let's introduce two formulas that we will use: Let t be a real number and A a matrix such that $A^2 = I$. Then

$$e^{iAt} = \cos(t)I + i\sin(t)A$$

For all Pauli terms, this $P_k^2 = I$ is true. So we can use this formula. For CNOT gate we have:

$$\text{CNOT} = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes \sigma_x$$

By taking these formulas into account let's show that the circuit implements the $e^{i\sigma_z\otimes\sigma_z t}$ Pauli term:

$$e^{i\sigma_z\otimes\sigma_z t} = \cos(t)I + i\sin(t)\sigma_z \otimes \sigma_z$$

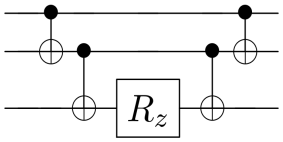
The circuit:

$$\begin{aligned} &\text{CNOT}\left(I \otimes e^{i\sigma_z t}\right)\text{CNOT} = \left[|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes \sigma_x\right] \\ &\left[\cos(t)I \otimes I + i\sin(t)I \otimes \sigma_z\right]\left[|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes \sigma_x\right] = \\ &= \cos(t)I + i\sin(t)\sigma_z \otimes \sigma_z \end{aligned}$$

So, the circuit implements what we want:

$$e^{i\sigma_z\otimes\sigma_z t} = \text{CNOT}\left(I \otimes e^{i\sigma_z t}\right)\text{CNOT}$$

Similarly for $e^{i\sigma_z\otimes\sigma_z\otimes\sigma_z t}$ the circuit will look like



This is can be easily generalized for $e^{i\sigma_z \otimes \sigma_z \otimes \ldots \otimes \sigma_z t}$.
Now for the case of one σ_x in the tensor product $P = P_1 \otimes \sigma_x^{(n)} \otimes P_2$, where P_1 and P_2 are also Pauli products, n is the qubit number. Note that:

$$\begin{aligned} e^{iP_1 \otimes \sigma_x^{(n)} \otimes P_2 t} &= \cos(t) I + i \sin(t) P_1 \otimes \sigma_x^{(n)} \otimes P_2 = \\ &= \cos(t) I + i \sin(t) P_1 \otimes \left(H \sigma_z^{(n)} H \right) \otimes P_2 = \\ &= H^{(n)} e^{iP_1 \otimes \sigma_z^{(n)} \otimes P_2 t} H^{(n)} \end{aligned}$$

where $H^{(n)}$ is the Hadamard gate acting on nth qubit. The same can be shown for σ_y:

$$e^{iP_1 \otimes \sigma_y^{(n)} \otimes P_2 t} = H_y^{(n)} e^{iP_1 \otimes \sigma_z^{(n)} \otimes P_2 t} H_y^{(n)}$$

where H_y is a self-inverse gate, which has this nice property $\sigma_y = H_y \sigma_z H_y$:

$$H_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix}$$

Now, we can simulate any Pauli term.
Hence by applying appropriate rotations, we can bring any Pauli term simulation problem to the simplest $e^{i\sigma_z \otimes \sigma_z \otimes \ldots \otimes \sigma_z t}$ Pauli term simulation problem, whose solution we already know. So with this approach, we can simulate any Pauli term, thus also any Hermitian operator.

6 Simulation using one hot encoding

6.1 Algebra for one hot encoding

When trying to simulate a quantum system on a quantum computer, we have a finite number of qubits at our disposal, hence when dealing with bosonic systems where the hamiltonian possesses an infinite number of energy eigenstates, we would need to truncate the number of basis states, that we use in our simulation[4]. We aim to simulate a system of N quantum harmonic oscillators where we can later add perturbations and small coupling terms and observe the time evolution of the initial state in these different cases.

Say we have decided to keep our upper limit to the basis states as N_p, and the number of oscillators as N hence for describing a state in this scheme, we could require $N(N_p + 1)$ qubits. The basis state for the i^{th} oscillator is of the form

$$\begin{aligned} |0\rangle_i &\leftrightarrow |00 \cdots 001\rangle_i \\ |1\rangle_i &\leftrightarrow |00 \cdots 010\rangle_i \\ |2\rangle_i &\leftrightarrow |00 \cdots 100\rangle_i \\ &\vdots \\ |N_{p-1}\rangle_i &\leftrightarrow |01 \cdots 000\rangle_i \\ |N_p\rangle_i &\leftrightarrow |10 \cdots 000\rangle_i \end{aligned}$$

Here we clearly see that for the basis states of a single oscillator, there is only one spin up state at a time and the index at which this spin up state is present determines the occupation number for this particular oscillator.The state of the entire system can just be obtained by taking a tensor product

of the individual states of each oscillator.The creation and annihilation operators for the i^{th} oscillator can be written as :

$$\bar{b}_i^\dagger = 1 \otimes \cdots \otimes 1 \otimes \underbrace{\hat{b}^\dagger}_{i^{\text{th}} \text{ factor}} \otimes 1 \otimes \cdots \otimes 1$$

where $\hat{b}^\dagger$ represents the creation operator for a single oscillator which is basically a $(N_p+1)*(N_p+1)$ matrix which looks like :

$$\hat{b}^\dagger = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \sqrt{2} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \sqrt{N_P} & 0 \end{pmatrix}$$

In terms of the σ_+ and the σ_- operators the creation operator becomes :

$$\bar{b}_i^\dagger = \sum_{n=0}^{N_P-1} \sqrt{n+1}\sigma_-^{n,i}\sigma_+^{n+1,i}$$

Subsequently the number operator for the i^{th} oscillator can be written as :

$$\bar{n}_i = \sum_{n=0}^{N_P} n\frac{1-\sigma_z^{n,i}}{2}$$

Here is the matrix representation of the Hamiltonian in σ_z basis for a single QHO, generated for $N_P = 3$ (4 states to be simulated, 4 qubits needed):

$$H = \begin{pmatrix} 0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4.5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6.5 \end{pmatrix} \tag{37}$$

The intersections of the highlighted lines form the matrix representation of the reduced Hamiltoian, they are obtained from the statevectors of interest, rest are redundant states that arise because of the chosen mapping scheme which does not include all the basis states of the computational basis. We could construct a reduced Hilbert space formed by these states and simulate that, but qiskit evolves all of the states, meaning a lot of computational power is wasted in evolving these redundant states. To tackle this issue we can choose a different encoding scheme that uses all of the basis states of the system of qubits. The number of redundant states will grow exponentially as the number of qubits increase.

6.2 Simulations for a single oscillator

Our aim to plot the expectation values of observables such as $\langle\hat{x}\rangle$, $\langle\hat{p}\rangle$ and $\langle\hat{H}\rangle$ varying with time.Here we shall display the results of our simulation for varies parameters and initial states , we shall perform

all our our runs for the duration $t_0 = 0$ s to $t_{final} = 4\pi$, the things we will adjust are:

- N_p
- N(But in this section we will be dealing with a a single oscillator so N=1)
- Number of points we want to plot in the given interval
- The inital state - We will be observing how the plots change when we start with a single basis state of the hamiltonian and when we start with a superposition of basis states
- We will observe how things change with adding $\hat{x}$ and $\hat{x}^3$ terms to the hamiltonian

Our simulation was carried out in the Qiskit library of python. First we wrote code to map the Hamiltonian of QHO (both single and coupled) to a sum of Pauli operators for any value of N_P, now we need to compute the exponential of the new Hamiltonian, we do this by using the Opflow module of Qiskit to Trotterize the Hamiltonian and compute the exponential of the individual Pauli operators in the sum using the procedure outlined in the previous section. Once the time evolution operator is obtained, we operate the same on different initial states to obtain the final state, which can be used to compute the expectation values of the required observables. Such expectation values are shown in the next section.

6.2.1 Time dependence of expectation values

We shall deal with the case of $N = 1$ and $N_p = 1$ and we shall see how the plot changes for 2 different initial states

- $|\psi(0)\rangle = |01\rangle$ (Ground state)
- $|\psi(0)\rangle = \frac{|01\rangle+|10\rangle}{\sqrt{2}}$ (Superposition of ground state and first excited state)

Before we move on to showing the plots, we can get the calculations analytically as they are very simple. Let us begin with the first initial condition :

$$\begin{aligned}
\langle\hat{x}(t)\rangle &= \langle\psi(t)|\hat{x}|\psi(t)\rangle \\
\langle\hat{x}(t)\rangle &= (\langle 0|e^{\frac{iE_0t}{\hbar}})\hat{x}(e^{\frac{-iE_0t}{\hbar}}|0\rangle) \\
\langle\hat{x}(t)\rangle &= \langle 0|e^{\frac{iE_0t}{\hbar}}(\hat{a}+\hat{a}^\dagger)e^{\frac{-iE_0t}{\hbar}}|0\rangle \\
\langle\hat{x}(t)\rangle &= 0
\end{aligned} \tag{38}$$

Similarly, its easy to show that $\langle\hat{p}(t)\rangle$ will also be 0 and that $\langle\hat{H}(t)\rangle$ will be $\frac{\hbar\omega}{2}$(ground state energy), where throughout our simulations we have kept parameters like $\hbar, \omega, m...$ as 1 for simplicity of working in atomic units. We can observe the same results in the Figure shown above.

Now for the case where our initial condition is a superposition state of the ground state and the first excited state The calculations for getting expectation values are shown below :

$$\langle\hat{x}(t)\rangle = \langle\psi(t)|\hat{x}|\psi(t)\rangle$$

$$\langle\hat{x}(t)\rangle = (\frac{\langle 0|e^{\frac{iE_0t}{\hbar}} + \langle 11e^{\frac{iE_1t}{\hbar}})}{\sqrt{2}})(\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^+\rangle)(\frac{|0\rangle e^{-\frac{iE_0t}{\hbar}} + |1\rangle e^{-\frac{iE_1t}{\hbar}}}{\sqrt{2}})$$

$$\langle\hat{x}(t)\rangle = \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}(\langle 0|e^{\frac{iE_0t}{\hbar}} + \langle 1|e^{\frac{iE_1t}{\hbar}})(|1\rangle e^{-\frac{iE_0t}{\hbar}} + |0\rangle e^{-\frac{iE_1t}{\hbar}})$$

$$E_1 - E_0 = \hbar\omega$$

$$\langle\hat{x}(t)\rangle = \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}(e^{i\omega t} + e^{-i\omega t})\langle\hat{x}(t)\rangle = \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}(2\cos\omega t)$$

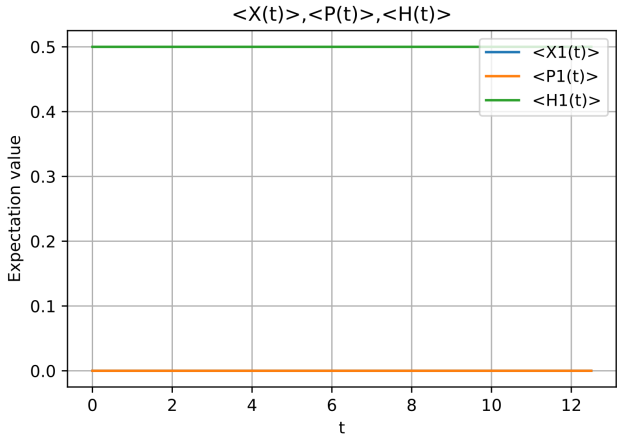


Figure 1: Expectation values for $|\psi(0)\rangle = |01\rangle$(Ground state)

$$\langle \hat{x}(t) \rangle = \sqrt{\frac{\hbar}{2m\omega}} \cos \omega t$$

Similarly we get the expectation value of the momentum operator as :

$$\langle \hat{p}(t) \rangle = -\sqrt{\frac{m\hbar\omega}{2}} \sin \omega t$$

And for the expectation of the hamiltonian, we get :

$$\langle \hat{H}(t) \rangle = \frac{E_0 + E_1}{2} = \hbar\omega$$

We can clearly see that our simulation matches the analytic results we expect. (Note that since we

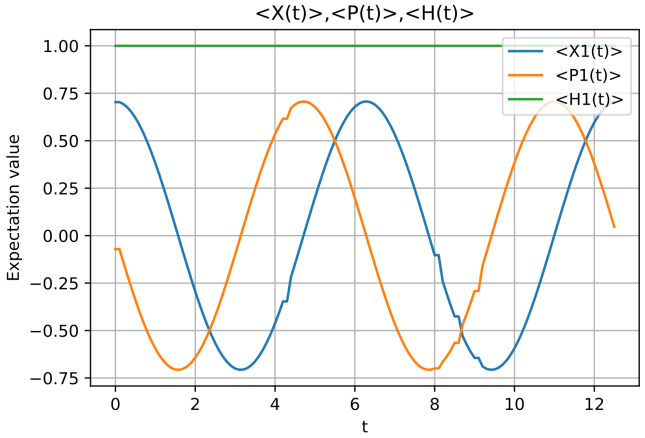


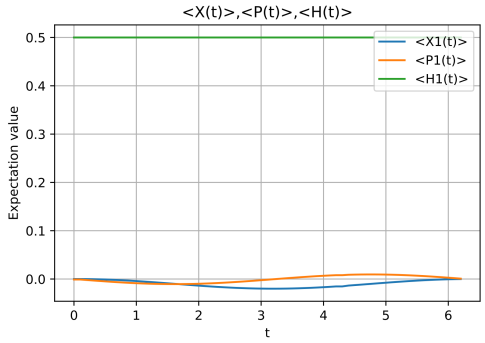
Figure 2: Expectation values for $|\psi(0)\rangle = \frac{|01\rangle+|10\rangle}{\sqrt{2}}$(Superposition of ground state and first excited state)

deal with a finite N_p when we apply the creation operator, say on $|1\rangle$ we get 0 instead of $|2\rangle$ for $N_p = 1$). We shall now move on to observe the changes for the case of perturbating the hamiltonian by $\hat{x}$ and $\hat{x}^3$

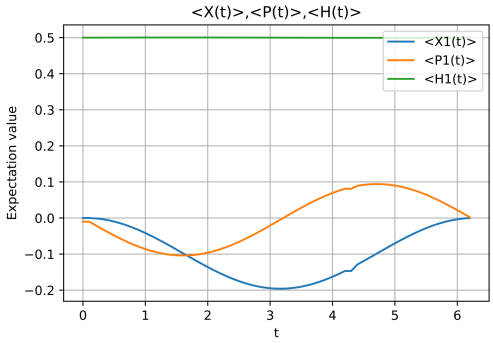
6.2.2 Adding perturbation to the hamiltonian

For the same initial conditions as the previous section, we will look at perturbations of the type $\hat{x}$ and $\hat{x}^3$. First we will look at $\hat{x}$, we will set the parameter values to $\lambda = 0.01, 0.1$ and 0.5:

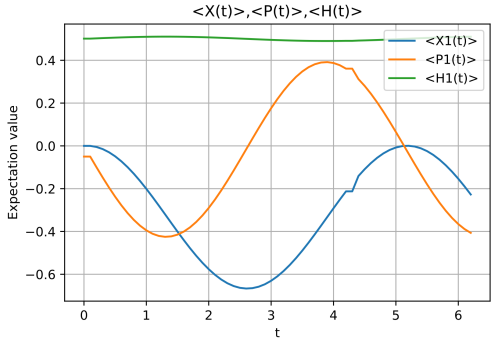
$$\hat{H} = \hat{H}_0 + \lambda\hat{x}$$
$$and\ \hat{H} = \hat{H}_0 + \lambda\hat{x}^3$$



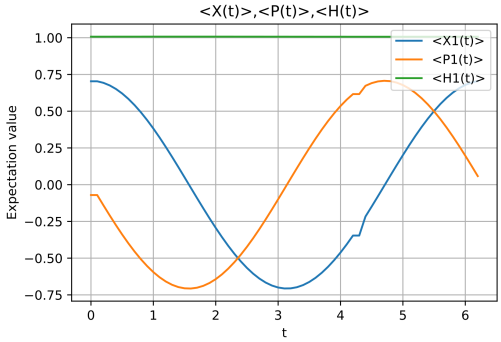
(a) $|\psi(0)\rangle = |01\rangle$ and $\lambda = 0.01$



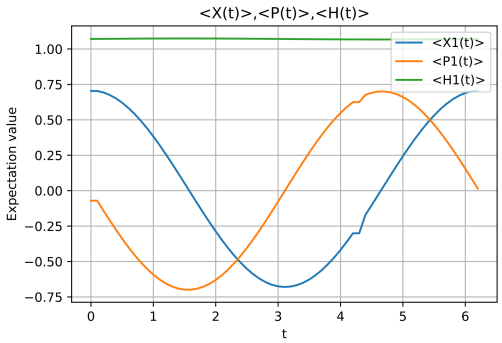
(b) $|\psi(0)\rangle = |01\rangle$ where $\lambda = 0.1$



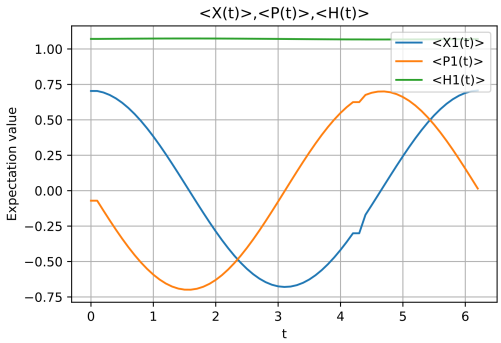
(c) $|\psi(0)\rangle = |01\rangle$ where $\lambda = 0.5$



(d) $|\psi(0)\rangle = \frac{|01\rangle+|10\rangle}{\sqrt{2}}$ and $\lambda = 0.01$



(e) $|\psi(0)\rangle = \frac{|01\rangle+|10\rangle}{\sqrt{2}}$ and $\lambda = 0.1$

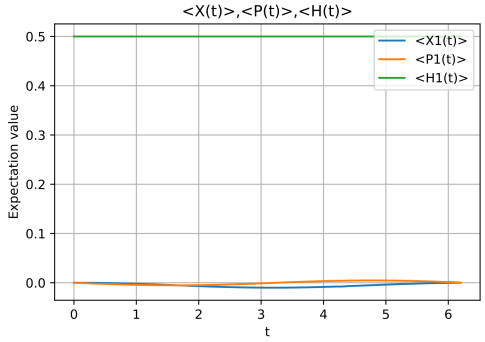


(f) $|\psi(0)\rangle = \frac{|01\rangle+|10\rangle}{\sqrt{2}}$ where $\lambda = 0.5$

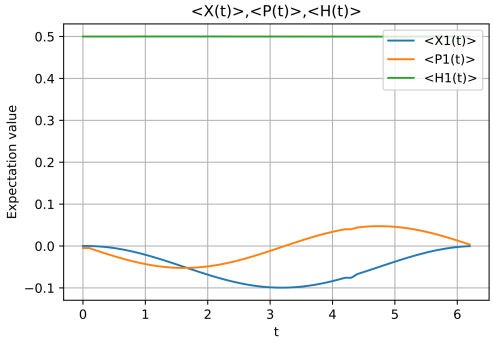
Figure 3: Expectation values for specific initial conditions and different values for $\lambda(\hat{x}$ perturbation)

Through first order Non-degenerate perturbation theory, we can analytically show that when we apply a perturbation of $\hat{x}$ there is no change in the behavior of the system apart from a uniform shift of all the energy levels by a constant term. This can, however, also be proved in a more simplistic nature

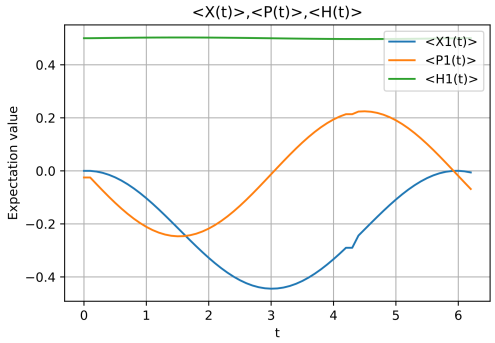
which gives the exact solution just by completing the square of the new hamiltonian and transforming the coordinates. Due to this, we may expect constant line graphs for the expectation values of $\hat{x}$,$\hat{p}$ and $\hat{H}$. However, since we are making measurements on the unperturbed hamiltonian basis, it is expected that one will not obtain such constant plots. It is quite obvious from the plots that the response of the system to the perturbation increases as we increase the value of the parameter; however, it is also interesting to note that these changes are only observable when we have our initial state as a single eigenstate of the unperturbed hamiltonian because when we choose a superposition state as our initial state, the order of magnitude of the expectation values is much higher than that of the changes produced due to the perturbation, this behavior carries over in the case of the $\hat{x}^3$ as well where we would need to apply perturbation theory in order to get the new energy eigenvalues and states. We won't be able to use any clever technique like for $\hat{x}^3$ to solve the hamiltonian exactly and will have to resort to perturbation theory.



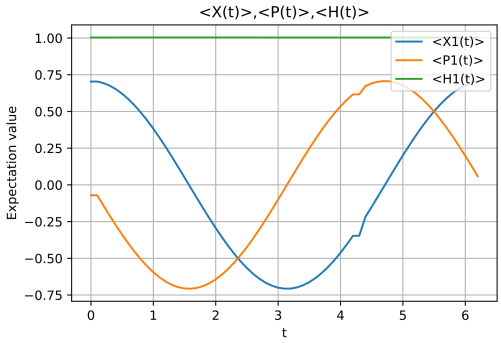
(a) $|\psi(0)\rangle = |01\rangle$ and $\lambda = 0.01$



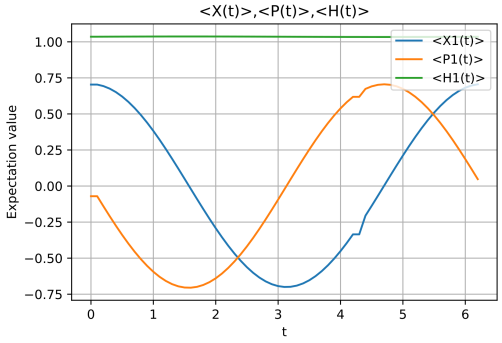
(b) $|\psi(0)\rangle = |01\rangle$ where $\lambda = 0.1$



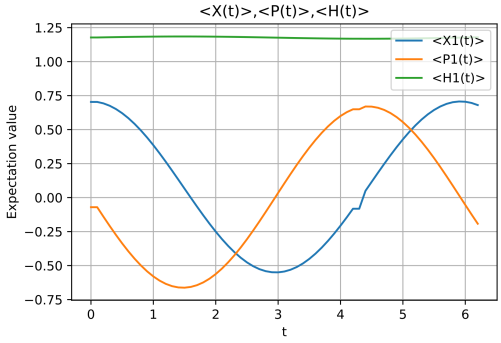
(c) $|\psi(0)\rangle = |01\rangle$ where $\lambda = 0.5$



(d) $|\psi(0)\rangle = \frac{|01\rangle+|10\rangle}{\sqrt{2}}$ and $\lambda = 0.01$



(e) $|\psi(0)\rangle = \frac{|01\rangle+|10\rangle}{\sqrt{2}}$ and $\lambda = 0.1$



(f) $|\psi(0)\rangle = \frac{|01\rangle+|10\rangle}{\sqrt{2}}$ where $\lambda = 0.5$

Figure 4: Expectation values for specific initial conditions and different values for $\lambda(\hat{x^3}$ perturbation)

7 Simulation using gray code encoding

As discussed in the previous section, to simulate a QHO on a quantum computer, we need to truncate the energy eigenstate spectrum to some max value N_P and map those to qubit states. For one hot encoding, we used mapping shown in Eqn (43) where N_P+1 qubits were needed to do the simulation; this is inefficient as there are $2^{N_P+1}-N_P-1$ unused states. We can resolve this issue by using a better encoding like the gray code encoding[5]. Gray code encoding is similar to binary encoding, but the numbers are ordered in a specific way, ensuring only one-bit changes when we go to the next number in the system.

7.1 Algebra for gray code encoding

In this encoding scheme, we map the state corresponding to j^{th} level in occupation number basis to its corresponding gray code digit. An example of such mapping is given below for the i^{th} oscillator where $N_P = 7$:

$$\begin{aligned}
|0\rangle_i &\leftrightarrow |\downarrow_2\downarrow_1\downarrow_0\rangle_i \\
|1\rangle_i &\leftrightarrow |\downarrow_2\downarrow_1\uparrow_0\rangle_i \\
|2\rangle_i &\leftrightarrow |\downarrow_2\uparrow_1\uparrow_0\rangle_i \\
|3\rangle_i &\leftrightarrow |\downarrow_2\uparrow_1\downarrow_0\rangle_i \\
|4\rangle_i &\leftrightarrow |\uparrow_2\uparrow_1\downarrow_0\rangle_i \\
|5\rangle_i &\leftrightarrow |\uparrow_2\uparrow_1\uparrow_0\rangle_i \\
|6\rangle_i &\leftrightarrow |\uparrow_2\downarrow_1\uparrow_0\rangle_i \\
|7\rangle_i &\leftrightarrow |\uparrow_2\downarrow_1\downarrow_0\rangle_i
\end{aligned} \tag{39}$$

In this encoding, to simulate N_P states of QHO, we would just need $log_2 N_P$ number of qubits as opposed to N_P qubits.
This can be extended to multiple oscillators by taking the tensor product of the encoded states of each individual oscillator. More formally a Gray code with bits, denoted G_η, is given by:

$$G_\eta = (g_0, g_1, \cdots, g_{2^\eta-1}) \tag{40}$$

For Eqn (50), the gray code sequence is given by

$$G_3 = (000, 001, 011, 010, 110, 111, 101, 100) \tag{41}$$

In addition, we can define a sequence called transition sequence, which denotes the position of the bit that changes when there is a transition. s_α corresponds to the position of the bit that changes when there is a transition from g_α to $g_{\alpha+1}$. The transition sequence S_{G_η} corresponding to the gray code sequence G_η are given by:

$$S_{G_\eta} = (s_0, s_1, \cdots, s_{2^\eta-1}) \tag{42}$$

$$s_i \in \{0, \cdots, \eta-1\} \ \forall\, i \ \in \{0, 1, \cdots, 2^\eta - 1\} \tag{43}$$

and the transition sequence for Eqn (52) is given by:

$$S_{G_3} = (0, 1, 0, 2, 0, 1, 0, 2)$$

Now we need to map the Hamiltonian of the QHO to a linear combination of Pauli terms. To do this, we will do the mapping for number operator and ladder operators first, similar to what was done in the previous section. To do this, we will define three operators A_α, B_α and C_α whose action is of the form $|\alpha\rangle\langle\alpha|$, $|\alpha+1\rangle\langle\alpha|$ and $|\alpha-1\rangle\langle\alpha|$ respectively. And finally we define two more projection operators $P^{(0)}$ and $P^{(1)}$ which project states to σ_z eigenstates:

$$\begin{aligned}
P^{(0)} &= |\downarrow\rangle\langle\downarrow| \\
P^{(1)} &= |\uparrow\rangle\langle\uparrow|
\end{aligned} \tag{44}$$

The A_α operator can be constructed as follows:

$$A_\alpha = \bigotimes_{n=0}^{\eta-1} P^{(g_\alpha,n)} \tag{45}$$

$$g_\alpha \in G_\eta \,\forall\ \alpha = \ (0, 1 \cdots, 2^\eta - 1) \tag{46}$$

Where $P^{(g_\alpha,n)}$ is $P^{(0)}$ if n^{th} bit of g_α is 0 or $P^{(1)}$ otherwise. Similarly B_α and C_α and be defined as:

$$B_\alpha = \left(\bigotimes_{i=0}^{s_\alpha-1} P^{(g_\alpha,i)}\right) \otimes \sigma_\pm \otimes \left(\bigotimes_{j=s_\alpha+1}^{\eta-1} P^{(g_\alpha,j)}\right); s_\alpha \in S_{G_\eta} \tag{47}$$

and

$$C_\alpha = \left(\bigotimes_{i=0}^{s_{\alpha-1}-1} P^{(g_\alpha,i)}\right) \otimes \sigma_\pm \otimes \left(\bigotimes_{j=s_{\alpha-1}+1}^{\eta-1} P^{(g_\alpha,j)}\right); s_{\alpha-1} \in S_{G_\eta} \tag{48}$$

Where σ_+ has to be chosen if the transition bit is going from 0 to 1, and σ_- is chosen if the transition bit is going from 1 to 0. The number operator for QHO can be constructed as follows:

$$N = \sum_{n=0}^{N_P} nA_n \tag{49}$$

and the ladder operators can be constructed as follows:

$$a^\dagger = \sum_{i=0}^{N_P} \sqrt{n+1} B_n \tag{50}$$

$$a = \sum_{i=0}^{N_P} \sqrt{n} C_n \tag{51}$$

And finally, the Hamiltonian of single uncoupled QHO can be easily obtained by:

$$\hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2}\right)$$

Here is an example of matrix representation of the Hamiltonian in σ_z basis for a single QHO, which was generated for $N_P = 3$ (4 states to be simulated and 2 qubits are needed):

$$H = \begin{pmatrix} 0.5 & 0 & 0 & 0 \\ 0 & 1.5 & 0 & 0 \\ 0 & 0 & 3.5 & 0 \\ 0 & 0 & 0 & 2.5 \end{pmatrix} \tag{52}$$

This is significantly smaller than the Hamiltonian matrix generated for one hot encoding as there are no redundant states and fewer qubits are needed to simulate same number of states. It can also be noted that the columns of the matrix may seem flipped, but this is due to the ordering of states chosen for the gray code encoding.

7.2 Simulations for a single oscillator

In this section, we will display the results of our simulation by plotting different expectation values such as $\langle\hat{x}\rangle, \langle\hat{p}\rangle$ and $\langle\hat{H}\rangle$ for different initial conditions similar to the previous section. We will not be repeating the procedure and analytical calculations done in previous section. Here is the result of the simulation for the QHO in ground state and simulation from t = 0 to t = 2π $|00\rangle$:

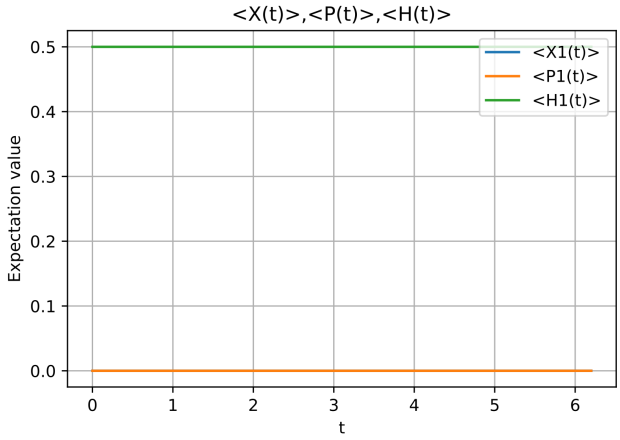


Figure 5: Expectation values for $|\psi(0)\rangle = |00\rangle$(Ground state)

We can observe that expectation values of x and p are zero and that of H is 0.5 as obtained from the analytical calculations. Similarly, here is the result for the case where the initial condition is the superposition of 1st and 2nd excited states $\frac{|00\rangle+|01\rangle}{\sqrt{2}}$: As this is a simple simulation, we see not many

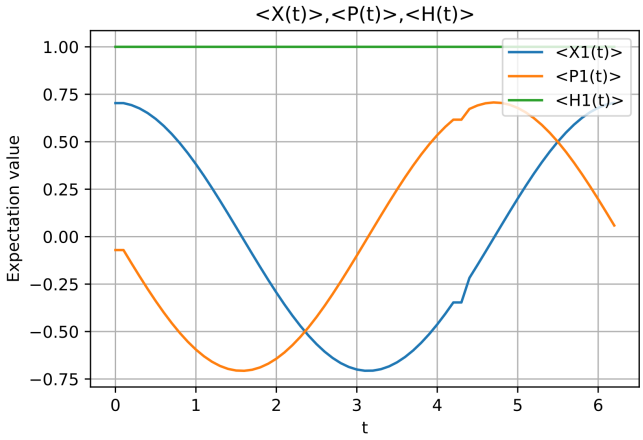


Figure 6: Expectation values for $|\psi(0)\rangle = \frac{|00\rangle+|01\rangle}{\sqrt{2}}$(Superposition of ground state and first excited state)

differences between the one hot encoding and gray code encoding. We will analyze the difference between the encoding schemes in the last section.

8 N Harmonic Oscillators

8.1 Independent Oscillators

In this section, we will be simulating the Hamiltonian of N-independent oscillators.

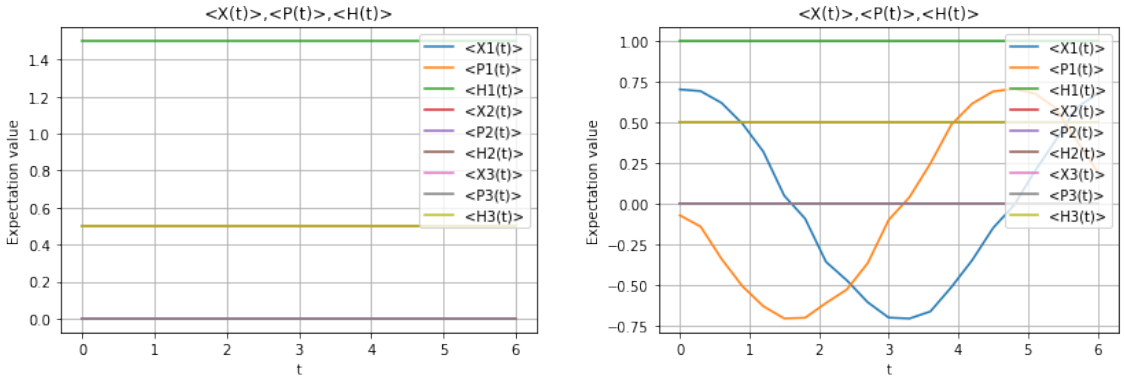
$$\hat{H} = \sum_j \frac{\hat{p}_j^2}{2m} + \frac{m\omega^2 \hat{x}_j^2}{2} \tag{53}$$

Now we will simulate this Hamiltonian in the gray code encoding and one hot encoding for two different initial states($N = 3$ and $N_p = 3$):

- $|\psi(0)\rangle = |000001\rangle$ (Gray Code) OR $|\psi(0)\rangle = |000100010010\rangle$ (One Hot)

- $|\psi(0)\rangle = \frac{|000001\rangle + |000000\rangle}{\sqrt{2}}$ (Gray Code) OR $|\psi(0)\rangle = \frac{|000100010010\rangle + |000100010001\rangle}{\sqrt{2}}$ (One Hot)

Results of the same are displayed in figure 7.



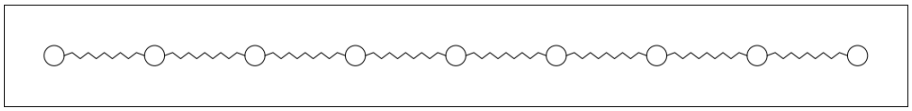
(a) First initial condition

(b) Second initial condition

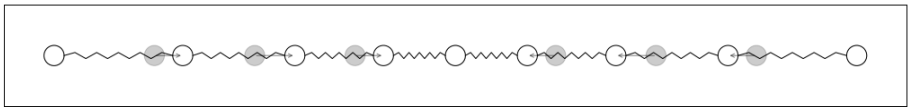
Figure 7: Expectation values for N independent oscillators with different initial conditions

8.2 Coupled Oscillators

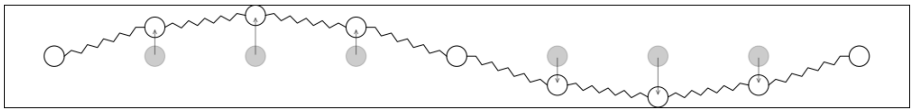
In this section, we will introduce a coupling term[6] to the Hamiltonian of N independent Harmonic Oscillator, which mimics the Hamiltonian of Phonons - quanta of sound. We will non-rigorously arrive at the Hamiltonian from a classical picture of sound. We can think of a mental model having a bunch of balls connected by a spring:



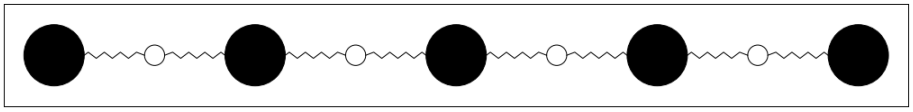
This will have two types of sound waves: longitudinal modes, where the atoms move in the direction of propagation:



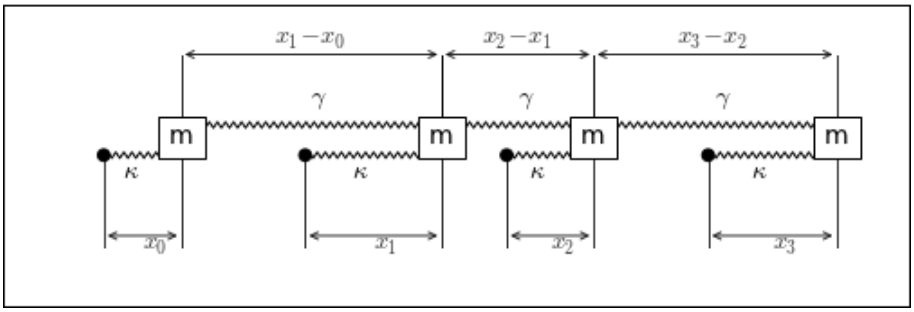
and transverse modes, where the atoms move perpendicular to the direction of motion:



Most materials have more than one type of atom. Thus our model should really have at least two different types of balls:



We are going to make a toy model of the longitudinal acoustic (all of the atoms move together) modes. We imagine that the heavy atoms are essentially stationary, and only the light atoms move. There will be a weak coupling between the light atoms, yielding a model something like:



We have added labels to show that the j'th particle is displaced by a distance x_j from its equilibrium position. It feels a restoring force with spring constant κ – representing the coupling with the heavy atoms. The j'th particle will also be attached by a spring to the $j+1$'th particle. These springs will have spring constant γ. We want a quantum description of this system. We start by writing the classical energy

$$E = \sum_j \frac{p_j^2}{2m} + \frac{\kappa}{2}x_j^2 + \frac{\gamma}{2}(x_j - x_{j-1})^2. \tag{54}$$

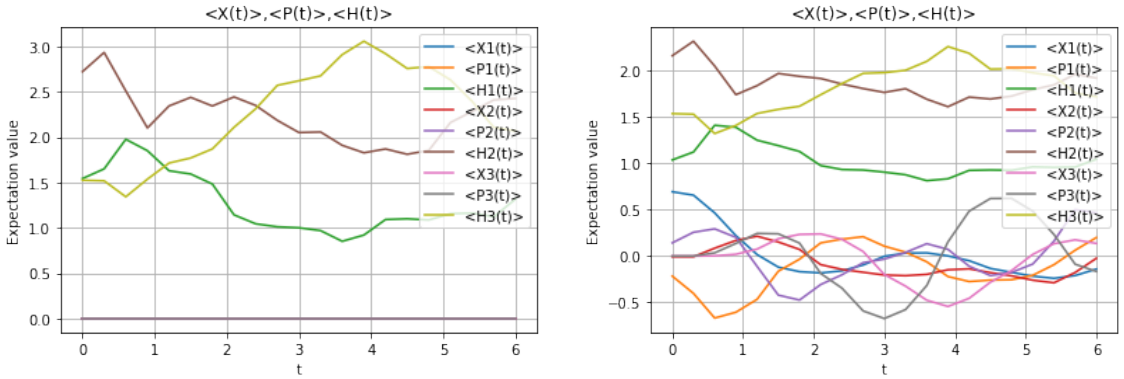
The quantum mechanical version of this just requires taking $p_j \to -i\partial_{x_j}$, and using this in a big Schrodinger equation $H\psi(x_1, x_2, \cdots, x_N) = E\psi(x_1, x_2, \cdots, x_N)$. Assigning 1 to all the parameters, we get the Hamiltonian as

$$\hat{H} = \sum_j \frac{\hat{p}_j^2}{2m} + \frac{m\omega^2}{2}\hat{x}_j^2 + \frac{1}{2}(\hat{x}_j - \hat{x}_{j-1})^2. \tag{55}$$

Now we will simulate this Hamiltonian in the gray code encoding and one hot encoding for two different initial states

- $|\psi(0)\rangle = |000001\rangle$ (Gray Code) OR $|\psi(0)\rangle = |000100010010\rangle$ (One Hot)
- $|\psi(0)\rangle = \frac{|000001\rangle + |000000\rangle}{\sqrt{2}}$ (Gray Code) OR $|\psi(0)\rangle = \frac{|000100010010\rangle + |000100010001\rangle}{\sqrt{2}}$ (One Hot)

Results of the same are displayed in figure 8.



(a) First initial condition

(b) Second initial condition

Figure 8: Expectation values for N coupled oscillators with different initial conditions

9 Comparison between one hot and gray code encoding

In the previous sections, we looked at results from the simulation of QHO and coupled QHOs under two different encoding schemes. In this section, we will analyze some parameters such as depth and

time taken to compare the two encoding schemes. We have already established that one hot encoding needs significantly more qubits to simulate the same number of energy eigenstates as compared to one hot encoding. Now we will establish some more differences, such as time taken and depth of the circuit. We have tabulated the parameters, such as circuit depth and time taken to execute the code. Note that to plot the different expectation values as shown above, the circuit has to be executed from the start at every time step and the time of execution shown is to display this graph, meaning the circuit was executed at each time step from the start. The simulation was done for t = 0 to t = 2π.

Nature of simulation	Depth of final step	Time for execution in seconds
Three independent oscillators one hot	61	27.73
Three independent oscillators gray code	240	17.69
Three coupled oscillators one hot	48185	818.97
Three coupled oscillators gray code	14041	205.51

From the above table, it can be observed that for the case of independent oscillators, depth for one hot encoding is lower, this is because the corresponding Hamiltonian only has σ_z terms which are encoded as simple R_z rotations. But for more complicated Hamiltonian such as for the case of coupled oscillators, gray code has significantly lower depth as it is a more efficient encoding with no unused states. Time for execution is higher for one hot encoding in both, such large difference could've arose, not only from lesser depth, but also from inefficiencies in our code in the case of one hot encoding as we had to specifically pick out the states of interest to run the simulation using opflow library. Given below a table for number of qubits required for simulation of N oscillators with N_P as the maximum occupation number:

Encoding Scheme	Total Qubits used	Total Qubits used per oscillator
one hot	$N(N_p + 1)$	$N_p + 1$
gray code	$N(\log_2(N_p + 1))$	$\log_2(N_p + 1)$

10 Conclusion

The simulation of bosonic systems such as the coupled quantum harmonic oscillator on a quantum computer requires a truncation of the energy spectrum, this truncation does not decrease the accuracy of any expectation values we choose to compute, but it just puts a restriction of the maximum possible energy, so if our bosonic system of interest only takes takes certain finite energy values, then it can be simulated accurately on a quantum computer. Once we have the spectrum of truncated occupation number spectrum, we can map these eigen states and the Hamiltonian to a system of qubits, there are various ways of doing the same. In this report we looked at two kinds of encoding schemes, one hot and gray code. While one hot encoding is simple to understand and implement, the results make it clear that gray code encoding is superior both in terms of time taken and depth of the resultant circuit. And finally the simulation can be carried out by simply computing the time evolution operator (for the case of time independent Hamiltonian) e^{iHt}, we have also shown a way to construct the time evolution operator as single and two qubit gates by Trotterizing it given that H is mapped onto a linear combination of Pauli operators. Once the time evolution operator is obtained, we can compute the states of system at any time and compute various expectation values to study the properties we desire.

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Google Colab link

- N-Coupled Harmonic Oscillators-One Hot
- N-Coupled Harmonic Oscillators-Gray Code