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RABI OSCILLATIONS AND ENTANGLEMENT BETWEEN TWO RYDBERG ATOMS IN AN OPTICAL CAVITY STUDIED BY THE JAYNES-CUMMINGS MODEL AND QUANTUM CIRCUITS ON QISKIT

A Thesis

by

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ABSTRACT

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Rydberg atoms are highly excited atoms in which one electron has a large principal quantum number. Due to their unusual atomic properties, Rydberg atoms are promising building blocks of two-qubit gates and light-atom quantum interfaces in quantum information processing. For two atoms at close distance (< 10 mm) the Rydberg blockade prevents the two atoms to be simultaneously in the excited state whereas this blockade is absent for atoms far apart. Recently, this effect was used to engineer a quantum processor based on two-dimensional arrays of neutral atoms which are trapped and transported by optical tweezers. Motivated by these experiments, we study the light-atom interaction and entanglement of two Rydberg atoms interacting by the Rydberg blockade in an optical cavity using the Jaynes-Cummings model. We find a rich variety of Rabi oscillations and entanglement as a function of initial conditions and interaction time, which may be used to generate two-qubit gates. Furthermore, we develop and simulate a quantum circuit of this system using Qiskit, an open-source software development kit designed to emulate the operation of a real Quantum Computer.

DEDICATION

I dedicate this work to my family: Mom, Dad, Angel you are all everything to me, Los quiero mucho.

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CHAPTER I

INTRODUCTION

1.1 Rydberg Atom and Jaynes Cummings Hamiltonian

Rydberg atoms are highly excited atoms with varying values of n (quantum principal numbers) that can range from a double-digit number to a three digit one; usually the higher the value of n, the farther away the electron is from the nucleus [5]. They have become a very interesting phenomena to study due to their exclusive properties, i.e., the size and dipole scaling as n^2 compared to the radiative lifetime scale and polarizability counterparts, their response to exterior magnetic and electric fields, the appearance of the well-known Rydberg Blockade [7] due to the latter property. The Rydberg Blockade (see Figure 1.1) happens when the atom is in a high energy Rydberg state that physically arise from an electron being in a high orbital; this one property will be the focus due to its replicability in the state space of our Hamiltonian [4].

We consider two Rydberg atoms inside a single quasi one-dimensional cavity of length L (See Figure 1.5). The atoms interact with each another and with one mode ω of the quantized field in the cavity.

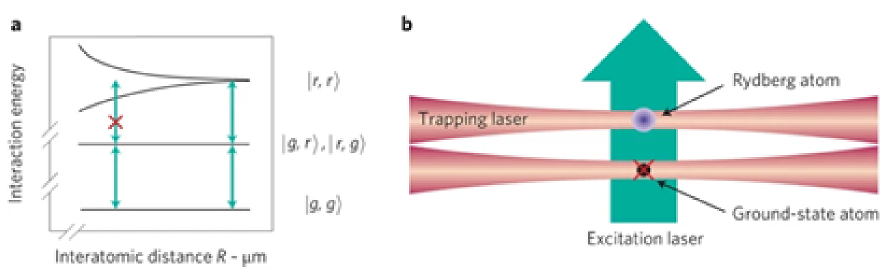

Figure 1.1: Rydberg Blockade and atom trap. a) describes the interaction energy as a function of inter-atomic distance, notice how any individual atom can be excited but not both simultaneously. b) Two atoms are trapped by an excitation laser independently. Taken from "There can only be one [8]".

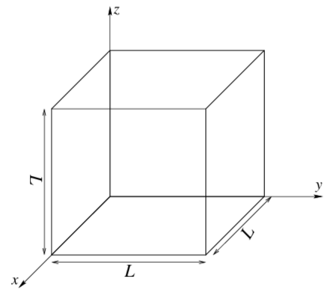

Figure 1.2: Linear Cavity. Cubic Volume of linear dimmensions L (Taken from Peter Lambropoulos, David Petrosyan, Fundamentals of Quantum Optics and Quantum Information [3])".

The Hamiltonian of this system has the following Jaynes-Cummings form:

$$\hat{H} = \hbar\omega\,\hat{a}^{\dagger}\hat{a} + \hat{H}_{2R} + \hat{H}_{RF} \tag{1.1}$$

where $\hat{a}^{\dagger}$, and $\hat{a}$ are the creation and annihilation operators respectively for the field mode with frequency ω in the cavity (See Appendix B for derivation). $\hat{H}_{2R}$ is the Hamiltonian for 2 interacting Rydberg atoms (2R) and $\hat{H}_{RF}$ is the interaction of the Rydberg atoms with the quantized field (RF).

For a Rydberg atom we associate the ground state $|g\rangle$ with qubit state $|0\rangle$ and the excited state $|r\rangle$ with qubit state $|1\rangle$. The following definitions are introduced:

$$\hat{\sigma}_{+} = \frac{1}{2}(\hat{\sigma}_x - i\hat{\sigma}_y) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{1.2}$$

$$\hat{\sigma}_{-} = \frac{1}{2}(\hat{\sigma}_x + i\hat{\sigma}_y) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{1.3}$$

Note that the signs in both (eq 1.2) and (eq 1.3) are inverted from those of spin raising/lowering operators, this is due to the definition of the qubit. (see Appendix A).

Obtaining,

$$\hat{\sigma}_{+}|0\rangle = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle, \tag{1.4}$$

$$\hat{\sigma}_{-}\left|1\right\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \left|0\right\rangle \tag{1.5}$$

which implies, $\hat{\sigma}_{+}\left|g\right\rangle = \left|r\right\rangle$ and $\hat{\sigma}_{-}\left|r\right\rangle = \left|g\right\rangle$ as desired. The Hamiltonian of a single Rydberg atom using qubit notation,

$$\begin{aligned} \hat{H}_R &= E_g\left|g\right\rangle\left\langle g\right| + E_r\left|r\right\rangle\left\langle r\right| = E_g\left|0\right\rangle\left\langle 0\right| + E_r\left|1\right\rangle\left\langle 1\right| = E_g\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + E_r\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} E_g & 0 \\ 0 & E_r \end{pmatrix} \equiv \begin{pmatrix} g & 0 \\ 0 & r \end{pmatrix} \end{aligned} \tag{1.6}$$

where we write $g := E_g$ and $r := E_r$ to simplify notation. Thus,

$$\begin{aligned} \hat{H}_R = \begin{pmatrix} g & 0 \\ 0 & r \end{pmatrix} &= \tfrac{1}{2}\begin{pmatrix} g+r & 0 \\ 0 & g+r \end{pmatrix} + \tfrac{1}{2}\begin{pmatrix} g-r & 0 \\ 0 & r-g \end{pmatrix} \\ &= \tfrac{1}{2}(g+r)\hat{I} + \tfrac{1}{2}(r-g)\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \equiv \tfrac{1}{2}gr\hat{I} - \tfrac{1}{2}\hbar\omega_0\hat{\sigma}_z \end{aligned} \tag{1.7}$$

with $gr \equiv g + r = E_g + E_r$ and $\hbar\omega_0 := r - g = E_r - E_g > 0$. The first term in the result of (1.7) corresponds to a global shift of energy so it can be neglected, resulting in,

$$\hat{H}_R = -\frac{1}{2}\hbar\omega_0\hat{\sigma}_z \tag{1.8}$$

Thus, for single atoms, transitions between $\left|g\right\rangle$ and $\left|r\right\rangle$ can be induced by excitation with light of frequency ω_0 including the interaction with photons results in the Jaynes–Cummings Hamiltonian (for single atoms) as described in Appendix B.

1.2 Two Interacting Rydberg Atoms

Consider two Rydberg atoms a, b with states $\left|a\right\rangle \otimes \left|b\right\rangle = \left|ab\right\rangle$. The Hamiltonian of two interacting atoms can be expressed as the sum of the Hamiltonians for two independent atoms plus an interaction term for the state $|rr\rangle$ in which both atoms are excited. The interaction is due to the Rydberg blockade, and it modifies only the energy of the state $|rr\rangle$. Thus, we obtain for two interacting Rydberg atoms (2R),

$$\begin{aligned}\hat{H}_{2R} &= \hat{H}_R^{(a)} \otimes \hat{I}^{(b)} + \hat{I}^{(a)} \otimes \hat{H}_R^{(b)} + \varepsilon \, |r\rangle \langle r|^{(a)} \otimes |r\rangle \langle r|^{(b)} \\ &\equiv \hat{H}_R \otimes \hat{I} + \hat{I} \otimes \hat{H}_R + \varepsilon \, |rr\rangle \langle rr|\end{aligned} \tag{1.9}$$

To simplify notation, in the second line we use the convention that the left side of tensor products $\otimes$ always applies to atom a and the right side to atom b. Note that, $|i\rangle \langle j| \otimes |k\rangle \langle l| = |ik\rangle \langle jl|$ (See Appendix A1.4). For $\varepsilon = 0$, Equation (1.9) corresponds to two independent atoms. For $\varepsilon > 0$, the energy of the state $|rr\rangle$ is $E_{rr} = 2E_r + \varepsilon$ and is shifted by an amount ε compared to two independent atoms. Thus, as long as both atoms are in the ground state or only one atom is excited, the two atoms are independent. Starting from the ground state $|gg\rangle$, each atom can be excited from its ground state $|g\rangle$ to its excited state $|r\rangle$ by light with frequency ω_0 . However, since $E_{rr} = 2E_r + \varepsilon$ the transition from $|gr\rangle$ or $|rg\rangle$ to $|rr\rangle$ is off-resonant and $|rr\rangle$ cannot be reached by light excitation with frequency ω_0 , this is the *Rydberg blockade*. For large ε the state $|rr\rangle$ is completely inaccessible. For small ε the state $|rr\rangle$ is accessible to some degree; furthermore, vε can be tuned by the distance between the atoms.

We can write $\hat{H}_{2R}$ in Equation (1.9) in matrix form, using Equation (1.6):

$$\begin{aligned}\hat{H}_{2R} &= \hat{H}_R \otimes \hat{I} + \hat{I} \otimes \hat{H}_R + \varepsilon \, |rr\rangle \langle rr| \\ &= \left(\tfrac{1}{2} gr\hat{I} - \tfrac{1}{2}\hbar\omega_0 \hat{\sigma}_z\right) \otimes \hat{I} + \hat{I} \otimes \left(\tfrac{1}{2} gr\hat{I} - \tfrac{1}{2}\hbar\omega_0 \hat{\sigma}_z\right) + \varepsilon \, |rr\rangle \langle rr| \\ &= gr\hat{I} \otimes \hat{I} - \hbar\omega_0 \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & 0 & \\ & & & -1 \end{pmatrix} + \varepsilon \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & 0 & \\ & & & 1 \end{pmatrix}\end{aligned} \tag{1.10}$$

[1] The first term $gr\hat{I}\otimes\hat{I}$ can again be neglected since it corresponds to a global shift in energy $gr\equiv g+r=E_g+E_r$ for the 2-atom system (is the average total energy for two independent atoms). Neglecting the term, we obtain in qubit notation:

$$\hat{H}_{2R}=-\hbar\omega_0\begin{pmatrix}1&&&\\&0&&\\&&0&\\&&&-1\end{pmatrix}+\varepsilon\begin{pmatrix}0&&&\\&0&&\\&&0&\\&&&1\end{pmatrix}=\begin{pmatrix}-\hbar\omega_0&&&\\&0&&\\&&0&\\&&&\hbar\left(\omega_0+\delta\omega\right)\end{pmatrix} \tag{1.11}$$

where we define the frequency shift $\delta\omega$ due to the Rydberg blockade by $\varepsilon=\hbar\delta\omega$. Recall that in qubit notation the top left entry corresponds to the ground state $|gg\rangle$ and the bottom right entry to the doubly excited state $|rr\rangle$. The diagonal elements in the middle correspond to $|rg\rangle$ and $|gr\rangle$, respectively. The zero point of energy is chosen as the average of the total energy for two independent atoms.

1.3 Interaction between Rydberg Atoms and Photons

1.3.1 One Atom

For a single atom at position z in the cavity, the Rydberg atom-field (RF) interaction in the dipole approximation is given by

$$H_{RF}=-\hat{\mathbf{d}}\cdot\hat{\mathbf{E}}\left(z\right)=-\hat{\mathbf{d}}\cdot\mathbf{E}_\omega\left(\hat{a}+\hat{a}^\dagger\right)\sin\left(kz\right)\equiv c\left(z\right)\hat{d}\left(\hat{a}+\hat{a}^\dagger\right) \tag{1.12}$$

Here $\hat{\mathbf{E}}\left(z\right)$ is the well known field operator and $\hat{\mathbf{d}}$ is the dipole operator of the atom, assumed to be parallel to $\hat{\mathbf{E}}$.

The coupling constant is given by

$$c\left(z\right)=-E_\omega\sin\left(kz\right) \tag{1.13}$$

[1] *Empty entries in matrices represent zeros*

The dipole operator $\hat{\mathbf{d}}$ is expressed as

$$\begin{aligned}\hat{d} &= |r\rangle\langle r|\hat{d}|g\rangle\langle g| + |g\rangle\langle g|\hat{d}|r\rangle\langle r| \\ &= d_{rg}|r\rangle\langle g| + d_{gr}|g\rangle\langle r| \\ &= d_{rg}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + d_{gr}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ &= d_{rg}\hat{\boldsymbol{\sigma}}_{+} + d_{gr}\hat{\boldsymbol{\sigma}}_{-}\end{aligned} \tag{1.14}$$

with the raising and lowering operators in qubit notation as

$$\hat{\boldsymbol{\sigma}}_{+} = |r\rangle\langle g| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad \hat{\boldsymbol{\sigma}}_{-} = |g\rangle\langle r| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{1.15}$$

Defining

$$d \equiv d_{gr} = \langle g|\hat{d}|r\rangle \tag{1.16}$$

and assuming without loss of generality that d is real; consequently, all the complex non-diagonal terms are real, which gives

$$\hat{d} = d\left(\hat{\boldsymbol{\sigma}}_{+} + \hat{\boldsymbol{\sigma}}_{-}\right) \tag{1.17}$$

Then using Equation (1.12) and Equation (1.17) the interaction Hamiltonian for a single atom

$$\begin{aligned}H_{RF} &= c(z)\,d\left(\hat{\boldsymbol{\sigma}}_{+} + \hat{\boldsymbol{\sigma}}_{-}\right)\left(\hat{a} + \hat{a}^{\dagger}\right) \\ &= \hbar\lambda(z)\left(\hat{\boldsymbol{\sigma}}_{+}\hat{a} + \hat{\boldsymbol{\sigma}}_{-}\hat{a} + \hat{\boldsymbol{\sigma}}_{+}\hat{a}^{\dagger} + \hat{\boldsymbol{\sigma}}_{-}\hat{a}^{\dagger}\right)\end{aligned} \tag{1.18}$$

with the coupling constant: $\hbar\lambda(z) = dc(z) = -dE_{\omega}\sin(kz)$.

1.3.2 Rotating Wave Approximation for One Atom

We now switch to the interaction picture. The photon operators with frequency ω gain the time dependence

$$\hat{a}(t) = \hat{a}\exp(-i\omega t) \qquad\qquad \hat{a}^{\dagger}(t) = \hat{a}^{\dagger}\exp(i\omega t) \tag{1.19}$$

Denoting $U_R(t) = \exp\left(-\frac{i}{\hbar}\hat{H}_R t\right)$ the free evolution operator for the atom, the transformation to the interaction picture is given by,

$$\begin{aligned} U_R^{\dagger}(t)\,\hat{\sigma}_+ U_R(t) &= \exp\left(\tfrac{i}{\hbar}\hat{H}_R t\right)|r\rangle\langle g|\exp\left(-\tfrac{i}{\hbar}\hat{H}_R t\right) \\ &= \exp\left(\tfrac{i}{\hbar}E_r' t\right)|r\rangle\langle g|\exp\left(-\tfrac{i}{\hbar}E_g t\right) \\ &= \hat{\sigma}_+\exp\left[\tfrac{i}{\hbar}\left(E_r' - E_g\right)t\right] \\ &= \hat{\sigma}_+\exp\left(i\omega' t\right) \end{aligned} \tag{1.20}$$

Thus,

$$\hat{\sigma}_+(t) = \hat{\sigma}_+\exp\left(i\omega' t\right) \tag{1.21}$$

Similarly it can be shown,

$$\hat{\sigma}_-(t) = \hat{\sigma}_-\exp\left(-i\omega' t\right) \tag{1.22}$$

where $\hbar\omega' = E_r' - E_g > 0$ is the energy difference between the excited state $|r\rangle$ of the atom relative to the ground state $|g\rangle$. For a single, free atom we have $\omega' = \omega_0$. However, for a system of 2 atoms, ω' for one atom depends on the state of the other atom:

$$\omega' = \begin{cases} \omega_0 \text{ if the other atom is in state } |g\rangle \\ \omega_0 + \delta\omega \text{ if the other atom is in state } |r\rangle \end{cases} \tag{1.23}$$

With these preparations, the interaction Hamiltonian for a single atom with transition frequency ω' is the same as the standard Jaynes-Cummings Hamiltonian. Using Equations (1.18), (1.19), (1.21) and (1.22),

$$H_{RF} = \hbar\lambda(z)\left[\hat{\sigma}_{+}\hat{a}\exp\left[i\left(\omega' - \omega\right)t\right] + \hat{\sigma}_{-}\hat{a}\exp\left[-i\left(\omega' + \omega\right)t\right] + \hat{\sigma}_{+}\hat{a}^{\dagger}\exp\left[i\left(\omega' + \omega\right)t\right] + \hat{\sigma}_{-}\hat{a}^{\dagger}\exp\left[-i\left(\omega' - \omega\right)t\right]\right] \tag{1.24}$$

In the rotating wave approximation, the fast oscillating terms (ω ,ω' appearing with same sign) are neglected:

$$H_{RF} = \hbar\lambda(z)\left[\hat{\sigma}_{+}\hat{a}\exp\left[i\left(\omega' - \omega\right)t\right] + \hat{\sigma}_{-}\hat{a}^{\dagger}\exp\left[-i\left(\omega' - \omega\right)t\right]\right] \tag{1.25}$$

Tuning the frequency of the light in the cavity so that $\omega = \omega_0$ (enabling transitions between ground state and excited state for free atoms), we obtain using (1.23),

$$H_{RF} = \hbar\lambda(z)\left(\hat{\sigma}_{+}\hat{a} + \hat{\sigma}_{-}\hat{a}^{\dagger}\right) \text{ if the other atom is in state } |g\rangle \tag{1.26}$$

$$H_{RF} = \hbar\lambda(z)\left[\hat{\sigma}_{+}\hat{a}\exp(i\delta\omega t) + \hat{\sigma}_{-}\hat{a}^{\dagger}\exp(-i\delta\omega t)\right] \text{ if the other atom is in state } |r\rangle \tag{1.27}$$

Equation (1.26) is the standard Jaynes-Cummings model after setting the detuning $\omega - \omega_0 = 0$. Equation (1.27) is a modified version of the JC model with oscillating terms $\exp(i\delta\omega t)$. If $\delta\omega$ is large enough then the transitions in Eq. (1.27) involving the state $|rr\rangle$ are essentially forbidden, which corresponds to the Rydberg blockade.

1.3.3 Two Atoms

We now assume for simplicity that the Rydberg blockade is in full effect, so that transitions $|g\rangle \to |r\rangle$ in one atom are forbidden if the other atom is in state $|r\rangle$. Using this constraint, we can construct the interaction Hamiltonian for two atoms using tensor products of 1-atom states as in the last section. To this end, we use the 1-atom Hamiltonian in (1.26) with (1.15), and the projection operator $\hat{P}_g = |g\rangle\langle g| = |0\rangle\langle 0|$ on the ground state of an atom to filter out the transitions that are forbidden by the Rydberg blockade. We also assume that atom a is at position z_a and atom b at position z_b in the cavity, and for simplicity we set $\lambda(z_a) = \lambda(z_b) = \lambda$ in (1.26). Then we obtain:

$$
\begin{aligned}
\hat{H}_{RF} &= \hbar\lambda\left(\hat{\sigma}_{+}\hat{a} + \hat{\sigma}_{-}\hat{a}^{\dagger}\right)\otimes\hat{P}_g + \hat{P}_g\otimes\hbar\lambda\left(\hat{\sigma}_{+}\hat{a} + \hat{\sigma}_{-}\hat{a}^{\dagger}\right)\\
&= \hbar\lambda\left(|r\rangle\langle g|\hat{a} + |g\rangle\langle r|\hat{a}^{\dagger}\right)\otimes\hat{P}_g + \hbar\lambda\hat{P}_g\otimes\left(|r\rangle\langle g|\hat{a} + |g\rangle\langle r|\hat{a}^{\dagger}\right)\\
&= \hbar\lambda\,|r\rangle\langle g|\otimes\hat{P}_g\hat{a} + \hbar\lambda\,|g\rangle\langle r|\otimes\hat{P}_g\hat{a}^{\dagger} + \hbar\lambda\hat{P}_g\otimes|r\rangle\langle g|\,\hat{a} + \hbar\lambda\hat{P}_g\otimes|g\rangle\langle r|\,\hat{a}^{\dagger}\\
&= \hbar\lambda\left[|r\rangle\langle g|\otimes\hat{P}_g + \hat{P}_g\otimes|r\rangle\langle g|\right]\hat{a} + \hbar\lambda\left[|g\rangle\langle r|\otimes\hat{P}_g + \hat{P}_g\otimes|g\rangle\langle r|\right]\hat{a}^{\dagger}\\
&= \hbar\lambda\left[\begin{pmatrix}0&0\\1&0\end{pmatrix}\otimes\begin{pmatrix}1&0\\0&0\end{pmatrix} + \begin{pmatrix}1&0\\0&0\end{pmatrix}\otimes\begin{pmatrix}0&0\\1&0\end{pmatrix}\right]\hat{a} +\\
&\hbar\lambda\left[\begin{pmatrix}0&1\\0&0\end{pmatrix}\otimes\begin{pmatrix}1&0\\0&0\end{pmatrix} + \begin{pmatrix}1&0\\0&0\end{pmatrix}\otimes\begin{pmatrix}0&1\\0&0\end{pmatrix}\right]\hat{a}^{\dagger}\\
&= \hbar\lambda\left[\begin{pmatrix} & & & \\ & & & \\ 1&0& & \\ 0&0& & \end{pmatrix} + \begin{pmatrix}0&0& & \\ 1&0& & \\ & & & \\ & & & \end{pmatrix}\right]\hat{a} + \\
&\hbar\lambda\left[\begin{pmatrix} & &1&0\\ & &0&0\\ & & & \\ & & & \end{pmatrix} + \begin{pmatrix}0&1& & \\ 0&0& & \\ & & & \\ & & & \end{pmatrix}\right]\hat{a}^{\dagger}\\
&= \hbar\lambda\begin{pmatrix} & & & \\ 1& & & \\ 1& & & \\ & & & \end{pmatrix}\hat{a} + \hbar\lambda\begin{pmatrix} &1&1& \\ & & & \\ & & & \\ & & & \end{pmatrix}\hat{a}^{\dagger}
\end{aligned}
\tag{1.28}
$$

Combining Eqs. (1.1), (1.26), (1.28) we obtain the full Hamiltonian:

$$\hat{H} = \hbar\omega\,\hat{a}^{\dagger}\hat{a} + \begin{pmatrix} -\hbar\omega_0 & & & \\ & 0 & & \\ & & 0 & \\ & & & \hbar\left(\omega_0 + \delta\omega\right) \end{pmatrix} + \hbar\lambda \begin{pmatrix} & & & \\ 1 & & & \\ 1 & & & \\ & & & \end{pmatrix} \hat{a} + \hbar\lambda \begin{pmatrix} & 1 & 1 & \\ & & & \\ & & & \\ & & & \end{pmatrix} \hat{a}^{\dagger} \tag{1.29}$$

$\hat{H}_{RF}$ was derived under the condition that transitions to $|rr\rangle = |11\rangle$ are forbidden due to the Rydberg blockade. This effectively reduces the system to a 3-state system with accessible states $|gg\rangle = |00\rangle$,$|gr\rangle = |01\rangle$,$|rg\rangle = |10\rangle$ while the state $|rr\rangle = |11\rangle$ can never be reached.

1.3.4 Towards a Quantum Circuit

For the *one atom* case using the free field hamiltonian $\hbar\omega\,\hat{a}^{\dagger}\hat{a}$, and Eqs (1.8) and (1.26) ,the Jaynes-Cummings Hamiltonian results to

$$\hat{H}/\hbar = \omega\,\hat{a}^{\dagger}\hat{a} - \frac{1}{2}\omega_0\hat{\sigma}_z + \lambda\left(\hat{\sigma}_+\hat{a} + \hat{\sigma}_-\hat{a}^{\dagger}\right) \tag{1.30}$$

which can be written using tensor products as,

$$\hat{H}/\hbar = \hat{I}\otimes\omega\,\hat{a}^{\dagger}\hat{a} - \frac{1}{2}\omega_0\hat{\sigma}_z\otimes\hat{I} + \lambda\left(\hat{\sigma}_+\hat{a} + \hat{\sigma}_-\hat{a}^{\dagger}\right) \tag{1.31}$$

For the *two atoms* case, the Hamiltonian in (1.29) acts on states $|a\rangle\otimes|b\rangle\otimes|\phi\rangle = |ab\phi\rangle$ where a , b are the atoms and $|\phi\rangle$ is the state of the photons. Using tensor products instead of matrices, the Hamiltonian in (1.1) has the form (using (1.10) and (1.28)),

$$\begin{aligned}\hat{H}/\hbar \,=\, & \omega \hat{I}\otimes\hat{I}\otimes \hat{a}^{\dagger}\hat{a} \,-\, \tfrac{1}{2}\omega_0\,\hat{\sigma}_z\otimes\hat{I}\otimes\hat{I}_P - \tfrac{1}{2}\omega_0\hat{I}\otimes\hat{\sigma}_z\otimes\hat{I}_P \\ & +\,\lambda\hat{\sigma}_+\otimes\hat{P}_g\otimes\hat{a} \,+\, \lambda\hat{\sigma}_-\otimes\hat{P}_g\otimes\hat{a}^{\dagger} \\ & +\,\lambda\hat{P}_g\otimes\hat{\sigma}_+\otimes\hat{a} + \lambda\hat{P}_g\otimes\hat{\sigma}_-\otimes\hat{a}^{\dagger}\end{aligned} \quad . \tag{1.32}$$

where $\hat{I}_P$ is the identity operator for the photons.

Now what remains is to build their respective quantum circuits, for that we need to express the operators in both (1.31) and (1.32) in terms of $\hat{\sigma}_x = X$, $\hat{\sigma}_y = Y$, $\hat{\sigma}_z = Z$, by no means a trivial task. We will continue onto the next chapter.

CHAPTER II

JAYNES CUMMINGS QUANTUM SIMULATION DERIVATION

The Hamiltonian of the Jaynes-Cummings model (JCM) for 1 atom in qubit notation is given by:

$$\hat{H}/\hbar = \omega \hat{a}^{\dagger}\hat{a} - \frac{1}{2}\omega_0 \hat{\sigma}_z + \lambda \left(\hat{\sigma}_+ \hat{a} + \hat{\sigma}_- \hat{a}^{\dagger} \right) \tag{2.1}$$

The Hamiltonian in (2.1) acts on 2-qubit states,

$$|\psi_2\rangle = |\text{atom}\rangle \otimes |\text{photon field}\rangle = |\psi_a\rangle \otimes |\psi_p\rangle \tag{2.2}$$

where a stands for atom and p stands for photon. (Here we assume that there is only one photon in the system; if there are more photons, we need more qubits to describe the photon field.) Both $|\psi_a\rangle$ and $|\psi_p\rangle$ are qubits and have the general form ,

$$|\psi_a\rangle = \alpha_a |0\rangle + \beta_a |1\rangle \qquad\qquad |\psi_p\rangle = \alpha_p |0\rangle + \beta_p |1\rangle \tag{2.3}$$

where $|0\rangle$, $|1\rangle$ means grounds state, excited state for the atom and no photon, one photon for the photon, respectively. Note that the 2-qubit state $|\psi_2\rangle$ may include entangled states, meaning that it cannot be factorized into a (tensor) product of the atom qubit and the photon qubit as in (2.2). The most general 2-qubit state is of the form,

$$|\psi_2\rangle = c_{00} |00\rangle + c_{01} |01\rangle + c_{10} |10\rangle + c_{11} |11\rangle \tag{2.4}$$

with $|ap\rangle = |a\rangle \otimes |p\rangle$ and complex coefficients c_{ap}.

2.1 Holstein Primakoff Transformation (HPT)

To construct a quantum cycle we need to transform the bosonic operators, this can be done with the help of the Holstein-Primakoff Transformation (HPT). The goal of the HPT is to map boson creation and annihilation operators $\hat{a}^\dagger$, $\hat{a}$, acting on the inifite-dimensional Fock space spanned by boson number states $\{|n\rangle_B; n = 0,1,2,\ldots\}$ to spin operators $\hat{S}_+$,$\hat{S}_-$,$\hat{S}_z$ acting on finite-dimensional spaces spanned by spin states $\{|s,m_s\rangle\,; s = 0,\, 1/2,\, 1,\, 3/2,\, \ldots\,; m_s = -s,\, -s+1,\, \ldots\,,\, s-1,\, s\}$. To this end, for given spin s the Fock space of bosons is truncated to a finite maximum number of bosons, $N = 2s$. The HPT then creates an isomorphism between the truncated Fock space $\{|n\rangle_B; n = 0,1,2,\ldots,N\}$ and spin states $\{|s,m_s\rangle\,; s = N/2\,; m_s = -s,\, -s+1,\, \ldots\,,\, s-1,\, s\}$. The precise mapping of states and operators in the HPT is described below.

2.1.1 Mapping of Spin States

Table 2.1: Map of Spin States

$\|s,m_s\rangle$ spin state $m_s = s-n$	$\|n\rangle_B$ boson number state n
s	0
$s-1$	1
$\vdots\ \vdots$	$\vdots$
$\hat{S}_+$	$\hat{a}^\dagger$
$\uparrow$	$\downarrow$
$\hat{S}_-$	$\hat{a}$
$\downarrow$	$\uparrow$
$\vdots$	$\vdots$
$-s+1$	$N-1$
$-s$	N

The operators $\hat{S}_+,\hat{S}_-$ create transitions $m_s \to m_s \pm 1$ between spin states and the operators $\hat{a}^\dagger,\hat{a}$ create transitions $n \to n \pm 1$ between boson number states as indicated. The spin state with maximum spin projection quantum number, $m_s = s$, is mapped to the vacuum state, $n = 0$, of bosons. The minimum (most negative) spin projection quantum number, $m_s = -s$, is mapped to the state with $N = 2s$ bosons.

2.1.2 Mapping of Operators

$$\hat{S}_{+} = \hbar\left(2s - \hat{a}^{\dagger}\hat{a}\right)^{1/2}\hat{a} \tag{2.5}$$

$$\hat{S}_{-} = \hbar\hat{a}^{\dagger}\left(2s - \hat{a}^{\dagger}\hat{a}\right)^{1/2} \tag{2.6}$$

$$\hat{S}_{z} = \hbar\left(s - \hat{a}^{\dagger}\hat{a}\right) \tag{2.7}$$

$$\hat{S}_{+} = \hat{S}_{x} + i\hat{S}_{y} \tag{2.8}$$

$$\hat{S}_{-} = \hat{S}_{x} - i\hat{S}_{y} \tag{2.9}$$

Using the bosonic commutation relation $\left[\hat{a},\hat{a}^{\dagger}\right] = 1$ one can verify the commutation relations required for spin operators $\left[\hat{S}_{+},\hat{S}_{-}\right] = 2\hbar\hat{S}_{z}$, $\left[\hat{S}_{z},\hat{S}_{+}\right] = \hbar\hat{S}_{+}$, $\left[\hat{S}_{z},\hat{S}_{-}\right] = -\hbar\hat{S}_{-}$.

For example, for a spin state $|s,m_s\rangle$ with state $\hat{S}_z|s,m_s\rangle = \hbar m_s|s,m_s\rangle$,the commutator relation $\left[\hat{S}_{z},\hat{S}_{+}\right] = \hbar\hat{S}_{+}$ implies $\hat{S}_z\hat{S}_+|s,m_s\rangle = \left(\hat{S}_+\hat{S}_z + \hbar\hat{S}_+\right)|s,m_s\rangle = \hbar\left(m_s+1\right)\hat{S}_+|s,m_s\rangle$.Thus, $\hat{S}_+|s,m_s\rangle$ is also an eigenstate of $\hat{S}_z$ where the eigenvalue has increased by one unit of $\hbar$.

2.2 HPT applied to the Subspaces $\mathscr{H}_n$ of JCH

In the HPT in the spin operators above $\hat{S}_{+}$, $\hat{S}_{-}$ depend on the boson number operator $\hat{n} = \hat{a}^{\dagger}\hat{a}$ in the square root. This makes the mapping $\hat{a}^{\dagger} \rightarrow \hat{S}_{+}$, $\hat{a} \rightarrow \hat{S}$ nonlinear, so that, in general, approximations are necessary, such as expanding the square roots. However, for the Jaynes-Cummings Hamiltonian (JCH) the mapping is exact, as we show below; this holds both for the original JCH for one atom (1.31), and our extension of the JCH to two atoms (1.32). The JCH for *one atom* the total Hilbert space of the system (atom, cavity field) decouples into subspaces $\mathscr{H}_n$= span$\{|e,n\rangle, |g,n+1\rangle\}$ for n = 0,1,2.. where n is the number of photons. Similarly, for our extension to 2 atoms, the total Hilbert space $\mathscr{H}$ of the system (atom a, atom b, cavity field) decouples into subspaces $\mathscr{H}_n = \text{span}\{|e,g,n\rangle, |g,e,n\rangle, |g,g,n+1\rangle\}$.

We now apply the HPT to the subspace $\mathscr{H}_\wr$ for given photon number n, for which the number of photons is restricted to n and $n+1$. To this end, we set the maximum number of photons to

$N = n+1$ and consider the HPT for the photon number states $n = N+1$ and $N-1 = n$ (Look at the last two lines in Table 1 above): Using (2.5),(2.6), and (2.7) with $/2s = N = n+1$ we find,

$\|s,m_s\rangle$ spin state $m_s = s-n$	$\|n\rangle$ boson number state n
$-s+1$	n
$-s$	$n+1$

Table 2.2: Truncated map

$$\hat{S}_+ = \hbar\left(n+1-\hat{a}^\dagger\hat{a}\right)^{1/2}\hat{a},\ \hat{S}_- = \hbar\hat{a}^\dagger\left(n+1-\hat{a}^\dagger\hat{a}\right)^{1/2},\ \hat{S}_z = \hbar\left(\frac{n+1}{2}-\hat{a}^\dagger\hat{a}\right) \tag{2.10}$$

These operators act on photon number states $|n\rangle$ and in the subspace $\mathscr{H}_n$ and $|n+1\rangle$ discussed above for 1 and 2 atoms; since the state of the atoms is not affected by the application of the cavity field operators, in the discussion below we only denote the photon number states $\mathscr{H}_n$ and $|n+1\rangle$ explicitly to simplify notation. In what follows, we apply the operators in (2.10) separately to the states $\mathscr{H}_n$ and $|n+1\rangle$ (for given states of the atom(s) in the subspace $\mathscr{H}_n$).

$$\begin{aligned}\hat{S}_+|n\rangle &= \hbar\left(n+1-\hat{a}^\dagger\hat{a}\right)^{1/2}\hat{a}\,|n\rangle = \hbar\left(n+1-\hat{a}^\dagger\hat{a}\right)^{1/2}\sqrt{n}\,|n-1\rangle \\ &= \hbar\,(n+1-(n-1))^{1/2}\sqrt{n}\,|n-1\rangle = \hbar\sqrt{2n}\,|n-1\rangle\end{aligned} \tag{2.11}$$

In the first line, we used $\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle$ and in the step to the second line we used that $\hat{a}^\dagger\hat{a} = \hat{n}$ is the number operator, thus $\hat{a}^\dagger\hat{a}\,|n-1\rangle = (n-1)\,|n-1\rangle$. Accordingly, the operation $\hat{S}_+|n\rangle$ results in a state $\propto |n-1\rangle$ not contained in $\mathscr{H}_n$). which reflects the fact that this process cannot occur in the system described by the JCH; for example, for the JCH with 1 atom, there is no mechanism by which a photon is annihilated (absorbed) when the atom is in the excited state $\propto |e\rangle$. Similarly, the operation,

$$\hat{S}_-|n+1\rangle = \hbar\hat{a}^\dagger\left(n+1-\hat{a}^\dagger\hat{a}\right)^{1/2}|n+1\rangle = \hbar\hat{a}^\dagger(n+1-(n+1))^{1/2}|n+1\rangle = 0 \tag{2.12}$$

cannot occur because there is no mechanism in the JCH by which a photon is created (emitted) when the atom(s) is (are) in the ground state $|g\rangle$. However, the following process is allowed:

$$\begin{aligned}\hat{S}_{+}|n+1\rangle &= \hbar\left(n+1-\hat{a}^{\dagger}\hat{a}\right)^{1/2}\hat{a}\,|n+1\rangle = \hbar\left(n+1-\hat{a}^{\dagger}\hat{a}\right)^{1/2}\sqrt{n+1}\,|n\rangle \\ &= \hbar\,(n+1-n)^{1/2}\sqrt{n+1}\,|n\rangle = \hbar\sqrt{n+1}\,|n\rangle \\ &= \hbar\hat{a}\,|n+1\rangle\end{aligned} \tag{2.13}$$

In the first line we used $\hat{a}\,|n+1\rangle = \sqrt{n+1}\,|n\rangle$. Thus, $\hat{S}_{+} = \hbar\hat{a}$ by the HPT when acting on the state $|n+1\rangle$. Similarly,

$$\begin{aligned}\hat{S}_{-}|n\rangle &= \hbar\hat{a}^{\dagger}\left(n+1-\hat{a}^{\dagger}\hat{a}\right)^{1/2}|n\rangle = \hbar\hat{a}^{\dagger}(n+1-n)^{1/2}|n\rangle = \hbar\hat{a}^{\dagger}|n\rangle \\ &= \hbar\sqrt{n+1}\,|n+1\rangle\end{aligned} \tag{2.14}$$

In the step to the second line we used $\hat{a}^{\dagger}|n\rangle = \sqrt{n+1}\,|n+1\rangle$. Thus,$\hat{S}_{-} = \hbar\hat{a}^{\dagger}$ by the HPT when acting on the state $|n\rangle$. In summary, the relations $\hat{a} = \hat{S}_{+}/\hbar$ and $\hat{a}^{\dagger} = \hat{S}_{-}/\hbar$ hold without approximation when applied to $\mathscr{H}_n$ for any $n = 0,1,2,....$ Finally, for $2s = N = n+1$, the operator relation, $\hat{S}_z = \hbar\left(\frac{n+1}{2} - \hat{a}^{\dagger}\hat{a}\right)$ in (2.10) is equivalent to the relation $m_s = s-n$ with $\hat{S}_z|s,m_s\rangle = \hbar m_s|s,m_s\rangle$ and $\hat{a}^{\dagger}\hat{a}\,|n\rangle = n\,|n\rangle$.

For each subspace $\mathscr{H}_n$ the quantized cavity field is spanned by the photon number states $|n\rangle$ and $|n+1\rangle$ representing a qubit $|\phi_c\rangle = \alpha_c|n\rangle + \beta_c|n+1\rangle$ with a spinor $\begin{pmatrix}\alpha_c\\ \beta_c\end{pmatrix} \in \mathscr{C}^2$. In the spinor representation, the basis of the qubit is given by $|n\rangle \triangleq \begin{pmatrix}1\\0\end{pmatrix}$ and $|n+1\rangle \triangleq \begin{pmatrix}0\\1\end{pmatrix}$.

In this basis, the operators $\hat{a}^{\dagger}$, $\hat{a}$, , and $\hat{a}^{\dagger}\hat{a} = \hat{n}$ take the form:

$$\hat{a}^{\dagger} = \sqrt{n+1}\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix} = \sqrt{n+1}\,\sigma_{+} \tag{2.15}$$

$$\hat{a} = \sqrt{n+1}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \sqrt{n+1}\,\sigma_- \tag{2.16}$$

and

$$\hat{n} \;=\; \hat{a}^\dagger \hat{a} \;=\; \begin{pmatrix} n & 0 \\ 0 & n+1 \end{pmatrix} \;=\; \frac{1}{2}\left[2n+1-\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] \;=\; \frac{1}{2}\,(2n+1-\sigma_z) \tag{2.17}$$

The qubit raising and lowering operators in (2.15), (2.16) are given in terms of Pauli matrices by

$$\sigma_+ = \frac{1}{2}\,(\sigma_x - i\sigma_y) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad \textit{and} \quad \sigma_- = \frac{1}{2}\,(\sigma_x + i\sigma_y) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{2.18}$$

For the special case $n = 0$ corresponding to the subspace $\mathscr{H}_0$ there is at most one photon in the system, so that the state $|\phi_c\rangle$of the cavity field is a superposition of $|0\rangle$ with no photon and $|1\rangle$ with one photon:

$$|\phi_c\rangle = \alpha_c\,|0\rangle + \beta_c\,|1\rangle \;\triangleq\; \begin{pmatrix} \alpha_c \\ \beta_c \end{pmatrix} \tag{2.19}$$

In this case,

$$\hat{a}^\dagger = \sigma_+, \quad \hat{a} = \sigma_-, \quad \hat{n} \;=\; \hat{a}^\dagger \hat{a} \;=\; \frac{1}{2}\,(1-\sigma_z) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{2.20}$$

Using $\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\;|n+1\rangle$ and $\hat{a}\,|n+1\rangle = \sqrt{n+1}\;|n\rangle$ one obtains:

$$\hat{a}^\dagger\,|0\rangle = |1\rangle\,, \quad \hat{a}\,|1\rangle = |0\rangle\,, \quad \hat{a}\,|0\rangle = 0, \quad \hat{a}^\dagger\,|1\rangle = \sqrt{2}\,|2\rangle \tag{2.21}$$

However, the two-photon state in the last line is not accessible to the system described by the JCH for the subspace $\mathscr{H}_\backslash$ as discussed above.

2.3 JCM for one Photon

Using (2.20) on the Jaynes Cummings Hamiltonian (2.1) becomes,

$$\hat{H}/\hbar = \hat{I} \otimes \frac{\omega}{2}\left(\hat{I} - \hat{\sigma}_z\right) - \frac{\omega_0}{2}\hat{\sigma}_z \otimes \hat{I} + \lambda\left(\hat{\sigma}_+ \otimes \hat{\sigma}_- + \hat{\sigma}_- \otimes \hat{\sigma}_+\right) \tag{2.22}$$

acting on states $|\psi_2\rangle = |\text{atom}\rangle \otimes |\text{photon field}\rangle = |\psi_a\rangle \otimes |\psi_p\rangle$ as in (2.2) (or on entangled states as in (2.4)). Thus, the left term in the tensor product $\otimes$ corresponds to the atom and the right term to the photon. The Hamiltonian can be simplified by disregarding a constant term $\hat{I} \otimes \omega \frac{1}{2} \hat{I}$ (first term on the right-hand side)[1] so that,

$$\hat{H}/\hbar = -\hat{I} \otimes \frac{\omega}{2}\hat{\sigma}_z - \frac{\omega_0}{2}\hat{\sigma}_z \otimes \hat{I} + \lambda\left(\hat{\sigma}_+ \otimes \hat{\sigma}_- + \hat{\sigma}_- \otimes \hat{\sigma}_+\right) \tag{2.23}$$

Using (2.18) and (2.20), the last term of eq (2.23) becomes,

$$\begin{aligned}
&\hat{\sigma}_+ \otimes \hat{\sigma}_- + \hat{\sigma}_- \otimes \hat{\sigma}_+ \\
&= \tfrac{1}{2}\left(\hat{\sigma}_x - i\hat{\sigma}_y\right) \otimes \tfrac{1}{2}\left(\hat{\sigma}_x + i\hat{\sigma}_y\right) + \tfrac{1}{2}\left(\hat{\sigma}_x + i\hat{\sigma}_y\right) \otimes \tfrac{1}{2}\left(\hat{\sigma}_x - i\hat{\sigma}_y\right) \\
&= \tfrac{1}{4}\left(\hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{\sigma}_y - i\hat{\sigma}_y \otimes \hat{\sigma}_x + i\hat{\sigma}_x \otimes \hat{\sigma}_y + \hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{\sigma}_y + i\hat{\sigma}_y \otimes \hat{\sigma}_x - i\hat{\sigma}_x \otimes \hat{\sigma}_y\right) \\
&= \tfrac{1}{2}\left(\hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{\sigma}_y\right)
\end{aligned} \tag{2.24}$$

The hamiltonian becomes,

$$\hat{H}/\hbar = -\hat{I} \otimes \frac{\omega}{2}\hat{\sigma}_z - \frac{\omega_0}{2}\hat{\sigma}_z \otimes \hat{I} + \frac{\lambda}{2}\left(\hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{\sigma}_y\right) \tag{2.25}$$

The deviation $\delta = \omega - \omega_0$ is the detuning parameter. Setting $\delta = 0$, i.e., $\omega = \omega_0$, then the Hamiltonian in (2.25) in units of $\hbar\omega$ becomes,

$$\frac{\hat{H}}{\hbar\omega} = -\frac{1}{2}\left(\hat{I} \otimes \hat{\sigma}_z + \hat{\sigma}_z \otimes \hat{I}\right) + \frac{\tilde{\lambda}}{2}\left(\hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{\sigma}_y\right) \tag{2.26}$$

[1] Identity matrices (I or $I \otimes I \otimes \ldots.$) stay constant since they have no effect on the quantum circuit.

with the dimensionless coupling constant,

$$\tilde{\lambda} = \frac{\lambda}{\omega} \tag{2.27}$$

2.3.1 Commutators

In what follows we assume that energies are given in units of $\hbar\omega$ and times in units of ω^{-1} and we skip the tilde symbol for $\tilde{\lambda}$ in (2.27) (assuming that λ is given in units of ω). The Hamiltonian in (2.26) then has the form,

$$\hat{H} = -\frac{1}{2}\left(\hat{I}\otimes\hat{\sigma}_z + \hat{\sigma}_z\otimes\hat{I}\right) + \frac{\lambda}{2}\left(\hat{\sigma}_x\otimes\hat{\sigma}_x + \hat{\sigma}_y\otimes\hat{\sigma}_y\right) \tag{2.28}$$

The only parameter is the dimensionless coupling constant λ. The Hamiltonian is a sum of terms $\hat{H}_k$:

$$\hat{H} = \sum_k \hat{H}_k \tag{2.29}$$

To implement a Hamiltonian of the form (2.29) in a quantum circuit we would like to express the evolution operator

$$\hat{U}(t) = \exp\left(-i\hat{H}t\right) \tag{2.30}$$

as a product of terms $\exp\left(-i\hat{H}_k t\right)$. This requires that the terms $\hat{H}_k$ commute. To proceed, we use the relation for operators (or matrices) A and B,

$$\exp(A+B) = \exp(A)\exp(B) \tag{2.31}$$

which holds if and only if A and B commute. [2]. We first show that the terms $A = \left(\hat{I}\otimes\,\hat{\sigma}_z + \hat{\sigma}_z\otimes\hat{I}\right)$ and $B = (\hat{\sigma}_x\otimes\hat{\sigma}_x +\,\hat{\sigma}_y\otimes\hat{\sigma}_y)$ in (2.28) commute.

$$\begin{aligned} [A,B] &= \left[\hat{I}\otimes\,\hat{\sigma}_z + \hat{\sigma}_z\otimes\hat{I},\;\hat{\sigma}_x\otimes\hat{\sigma}_x +\,\hat{\sigma}_y\otimes\hat{\sigma}_y\right] \\ &= \left[\hat{I}\otimes\,\hat{\sigma}_z,\;\hat{\sigma}_x\otimes\hat{\sigma}_x\right] + \left[\hat{I}\otimes\,\hat{\sigma}_z,\;\hat{\sigma}_y\otimes\hat{\sigma}_y\right] + \left[\hat{\sigma}_z\otimes\hat{I},\;\hat{\sigma}_x\otimes\hat{\sigma}_x\right] + \left[\hat{\sigma}_z\otimes\hat{I},\;\hat{\sigma}_y\otimes\hat{\sigma}_y\right] \end{aligned} \tag{2.32}$$

Using $(A\otimes B)(C\otimes D) = (AC)\otimes(BD)$ gives for the first term on the right-hand side of (2.32)

$$\begin{aligned} \left[\hat{I}\otimes\,\hat{\sigma}_z,\hat{\sigma}_x\otimes\hat{\sigma}_x\right] &= \left(\hat{I}\otimes\,\hat{\sigma}_z\right)(\hat{\sigma}_x\otimes\hat{\sigma}_x) - (\hat{\sigma}_x\otimes\hat{\sigma}_x)\left(\hat{I}\otimes\,\hat{\sigma}_z\right) \\ &= \hat{\sigma}_x\otimes\hat{\sigma}_z\hat{\sigma}_x - \hat{\sigma}_x\otimes\hat{\sigma}_x\hat{\sigma}_z = \hat{\sigma}_x\otimes[\hat{\sigma}_z,\hat{\sigma}_x] \;=\; 2i\hat{\sigma}_x\otimes\hat{\sigma}_y \end{aligned} \tag{2.33}$$

And similarly for the other terms in (2.32):

$$\begin{aligned} \left[\hat{I}\otimes\,\hat{\sigma}_z,\hat{\sigma}_y\otimes\hat{\sigma}_y\right] &= \left(\hat{I}\otimes\,\hat{\sigma}_z\right)(\hat{\sigma}_y\otimes\hat{\sigma}_y) - (\hat{\sigma}_y\otimes\hat{\sigma}_y)\left(\hat{I}\otimes\,\hat{\sigma}_z\right) \\ &= \hat{\sigma}_y\otimes\hat{\sigma}_z\hat{\sigma}_y - \hat{\sigma}_y\otimes\hat{\sigma}_y\hat{\sigma}_z = \hat{\sigma}_y\otimes[\hat{\sigma}_z,\hat{\sigma}_y] \;=\; -2i\hat{\sigma}_y\otimes\hat{\sigma}_x \end{aligned} \tag{2.34}$$

$$\begin{aligned} \left[\hat{\sigma}_z\otimes\hat{I},\hat{\sigma}_x\otimes\hat{\sigma}_x\right] &= \left(\hat{\sigma}_z\otimes\hat{I}\right)(\hat{\sigma}_x\otimes\hat{\sigma}_x) - (\hat{\sigma}_x\otimes\hat{\sigma}_x)\left(\hat{\sigma}_z\otimes\hat{I}\right) \\ &= \hat{\sigma}_z\hat{\sigma}_x\otimes\hat{\sigma}_x - \hat{\sigma}_x\hat{\sigma}_z\otimes\hat{\sigma}_x = [\hat{\sigma}_z,\hat{\sigma}_x]\otimes\hat{\sigma}_x \;=\; 2i\hat{\sigma}_y\otimes\hat{\sigma}_x \end{aligned} \tag{2.35}$$

$$\begin{aligned} \left[\hat{\sigma}_z\otimes\hat{I},\hat{\sigma}_y\otimes\hat{\sigma}_y\right] &= \left(\hat{\sigma}_z\otimes\hat{I}\right)(\hat{\sigma}_y\otimes\hat{\sigma}_y) - (\hat{\sigma}_y\otimes\hat{\sigma}_y)\left(\hat{\sigma}_z\otimes\hat{I}\right) \\ &= \hat{\sigma}_z\hat{\sigma}_y\otimes\hat{\sigma}_y - \hat{\sigma}_y\hat{\sigma}_z\otimes\hat{\sigma}_y = [\hat{\sigma}_z,\hat{\sigma}_y]\otimes\hat{\sigma}_y \;=\; -2i\hat{\sigma}_x\otimes\hat{\sigma}_y \end{aligned} \tag{2.36}$$

Inserting (2.33) – (2.36) in (2.32) gives

$$\begin{aligned} [A,B] &= \left[\hat{I}\otimes\,\hat{\sigma}_z + \hat{\sigma}_z\otimes\hat{I},\;\hat{\sigma}_x\otimes\hat{\sigma}_x +\,\hat{\sigma}_y\otimes\hat{\sigma}_y\right] \\ &= 2i\hat{\sigma}_x\otimes\hat{\sigma}_y - 2i\hat{\sigma}_y\otimes\hat{\sigma}_x + 2i\hat{\sigma}_y\otimes\hat{\sigma}_x - 2i\hat{\sigma}_x\otimes\hat{\sigma}_y = 0 \end{aligned} \tag{2.37}$$

This is a nontrivial cancellation of terms. Note that $[A,B] = 0$ only holds for the full form of the terms A and B. Using only one of the terms in B, for example gives $\left[\hat{I}\otimes\,\hat{\sigma}_z + \hat{\sigma}_z\otimes\hat{I},\;\hat{\sigma}_x\otimes\hat{\sigma}_x\right] \neq 0$

[2] If terms do not commute, we may use Trotter decomposition, more on that later

Using (2.31) and (2.37) we obtain for the Hamiltonian in (2.28)

$$\hat{U}(t) = \exp\left(-i\hat{H}t\right) = \exp\left[it\frac{1}{2}\left(\hat{I}\otimes\hat{\sigma}_z + \hat{\sigma}_z\otimes\hat{I}\right)\right]\exp\left[-it\frac{\lambda}{2}\left(\hat{\sigma}_x\otimes\hat{\sigma}_x + \hat{\sigma}_y\otimes\hat{\sigma}_y\right)\right] \tag{2.38}$$

Now we can decompose the terms in (2.38) even further. To this end we show:

$$1.\ \left[\hat{I}\otimes\hat{\sigma}_z, \hat{\sigma}_z\otimes\hat{I}\right] = 0: \quad \begin{aligned}\left[\hat{I}\otimes\hat{\sigma}_z, \hat{\sigma}_z\otimes\hat{I}\right] &= \left(\hat{I}\otimes\hat{\sigma}_z\right)\otimes\left(\hat{\sigma}_z\otimes\hat{I}\right) - \left(\hat{\sigma}_z\otimes\hat{I}\right)\left(\hat{I}\otimes\hat{\sigma}_z\right)\\ &= \hat{\sigma}_z\otimes\hat{\sigma}_z - \hat{\sigma}_z\otimes\hat{\sigma}_z = 0\end{aligned} \tag{2.39}$$

$$2.\ \left[\hat{\sigma}_x\otimes\hat{\sigma}_x, \hat{\sigma}_y\otimes\hat{\sigma}_y\right] = 0 \tag{2.40}$$

For this we use the following definition:

$$\left[\hat{\sigma}_a\otimes\hat{\sigma}_c, \hat{\sigma}_b\otimes\hat{\sigma}_d\right] = 2i\varepsilon_{abe}\delta_{cd}\left(\hat{\sigma}_e\otimes\hat{I}\right) + 2i\varepsilon_{cdf}\delta_{ab}\left(\hat{I}\otimes\hat{\sigma}_f\right) \tag{2.41}$$

Using (2.41) with a = c = x, b = d = y gives,

$$\left[\hat{\sigma}_x\otimes\hat{\sigma}_x, \hat{\sigma}_y\otimes\hat{\sigma}_y\right] = 2i\varepsilon_{xye}\delta_{xy}\left(\hat{\sigma}_e\otimes\hat{I}\right) + 2i\varepsilon_{xyf}\delta_{xy}\left(\hat{I}\otimes\hat{\sigma}_f\right) = 0 \tag{2.42}$$

because $\delta_{xy} = 0$ in both terms. Using again (2.31), but this time with (2.40), (2.42), we obtain for (2.38),

$$\begin{aligned}\hat{U}(t) = \exp\left(-i\hat{H}t\right) = \exp\left(it\frac{1}{2}\hat{I}\otimes\hat{\sigma}_z\right)\exp\left(it\frac{1}{2}\hat{\sigma}_z\otimes\hat{I}\right)\cdot\ldots\\ \ldots\exp\left(-it\frac{\lambda}{2}\hat{\sigma}_x\otimes\hat{\sigma}_x\right)\exp\left(-it\frac{\lambda}{2}\hat{\sigma}_y\otimes\hat{\sigma}_y\right)\end{aligned} \tag{2.43}$$

It is interesting to note that (2.43) holds even though some of the factors in (2.43) do not commute. For example, $\hat{\sigma}_z\otimes\hat{I}$ does not commute with $\hat{\sigma}_x\otimes\hat{\sigma}_x$, thus the second and third exponential factors in (2.43) do not commute. One needs to perform the two-step process first deriving (2.38) and then (2.43) as shown above.

2.4 Single Atom Quantum Circuit

To translate the evolution operator in (2.43) into a quantum circuit, we need to present some definitions,

Rotation Operator:

$$R_\alpha(\theta) = \exp\left(-i\frac{\theta}{2}\sigma_\alpha\right) \quad where \quad \alpha = x, y, z \tag{2.44}$$

We also define:

$$H\sigma_z H = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \sigma_x \tag{2.45}$$

$$U'\sigma_z U' = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix} = \sigma_y \tag{2.46}$$

[3] Where U' is defined as:

$$U(\theta,\phi,\lambda) = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -\exp(i\lambda)\sin\left(\frac{\theta}{2}\right) \\ \exp(i\phi)\sin\left(\frac{\theta}{2}\right) & \exp(i(\phi+\lambda))\cos\left(\frac{\theta}{2}\right) \end{pmatrix}$$
$$U'\left(\frac{\pi}{2},\frac{\pi}{2},\frac{\pi}{2}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \tag{2.47}$$

Using [4]

$$\exp(iAx) = \cos(x)I + i\sin(x)A \tag{2.48}$$

where A is a matrix such that $A^(2) = I$ We can conclude,

$$\exp\left(-i\delta\sigma_\alpha \otimes \sigma_\beta\right) = \cos(-\delta)I \otimes I + i\sin(-\delta)\sigma_\alpha \otimes \sigma_\beta \tag{2.49}$$

[3]Note: The definitions stated here can vary, for example one can use the definitions stated in [9] (which are the ones stated above) or one can use the definitions stated in [6] which are different but should portray similar results.

which holds because,

$$\left(\sigma_\alpha \otimes \sigma_\beta\right)^2 = \left(\sigma_\alpha\right)^2 \otimes \left(\sigma_\beta\right)^2 = I \otimes I = I_4 \tag{2.50}$$

Let us consider the following expression:

$$[U' \otimes U']CNOT[I \otimes R_Z(2\delta)]CNOT[U' \otimes U'] \tag{2.51}$$

Using $R_z(2\delta) = \exp(-i\delta\sigma_z)$ and the result for the first circuit in [6] we obtain the middle part in (2.51),

$$\begin{aligned} &CNOT[I \otimes R_Z(2\delta)]CNOT = CNOT[I \otimes \exp(-i\delta\sigma_z)]CNOT \\ &= \exp(-i\delta\sigma_z \otimes \sigma_z) = \cos(-\delta)I \otimes I + i\sin(-\delta)\sigma_z \otimes \sigma_z \end{aligned} \tag{2.52}$$

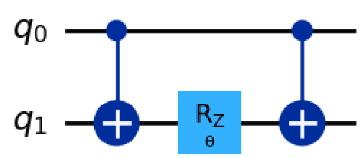

Figure 2.1: $\exp(-i\delta\sigma_z \otimes \sigma_z)$

Inserting (2.52) in (2.51) and multiplying out we obtain,

$$\begin{aligned} &[U' \otimes U'][\cos(-\delta)I \otimes I + i\sin(-\delta)\sigma_z \otimes \sigma_z][U' \otimes U'] \\ &= [\cos(-\delta)U' \otimes U' + i\sin(-\delta)(U'\sigma_z) \otimes (U'\sigma_z)][U' \otimes U'] \\ &= \cos(-\delta)I \otimes I + i\sin(-\delta)(U'\sigma_z U') \otimes (U'\sigma_z U') \\ &= \cos(-\delta)I \otimes I + i\sin(-\delta)\sigma_y \otimes \sigma_y \\ &= \exp(-i\delta\sigma_y \otimes \sigma_y) \end{aligned} \tag{2.53}$$

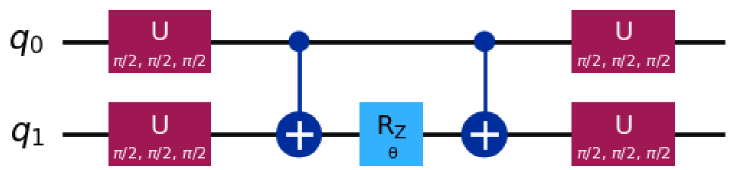

Figure 2.2: $\exp(-i\delta\sigma_y \otimes \sigma_y)$

Similarly it can be shown,

$$\exp(-i\delta\sigma_x \otimes \sigma_x) = [H \otimes H]CNOT[I \otimes R_Z(2\delta)]CNOT[H \otimes H] \tag{2.54}$$

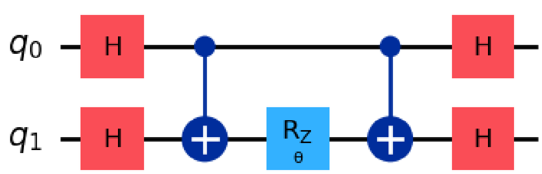

Figure 2.3: $\exp(-i\delta\sigma_x \otimes \sigma_x)$

Thus, we can express $\hat{U}(t)$ in (2.43) by using (2.52), (2.53), (2.54) and gates (2.44): [4]

$$\boxed{\hat{U}(t) = \begin{array}{r} R_z(-t) \otimes R_z(-t) \\ [H \otimes H]\text{CNOT}[I \otimes R_z(2\delta)]\text{CNOT}[H \otimes H] \\ [U' \otimes U']\text{CNOT}[I \otimes R_z(2\delta)]\text{CNOT}[U' \otimes U'] \end{array}} \tag{2.55}$$

where $\delta = t\frac{\lambda}{2}$, due to the definition of (2.43).

[4]We shall comeback for more context in the next chapter, for now we will focus on the derivation only on the final result.

2.5 Towards a Rydberg Blockade Hamiltonian Quantum Circuit (RBH)

With that being said, we are now ready to explore more interesting Hamiltonian, let us go back to eq. (1.32),

$$\begin{aligned}\hat{H}/\hbar \,=\, &\omega \hat{I}\otimes\hat{I}\otimes \hat{a}^{\dagger}\hat{a} \,-\, \tfrac{1}{2}\omega_0\,\hat{\sigma}_z\otimes\hat{I}\otimes\hat{I}_P - \tfrac{1}{2}\omega_0\hat{I}\otimes\hat{\sigma}_z\otimes\hat{I}_P \\ &+\, \lambda\,\hat{\sigma}_+\otimes\hat{P}_g\otimes\hat{a} \,+\, \lambda\,\hat{\sigma}_-\otimes\hat{P}_g\otimes\hat{a}^{\dagger} \\ &+\, \lambda\hat{P}_g\otimes\hat{\sigma}_+\otimes\hat{a} + \lambda\hat{P}_g\otimes\hat{\sigma}_-\otimes\hat{a}^{\dagger}\end{aligned} \quad . \tag{2.56}$$

Where $\hat{I}_P$ is the identity operator for the photons (in what follows we write $\hat{I}=\hat{I}_p$) and $\tilde{\lambda}=\frac{\lambda}{\omega}$.

The Hamiltonian (2.56) acts on states $|a\rangle\otimes|b\rangle\otimes|\phi\rangle = |ab\phi\rangle$ where a,b are the atoms and $|\phi\rangle$ is the state of the photons. If the Rydberg blockade is in full effect, a state in which both atoms are excited cannot be reached: if one atom is excited, the other atom must be in the ground state. If there is one excitation in the system, for example by using the initial condition: $|\phi\rangle = |001\rangle$ (at t=0) corresponding to “both atoms in ground state, 1 photon”, this one excitation will be conserved, that is, the space of accessible states is confined to the subspace spanned by the 3 basis states. (In this order)

$$|001\rangle\,,|010\rangle\,,|100\rangle \tag{2.57}$$

A general state accessible to the system can then be expanded as

$$|\psi\rangle = c_1\,|001\rangle + c_2\,|010\rangle + c_3\,|100\rangle \tag{2.58}$$

using the notation: $c_1 = c_{001}, \quad c_2 = c_{010}, \quad c_3 = c_{100}$

The use of the projection operators $\hat{P}_g$ to the ground states of the atoms in (2.56) is actually not necessary, and can be replaced by the identity operator $\hat{I}$. To see this, consider for example the term $\lambda\hat{\sigma}_+\otimes\hat{P}_g\otimes\hat{a}$ in (2.56). It describes a process where atom a absorbs a photon and thereby is excited from the ground state to the excited state (described by $\hat{\sigma}_+$) while the photon is destroyed (described by $\hat{a}$). This is only possible if initially atom a was in the ground state and one photon was present. [5] This corresponds to a transition between basis states $|001\rangle \rightarrow |100\rangle$ where atom b (the middle entry) remains in the ground state.

Replacing in (2.56) by $\hat{I}$ and setting $\omega = \omega_0$ (zero detuning) we obtain

$$\begin{aligned} \frac{\hat{H}}{\hbar\omega} &= \hat{I}\otimes\hat{I}\otimes\hat{a}^{\dagger}\hat{a} - \tfrac{1}{2}\hat{\sigma}_z\otimes\hat{I}\otimes\hat{I} - \tfrac{1}{2}\hat{I}\otimes\hat{\sigma}_z\otimes\hat{I} \\ &+ \tilde{\lambda}\hat{\sigma}_+\otimes\hat{I}\otimes\hat{a} + \tilde{\lambda}\hat{\sigma}_-\otimes\hat{I}\otimes\hat{a}^{\dagger} \\ &+ \tilde{\lambda}\hat{I}\otimes\hat{\sigma}_+\otimes\hat{a} + \tilde{\lambda}\hat{I}\otimes\hat{\sigma}_-\otimes\hat{a}^{\dagger} \end{aligned} \tag{2.59}$$

with $\tilde{\lambda} = \frac{\lambda}{\omega}$. In what follows we simplify notation by writing $\lambda = \tilde{\lambda}$ (omitting the tilde). Using (2.20), and disregarding the constant term $\hat{I}\otimes\hat{I}\otimes\frac{1}{2}\hat{I}$ (for fixed ω) we find:

$$\begin{aligned} \frac{\hat{H}}{\hbar\omega} &= -\tfrac{1}{2}\left(\hat{I}\otimes\hat{I}\otimes\hat{\sigma}_z + \hat{\sigma}_z\otimes\hat{I}\otimes\hat{I} + \hat{I}\otimes\hat{\sigma}_z\otimes\hat{I}\right) \\ &+ \lambda\left(\hat{\sigma}_+\otimes\hat{I}\otimes\hat{a} + \hat{\sigma}_-\otimes\hat{I}\otimes\hat{a}^{\dagger} + \hat{I}\otimes\hat{\sigma}_+\otimes\hat{a} + \hat{I}\otimes\hat{\sigma}_-\otimes\hat{a}^{\dagger}\right) \end{aligned} \tag{2.60}$$

Note that in (2.60) we still use $\hat{a},\hat{a}^{\dagger}$ operators for the photon. The first two terms in the 2$^{\text{nd}}$ line of (2.60) describe the interaction of the photon with atom a, and the last two terms describe the interaction of the photon with atom b.

2.5.1 Commutator Issue

We can write eq. (2.60) as $\frac{\hat{H}}{\hbar\omega} = -\frac{1}{2}\hat{A} + \frac{\lambda}{2}\hat{B}$ with,

$$\hat{A} = \hat{I}\otimes\hat{I}\otimes\hat{\sigma}_z + \hat{\sigma}_z\otimes\hat{I}\otimes\hat{I} + \hat{I}\otimes\hat{\sigma}_z\otimes\hat{I} \tag{2.61}$$

$$\hat{B} = \hat{\sigma}_+\otimes\hat{I}\otimes\hat{a} + \hat{\sigma}_-\otimes\hat{I}\otimes\hat{a}^{\dagger} + \hat{I}\otimes\hat{\sigma}_+\otimes\hat{a} + \hat{I}\otimes\hat{\sigma}_-\otimes\hat{a}^{\dagger} \tag{2.62}$$

[5] Because $\hat{\sigma}_+|1\rangle_a = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$ and $\hat{a}|0\rangle_P = 0$

Since $\hat{A}$ corresponds to the "total excitation number" of atoms and photons, which is conserved and equal to 1 in the present system, and since $\hat{A}$ conserves this number, it can be shown that

$$\left[\hat{A},\hat{B}\right]=0 \tag{2.63}$$

Furthermore, it is easy to see that the three terms in $\hat{A}$ pairwise commute among each other. For example,

$$\begin{aligned}&\left[\hat{I}\otimes\hat{I}\otimes\ \hat{\sigma}_z\,,\ \hat{\sigma}_z\otimes\hat{I}\otimes\hat{I}\right]\\&=\left(\hat{I}\otimes\hat{I}\otimes\ \hat{\sigma}_z\right)\left(\hat{\sigma}_z\otimes\hat{I}\otimes\hat{I}\right)-\left(\hat{\sigma}_z\otimes\hat{I}\otimes\hat{I}\right)\left(\hat{I}\otimes\hat{I}\otimes\ \hat{\sigma}_z\right)\\&=\hat{\sigma}_z\otimes\hat{I}\otimes\ \hat{\sigma}_z-\hat{\sigma}_z\otimes\hat{I}\otimes\ \hat{\sigma}_z=0\end{aligned} \tag{2.64}$$

We can therefore write,

$$\begin{aligned}\exp\left(\hat{A}\right)\ &=\exp\ \left(\hat{I}\otimes\hat{I}\otimes\ \hat{\sigma}_z+\ \hat{\sigma}_z\otimes\hat{I}\otimes\hat{I}+\ \hat{I}\otimes\hat{\sigma}_z\otimes\hat{I}\right)\\&=\exp\left(\hat{I}\otimes\hat{I}\otimes\ \hat{\sigma}_z\right)\ \exp\left(\hat{\sigma}_z\otimes\hat{I}\otimes\hat{I}\right)\ \exp\left(\hat{\sigma}_z\otimes\hat{I}\otimes\hat{I}\right)\end{aligned} \tag{2.65}$$

similar to the first two terms in (2.43).

Next we consider the operator B in (2.62). Similarly as in (2.65) we would like to write $\exp\left(\hat{B}\right)$ as a product of exponentials of single operators. However, this does not seem to be possible because the operators in $\hat{B}$ do not commute. Consider the commutator,

$$\left[\hat{\sigma}_+\otimes\hat{I}\otimes\ \hat{a}\ +\ \hat{\sigma}_-\otimes\hat{I}\otimes\ \hat{a}^\dagger\,,\ \hat{I}\otimes\hat{\sigma}_+\otimes\hat{a}\ +\ \hat{I}\otimes\hat{\sigma}_-\otimes\ \hat{a}^\dagger\right] \tag{2.66}$$

we want to see if the overall interaction of the photon with atom a commutes with the interaction of the photon with atom b. To simplify notation, we temporarily omit the $\otimes$ symbol, keeping in mind that the terms are tensor product of three operators in the given order,

$$
\begin{aligned}
&\left[\hat{\sigma}_+ \otimes \hat{I} \otimes \hat{a} + \hat{\sigma}_- \otimes \hat{I} \otimes \hat{a}^\dagger , \hat{I} \otimes \hat{\sigma}_+ \otimes \hat{a} + \hat{I} \otimes \hat{\sigma}_- \otimes \hat{a}^\dagger\right] \\
&= \left[\hat{\sigma}_+ \hat{I} \hat{a} + \hat{\sigma}_- \hat{I} \hat{a}^\dagger , \hat{I} \hat{\sigma}_+ \hat{a} + \hat{I} \hat{\sigma}_- \hat{a}^\dagger\right] \\
&= \left(\hat{\sigma}_+ \hat{I} \hat{a} + \hat{\sigma}_- \hat{I} \hat{a}^\dagger\right)\left(\hat{I} \hat{\sigma}_+ \hat{a} + \hat{I} \hat{\sigma}_- \hat{a}^\dagger\right) - \left(\hat{I} \hat{\sigma}_+ \hat{a} + \hat{I} \hat{\sigma}_- \hat{a}^\dagger\right)\left(\hat{\sigma}_+ \hat{I} \hat{a} + \hat{\sigma}_- \hat{I} \hat{a}^\dagger\right)
\end{aligned}
\tag{2.67}
$$

$$
\begin{aligned}
&= \hat{\sigma}_+ \hat{\sigma}_+ (\hat{a}\hat{a}) + \hat{\sigma}_- \hat{\sigma}_- \left(\hat{a}^\dagger \hat{a}^\dagger\right) + \hat{\sigma}_+ \hat{\sigma}_- \left(\hat{a}\hat{a}^\dagger\right) + \hat{\sigma}_- \hat{\sigma}_+ \left(\hat{a}^\dagger \hat{a}\right) \\
&- \hat{\sigma}_+ \hat{\sigma}_+ (\hat{a}\hat{a}) - \hat{\sigma}_- \hat{\sigma}_- \left(\hat{a}^\dagger \hat{a}^\dagger\right) - \hat{\sigma}_- \hat{\sigma}_+ \left(\hat{a}\hat{a}^\dagger\right) - \hat{\sigma}_+ \hat{\sigma}_- \left(\hat{a}^\dagger \hat{a}\right)
\end{aligned}
$$

The four terms on the left cancel, and using $\hat{a}\hat{a}^\dagger = \hat{a}^\dagger \hat{a} + \hat{I}$ (from $\left[\hat{a}, \hat{a}^\dagger\right] = \hat{I}$) the remaining terms give

$$
\begin{aligned}
&= \hat{\sigma}_+ \hat{\sigma}_- \left(\hat{a}^\dagger \hat{a} + \hat{I}\right) + \hat{\sigma}_- \hat{\sigma}_+ \left(\hat{a}^\dagger \hat{a}\right) - \hat{\sigma}_- \hat{\sigma}_+ \left(\hat{a}^\dagger \hat{a} + \hat{I}\right) - \hat{\sigma}_+ \hat{\sigma}_- \left(\hat{a}^\dagger \hat{a}\right) \\
&= \hat{\sigma}_+ \hat{\sigma}_- \hat{I} - \hat{\sigma}_- \hat{\sigma}_+ \hat{I} \\
&= \hat{\sigma}_+ \otimes \hat{\sigma}_- \otimes \hat{I} - \hat{\sigma}_- \otimes \hat{\sigma}_+ \otimes \hat{I} \neq 0
\end{aligned}
\tag{2.68}
$$

So (2.66) does not commute. We can try transform the $\hat{\sigma}_+$, $\hat{\sigma}_-$ operators in B to $\hat{\sigma}_x$, $\hat{\sigma}_y$ operators and $\hat{a}^\dagger = \hat{\sigma}_+$, $\hat{a} = \hat{\sigma}_-$ for the photon operators.

Let us try,

$$
\begin{aligned}
2\hat{B} &= \hat{\sigma}_x \otimes \hat{I} \otimes \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{I} \otimes \hat{\sigma}_y + \hat{I} \otimes \hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{I} \otimes \hat{\sigma}_y \otimes \hat{\sigma}_y \\
&= \hat{C}' + \hat{D}'
\end{aligned}
\tag{2.69}
$$

with $\hat{C}' = \hat{\sigma}_x \otimes \hat{I} \otimes \hat{\sigma}_x + \hat{I} \otimes \hat{\sigma}_y \otimes \hat{\sigma}_y$, $\quad \hat{D}' = \hat{\sigma}_y \otimes \hat{I} \otimes \hat{\sigma}_y + \hat{I} \otimes \hat{\sigma}_x \otimes \hat{\sigma}_x$.

Now we find

$$
\begin{aligned}
\left[\hat{C}', \hat{D}'\right] \ &= \ \left[\hat{\sigma}_x \otimes \hat{I} \otimes \ \hat{\sigma}_x \ + \ \hat{I} \otimes \hat{\sigma}_y \otimes \ \hat{\sigma}_y, \ \hat{\sigma}_y \otimes \hat{I} \otimes \ \hat{\sigma}_y \ + \ \hat{I} \otimes \hat{\sigma}_x \otimes \ \hat{\sigma}_x\right] \\
&= \ \left(\hat{\sigma}_x \otimes \hat{I} \otimes \ \hat{\sigma}_x \ + \hat{I} \otimes \hat{\sigma}_y \otimes \ \hat{\sigma}_y\right)\left(\hat{\sigma}_y \otimes \hat{I} \otimes \ \hat{\sigma}_y \ + \hat{I} \otimes \hat{\sigma}_x \otimes \ \hat{\sigma}_x\right) \\
&- \ \left(\hat{\sigma}_y \otimes \hat{I} \otimes \ \hat{\sigma}_y \ + \hat{I} \otimes \hat{\sigma}_x \otimes \ \hat{\sigma}_x\right)\left(\hat{\sigma}_x \otimes \hat{I} \otimes \ \hat{\sigma}_x \ + \hat{I} \otimes \hat{\sigma}_y \otimes \ \hat{\sigma}_y\right) \\
&= \ \hat{\sigma}_x \hat{\sigma}_y \otimes \hat{I} \otimes \ \hat{\sigma}_x \hat{\sigma}_y \ + \hat{I} \otimes \hat{\sigma}_y \hat{\sigma}_x \otimes \hat{\sigma}_y \hat{\sigma}_x \ + \ \hat{\sigma}_x \otimes \hat{\sigma}_x \otimes \ \hat{\sigma}_x \hat{\sigma}_x \ + \ \hat{\sigma}_y \otimes \ \hat{\sigma}_y \otimes \ \hat{\sigma}_y \hat{\sigma}_y \\
&- \hat{\sigma}_y \hat{\sigma}_x \otimes \hat{I} \otimes \ \hat{\sigma}_y \hat{\sigma}_x - \ \hat{I} \otimes \hat{\sigma}_x \hat{\sigma}_y \otimes \hat{\sigma}_x \hat{\sigma}_y \ - \ \hat{\sigma}_y \otimes \ \hat{\sigma}_y \otimes \ \hat{\sigma}_y \hat{\sigma}_y - \ \hat{\sigma}_x \otimes \hat{\sigma}_x \otimes \ \hat{\sigma}_x \hat{\sigma}_x \\
&= 0
\end{aligned}
\tag{2.70}
$$

The four terms on the left cancel again because of $\hat{\sigma}_y \hat{\sigma}_x = - \ \hat{\sigma}_x \hat{\sigma}_y$ (from $\left\{\hat{\sigma}_x, \hat{\sigma}_y\right\} = 0$), the four terms on the right cancel directly.

Therefore we derive the following expression by substituting back,

$$
\begin{aligned}
\frac{\hat{H}}{\hbar\omega} \ = \ -\tfrac{1}{2}\left(\hat{I} \otimes \hat{I} \otimes \ \hat{\sigma}_z + \ \hat{\sigma}_z \otimes \hat{I} \otimes \hat{I} + \ \hat{I} \otimes \hat{\sigma}_z \otimes \hat{I}\right) + \\
\tfrac{\lambda}{4}\left(\hat{\sigma}_x \otimes \hat{I} \otimes \ \hat{\sigma}_x \ + \ I \otimes \hat{\sigma}_y \otimes \ \hat{\sigma}_y \ + \ I \otimes \hat{\sigma}_x \otimes \ \hat{\sigma}_x \ + \hat{\sigma}_y \otimes \hat{I} \otimes \ \hat{\sigma}_y\right)
\end{aligned}
\tag{2.71}
$$

Using (2.30),

$$
\begin{aligned}
&\exp(-i\hat{H}t) = \exp\left(it\tfrac{1}{2}\hat{I} \otimes \hat{I} \otimes \ \hat{\sigma}_z\right) \ \exp\left(it\tfrac{1}{2}\hat{I} \otimes \ \hat{\sigma}_z \otimes I\right) \exp\left(it\tfrac{1}{2}\,\hat{\sigma}_z \otimes I \otimes I\right) \\
&\exp\left(-it\tfrac{\lambda}{4}\left(\hat{\sigma}_x \otimes \hat{I} \otimes \ \hat{\sigma}_x + I \otimes \hat{\sigma}_y \otimes \ \hat{\sigma}_y \ \right)\right) \exp\left(-it\tfrac{\lambda}{4}\left(I \otimes \hat{\sigma}_x \otimes \ \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{I} \otimes \ \hat{\sigma}_y\right)\right)
\end{aligned}
\tag{2.72}
$$

The last two terms of eq. (2.72) have terms that do not commute each other, and for this we make use of Trotter decomposition [6].

[6] See Appendix C

2.5.2 Trotter and Final Result

Trotter Formula of the first order:

$$\begin{aligned}
&\exp(\hat{A}+\hat{B}) = \lim_{n\to\infty}\left(\exp\left(\tfrac{\hat{A}}{n}\right)\exp\left(\tfrac{\hat{B}}{n}\right)\right)^n \\
&\textit{where} \\
&\exp(\delta(\hat{A}+\hat{B})) = \exp(\delta\hat{A})\exp(\delta\hat{B}) + O(\delta^2)
\end{aligned} \tag{2.73}$$

applying (2.73) to the last two terms of (2.72) yields,

$$\begin{aligned}
&\exp(-it\tfrac{\lambda}{4}\,(\hat{\sigma}_x\otimes\hat{I}\otimes\ \hat{\sigma}_x + I\otimes\hat{\sigma}_y\otimes\ \hat{\sigma}_y\ )) = \\
&\lim_{n\to\infty}\left(\exp\left(\tfrac{-i\lambda t}{4n}\right)(\hat{\sigma}_x\otimes\hat{I}\otimes\ \hat{\sigma}_x)\exp\left(\tfrac{-i\lambda t}{4n}\right)(I\otimes\hat{\sigma}_y\otimes\ \hat{\sigma}_y)\right)^n
\end{aligned} \tag{2.74}$$

$$\begin{aligned}
&\exp(-it\tfrac{\lambda}{4}\,(I\otimes\hat{\sigma}_x\otimes\ \hat{\sigma}_x + \hat{\sigma}_y\otimes\hat{I}\otimes\ \hat{\sigma}_y)) = \\
&\lim_{n\to\infty}\left(\exp\left(\tfrac{-i\lambda t}{4n}\right)(I\otimes\hat{\sigma}_x\otimes\ \hat{\sigma}_x)\exp\left(\tfrac{-i\lambda t}{4n}\right)(\hat{\sigma}_y\otimes\hat{I}\otimes\ \hat{\sigma}_y)\right)^n
\end{aligned} \tag{2.75}$$

Applying both (2.74) and (2.75) into (2.72),

$$\begin{aligned}
&\exp(-i\hat{H}t) = \exp(it\tfrac{1}{2}\hat{I}\otimes\hat{I}\otimes\ \hat{\sigma}_z)\ \exp(it\tfrac{1}{2}\hat{I}\otimes\ \hat{\sigma}_z\otimes I)\ \exp(it\tfrac{1}{2}\,\hat{\sigma}_z\otimes I\otimes I) \\
&\lim_{n\to\infty}\left(\exp\left(\tfrac{-i\lambda t}{4n}\right)(\hat{\sigma}_x\otimes\hat{I}\otimes\ \hat{\sigma}_x)\exp\left(\tfrac{-i\lambda t}{4n}\right)(I\otimes\hat{\sigma}_y\otimes\ \hat{\sigma}_y)\right)^n \\
&\lim_{n\to\infty}\left(\exp\left(\tfrac{-i\lambda t}{4n}\right)(I\otimes\hat{\sigma}_x\otimes\ \hat{\sigma}_x)\exp\left(\tfrac{-i\lambda t}{4n}\right)(\hat{\sigma}_y\otimes\hat{I}\otimes\ \hat{\sigma}_y)\right)^n
\end{aligned} \tag{2.76}$$

Equation (2.76) is the operator for RBH. Following the same process as with the single atom circuit, we proceed to convert everything to quantum gates, using (2.45) and (2.46),

$$\boxed{\begin{aligned}
&\hat{U}(t) = R_z(-t)\otimes R_z(-t)\otimes R_z(-t) \\
&\left(\begin{aligned}&(H\otimes I\otimes H)(CNOT_{1,3})\left(I\otimes I\otimes R_z\left(\tfrac{2\delta}{n}\right)\right)(CNOT_{1,3})(H\otimes I\otimes H) \\ &(I\otimes U'\otimes U')(I\otimes CNOT_{2,3})\left(I\otimes I\otimes R_z\left(\tfrac{2\delta}{n}\right)\right)(I\otimes CNOT_{2,3})(I\otimes U'\otimes U')\end{aligned}\right)^n \\
&\left(\begin{aligned}&(I\otimes H\otimes H)(I\otimes CNOT_{2,3})\left(I\otimes I\otimes R_z\left(\tfrac{2\delta}{n}\right)\right)(I\otimes CNOT_{2,3})(I\otimes H\otimes H) \\ &(U'\otimes I\otimes U')(CNOT_{1,3})\left(I\otimes I\otimes R_z\left(\tfrac{2\delta}{n}\right)\right)(CNOT_{1,3})(U'\otimes I\otimes U')\end{aligned}\right)^n
\end{aligned}} \tag{2.77}$$

CHAPTER III

QISKIT'S QUANTUM CIRCUITS AND PLOTS

We will be using Qiskit to build and run Quantum Circuits, Qiskit is an open-source software development kit for working with quantum computers.

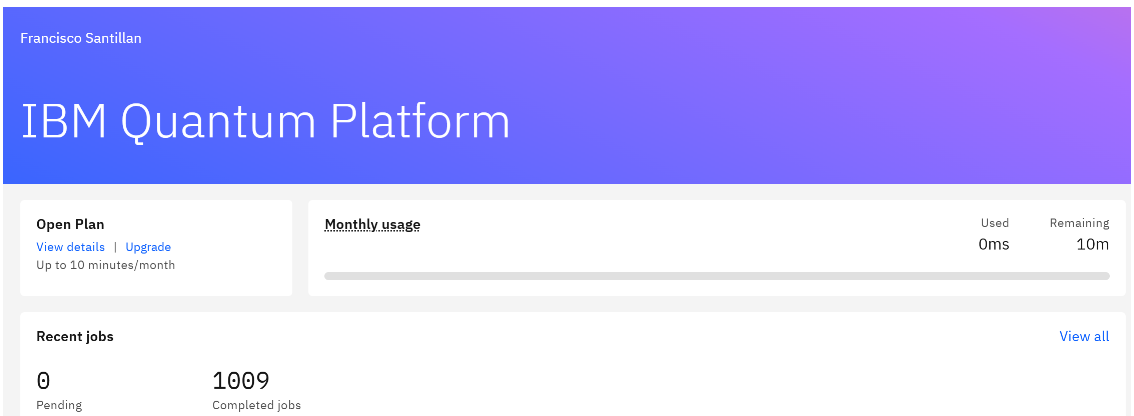

Figure 3.1: IBM login page. Taken from IBM Quantum Lab

By the time I was working on the circuit, the IBM quantum lab was available, but at the time of writing since it has been deprecated, the best bet is to download Qiskit locally, for this follow https://www.ibm.com/quantum/qiskit. [2]

3.0.1 JCH Circuit and Plot

Now it is turn to analyze the equations previously derived, for this we go back to equation (2.55),

$$\begin{aligned} & R_z(-t) \otimes R_z(-t) \\ \hat{U}(t) = \quad & [H \otimes H]\text{CNOT}[I \otimes R_z(2\delta)]\text{CNOT}[H \otimes H] \\ & [U' \otimes U']\text{CNOT}[I \otimes R_z(2\delta)]\text{CNOT}[U' \otimes U'] \end{aligned} \tag{3.1}$$

Equation (3.1) gives the time evolution operator $\hat{U}(t) = \exp\left(-i\hat{H}t\right)$ in quantum circuit form. Using Qiskit and drawing the circuit,

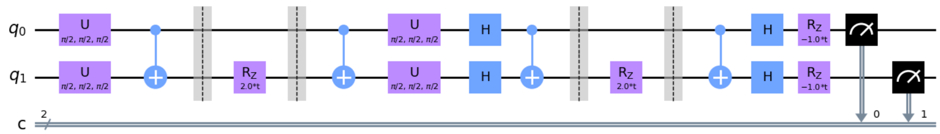

Figure 3.2: Jaynes Cummings Quantum Circuit

The circuit in Figure 3.2 effectively runs Equation (3.1). To this end, we need to introduce the concept of *Rabi Oscillations*. Rabi Oscillations are the consequence of an external light field interacting with a two-level quantum system, when the Hamiltonian is known, we apply the previously mentioned time evolution operator. To effectively extract Rabi Oscillations, first, we need to initialize it (to 01, or 10) (01 for atom excited, no photon, and 10 for atom in ground state and photon is present) and then, we need to run the circuit in the simulator for each data point t, on a chosen interval of time.

For Figure (3.3), there are a few key points to mention: time is t $\in$ 0,5 and its mutually exclusive value from the Hamiltonian, meaning that time can be chosen at any interval, as long as a whole complete period is shown, the time interval must be sliced equally between points for a symmetric plot, otherwise the data will not make sense (other than by extrapolating). Second, the dashed lines in the figure represent simulation of the circuit using Aer Simulator, and the squares represent real jobs ran in ibmq_lima available at the time of the job. Third, observe how the real measurement follows the pattern of the simulated photon/atom, but as time progresses, the real measurement loses number of counts yet still follows the pattern, this is due to decoherence of the quantum device.

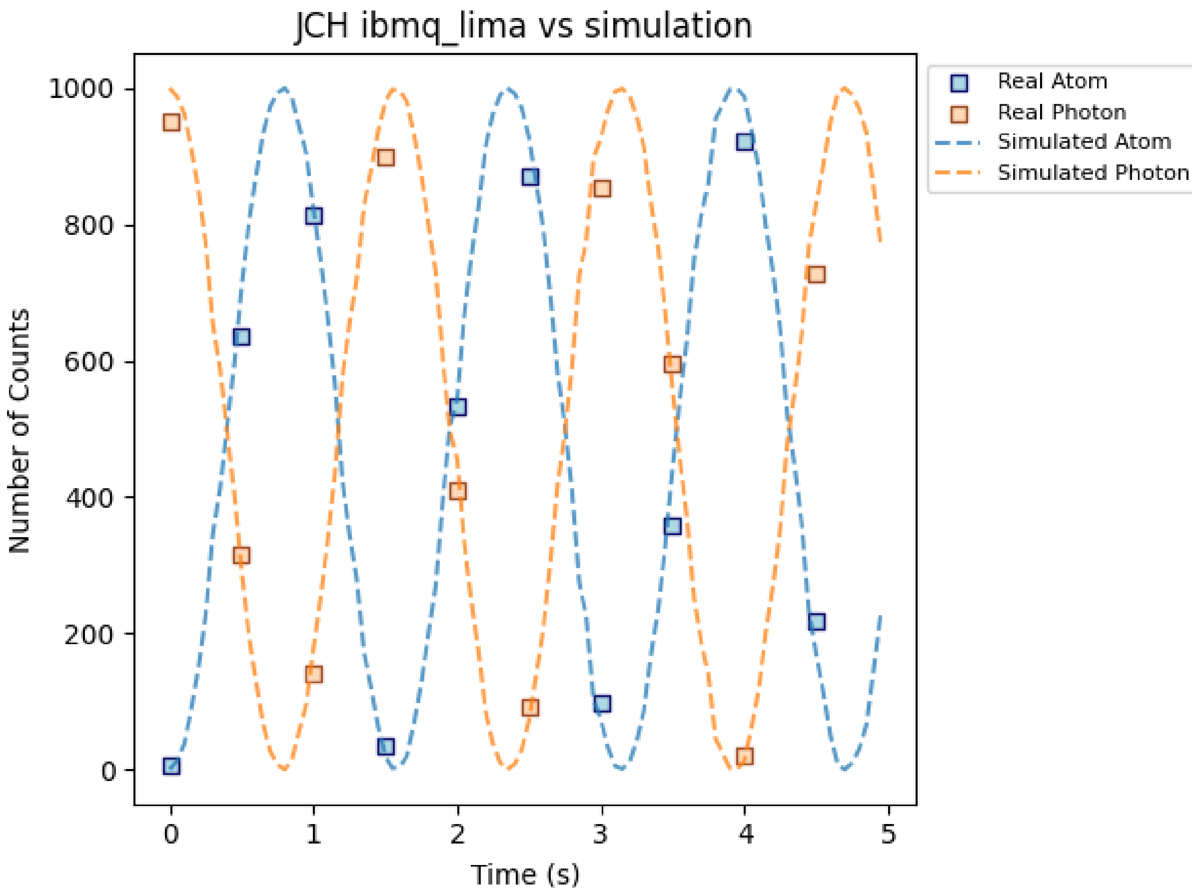

Figure 3.3: Rabi Oscillations Plot for JCH

This is the behavior expected for a single atom JCH, implementing the evolution operator (2.43) directly yields,

$$\hat{U} = \begin{pmatrix} \exp(it) & & & \\ & \cos(\lambda t) & -i\sin(\lambda t) & \\ & -i\sin(\lambda t) & \cos(\lambda t) & \\ & & & \exp(-it) \end{pmatrix} \tag{3.2}$$

In what follows we focus on superpositions of states $|01\rangle$ = "atom in ground state, 1 photon" and $|01\rangle$ = "atom in excited state, no photon":

$$|\psi_2\rangle = c_{01}|01\rangle + c_{10}|10\rangle \tag{3.3}$$

That is, we omit the states $|00\rangle$ and $|11\rangle$ because they cannot be reached if the system is prepared in a state of the form (48). In this case, we can consider the truncated evolution operator,

$$\hat{U}(t) = \begin{pmatrix} \cos(\lambda t) & -i\sin(\lambda t) \\ -i\sin(\lambda t) & \cos(\lambda t) \end{pmatrix} \tag{3.4}$$

acting on states,

$$|\psi(t)\rangle = \begin{pmatrix} c_{01}(t) \\ c_{10}(t) \end{pmatrix} \tag{3.5}$$

Where λ is the frequency of the Rabi Oscillations for the case in which the detuning $\delta = \omega - \omega_0$ is zero. Physically, the atom and the photon both oscillate as two-level quantum system, either the atom absorbs the photon and is in an excited state, or the atom is in ground state and the photon is non-absorbed and around.

3.0.2 RBH Circuit and Plot

For the next Hamiltonian let us go back to Equation (2.77):

$$\begin{aligned} \hat{U}(t) = {} & R_z(-t)\otimes R_z(-t)\otimes R_z(-t) \\ & \begin{pmatrix} (H\otimes I\otimes H)(CNOT_{1,3})\left(I\otimes I\otimes R_z\left(\frac{2\delta}{n}\right)\right)(CNOT_{1,3})(H\otimes I\otimes H) \\ (I\otimes U'\otimes U')(I\otimes CNOT_{2,3})\left(I\otimes I\otimes R_z\left(\frac{2\delta}{n}\right)\right)(I\otimes CNOT_{2,3})(I\otimes U'\otimes U') \end{pmatrix}^n \\ & \begin{pmatrix} (I\otimes H\otimes H)(I\otimes CNOT_{2,3})\left(I\otimes I\otimes R_z\left(\frac{2\delta}{n}\right)\right)(I\otimes CNOT_{2,3})(I\otimes H\otimes H) \\ (U'\otimes I\otimes U')(CNOT_{1,3})\left(I\otimes I\otimes R_z\left(\frac{2\delta}{n}\right)\right)(CNOT_{1,3})(U'\otimes I\otimes U') \end{pmatrix}^n \end{aligned} \tag{3.6}$$

Before doing an analysis on the results, let us fold back and analyze (3.6). First, notice how we have $CNOT_{1,3}$ and $CNOT_{2,3}$, you may recognize that for the underscripts the first number is the control qubit and the other is the target qubit; nonetheless analyzing closely one can see that both are 8x8 and 4x4 matrix respectively, that is because, $CNOT_{1,3}$ not only works with the first and third qubit, but passes through the second qubit, and this happens exclusively in this gate, i.e if we had $CNOT_{2,5}$ then we would have a 16x16 matrix.

Second, notice n exponent on the top, this is the trotter formula applied to the circuit, where n is the trotter number, it can be chosen depending on the result that is needed and/or the resources available.

For the RBH circuit, and similar to JCH, by drawing (3.6),

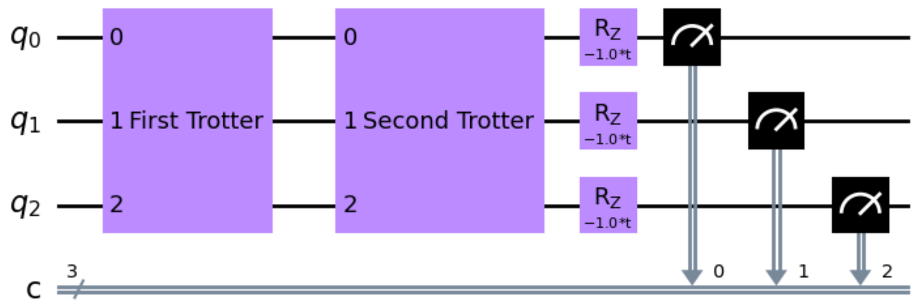

Figure 3.4: RBH Quantum Circuit

Figure (3.4) shows the quantum circuit for (3.6) in a much simplified manner. Reading from right to left (because these are matrices [1]) We can see the two blocks as First Trotter and Second Trotter respectively.

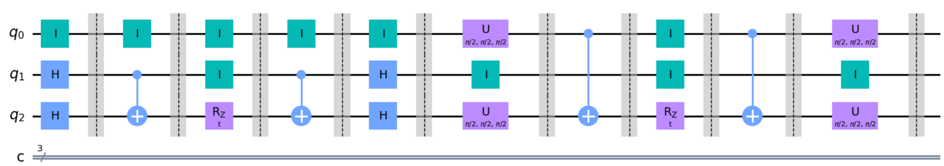

Figure 3.5: First Trotter Circuit

[1]See Appendix A

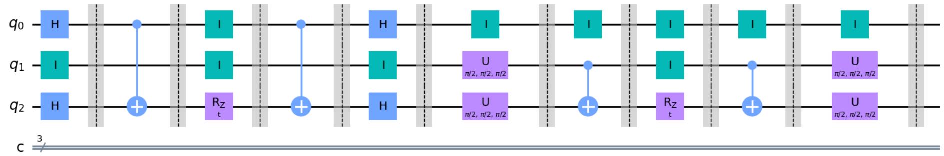

Figure 3.6: Second Trotter Circuit

Both Figures 3.5 and 3.6 constitute the blocks in Figure 3.4; furthermore, these blocks are ran on the circuit n amount of times depending on the trotter number i.e. if $n = 2$ for First Trotter and $n = 5$ for Second Trotter then, First Trotter is repeated two times in Figure 3.4 followed by a Second Trotter being repeated five times.

The following are plots of Rabi Oscillations for RBH with different trotter numbers n:

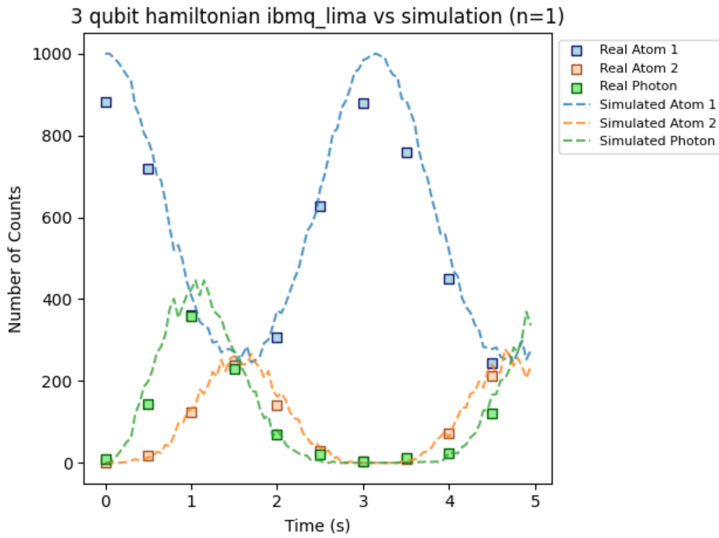

Figure 3.7: Rabi Oscillations for n=1

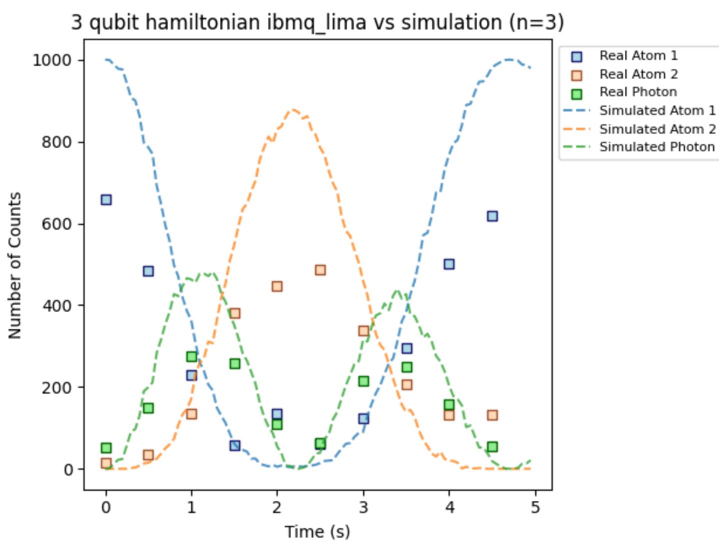

Figure 3.8: Rabi Oscillations for n=3

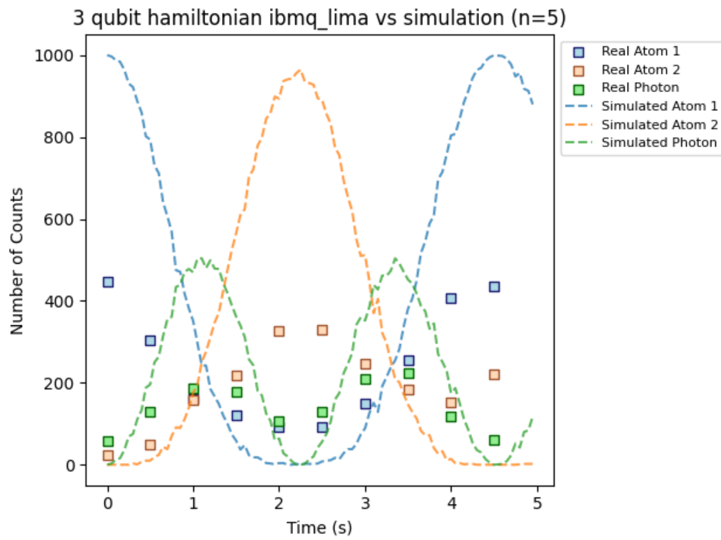

Figure 3.9: Rabi Oscillations for n=5

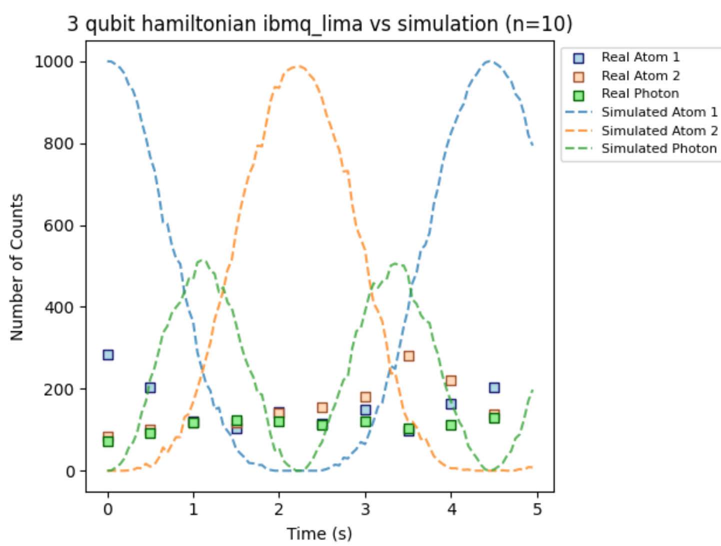

Figure 3.10: Rabi Oscillations for n=10

These plots provide the "same" oscillations for different n values yet we have different results for each one of them. For $n = 1$, the pattern real device measurements follow is quite similar yet physically it does not mean anything. For $n = 3$, you can start to see more decoherence effects and the real device measurements still keeping the shape but slowly losing it; all the way to $n = 10$, where we have an almost perfect simulation, yet the real device measurements are almost lost. The RBH circuit has an initial depth of 13 for $n = 1$, yet the depth value is increased exponentially as n is increased, allowing for decoherence effects to measure forbidden states other than $|001\rangle$, $|010\rangle$, $|100\rangle$.

CHAPTER IV

ENTANGLEMENT AND CONCLUSION

4.1 Entangled or not?

Consider a composite AB system consisting of 2 subsystems A (Alice) and B (Bob). Each subsystem is a 2-state system with states $|0\rangle$, $|1\rangle$.
A product state in the composite system is for example the tensor product,

$$|\Phi\rangle_{AB} = |0\rangle_A \otimes |1\rangle_B = |01\rangle \tag{4.1}$$

We use the convention that the left entry refers to subsystem A and the right entry to B. $|\Phi\rangle_{AB}$ is a tensor product, thus the two subsystems are separated (not entangled). Another state in the composite system is the Bell state

$$\left|\Psi^+\right\rangle_{AB} = \frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right) \tag{4.2}$$

This state cannot be written as a single tensor product $|a\rangle_A \otimes |b\rangle_B$ and is thus entangled. Given an arbitrary state $|\Omega\rangle_{AB}$in the composite system AB, how can we tell if $|\Omega\rangle_{AB}$ is entangled?

Note that both $|\Phi\rangle_{AB}$ and $|\Psi^+\rangle_{AB}$ are pure states in the composite system AB. Thus we will find for both density matrices $\hat{\rho}_{AB}(\Phi) = |\Phi\rangle\langle\Phi|$ and $\hat{\rho}_{AB}(\Psi^+) = |\Psi^+\rangle\langle\Psi^+|$ that $\hat{\rho}_{AB}^2 = \hat{\rho}_{AB}$. Thus calculating $\hat{\rho}_{AB}^2$ and comparing it with $\hat{\rho}_{AB}$ does not tell us if the state in the composite system is entangled.

However, let's consider the reduced density matrix $\hat{\rho}_B = \underset{A}{\mathrm{tr}}(\hat{\rho}_{AB})$ of one subsystem (say B) after tracing out the other subsystem (say A). If the original state $|\Omega\rangle_{AB}$ is a product state such $|\Phi\rangle_{AB} = |0\rangle_A \otimes |1\rangle_B = |01\rangle$ in (4.1), then the reduced density matrix $\hat{\rho}_B$ describes a pure state in subsystem B, and we obtain $\hat{\rho}_B^2 = \hat{\rho}_B$:

$$\begin{aligned}\hat{\rho}_B &= \underset{A}{\mathrm{tr}}(\hat{\rho}_{AB}) = \underset{A}{\mathrm{tr}}(|01\rangle\langle 01|) = \underset{A}{\mathrm{tr}}[(|0\rangle\otimes|1\rangle)(\langle 0|\otimes\langle 1|)] \\ &= (\langle 0\mid 0\rangle\otimes|1\rangle)(\langle 0\mid 0\rangle\otimes\langle 1|) + (\langle 1\mid 0\rangle\otimes|1\rangle)(\langle 0\mid 1\rangle\otimes\langle 1|) \\ &= (|1\rangle\langle 1|)_B\end{aligned} \tag{4.3}$$

As expected, subsystem B ends up in the pure state $|1\rangle$, and $\hat{\rho}_B^2 = |1\rangle\langle 1\mid 1\rangle\langle 1| = |1\rangle\langle 1| = \hat{\rho}_B$. This is expected since the two subsystems are separated and independent, thus Bob just keeps his pure state $|1\rangle$ independent of what Alice is doing.

However, if the original state $|\Omega\rangle_{AB}$ is an entangled state such as $|\Psi^+\rangle_{AB} = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ in (4.2) then the reduced density matrix $\hat{\rho}_B$ actually describes a mixed state in subsystem B, $\hat{\rho}_B^2 \neq \hat{\rho}_B$: and we obtain $\hat{\rho}_B^2 \neq \hat{\rho}_B$:

$$\begin{aligned}\hat{\rho}_B &= \underset{A}{\mathrm{tr}}(\hat{\rho}_{AB}) = \underset{A}{\mathrm{tr}}\left(\tfrac{1}{\sqrt{2}}(|00\rangle + |11\rangle)\tfrac{1}{\sqrt{2}}(\langle 00| + \langle 11|)\right) \\ &= \underset{A}{\mathrm{tr}}\left(\tfrac{1}{2}(|0\rangle\otimes|0\rangle + |1\rangle\otimes|1\rangle)(\langle 0|\otimes\langle 0| + \langle 1|\otimes\langle 1|)\right) \\ &= \tfrac{1}{2}(\langle 0\mid 0\rangle\otimes|0\rangle + \langle 0\mid 1\rangle\otimes|1\rangle)(\langle 0\mid 0\rangle\otimes\langle 0| + \langle 1\mid 0\rangle\otimes\langle 1|) \\ &+ \tfrac{1}{2}(\langle 1\mid 0\rangle\otimes|0\rangle + \langle 1\mid 1\rangle\otimes|1\rangle)(\langle 0\mid 1\rangle\otimes\langle 0| + \langle 1\mid 1\rangle\otimes\langle 1|) \\ &= \tfrac{1}{2}(|0\rangle\langle 0|) + \tfrac{1}{2}(|1\rangle\langle 1|)_B \\ &= \tfrac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)_B\end{aligned} \tag{4.4}$$

It is easy to see that $\underset{B}{\mathrm{tr}}(\hat{\rho}_B) = 1$, showing that $\underset{AB}{\mathrm{tr}}(\hat{\rho}_{AB}) = 1$ for the pure state $|\Psi^+\rangle_{AB}$ in the composite system AB. However, $\hat{\rho}_B$ in subsystem B is a density matrix describing a mixture of states $|0\rangle$ and $|1\rangle$, each with probability 1/2. We obtain:

$$\begin{aligned}
\hat{\rho}_B^2 &= \tfrac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)\ \tfrac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) \\
&= \tfrac{1}{4}(|0\rangle\langle 0 \mid 0\rangle\langle 0| + |0\rangle\langle 0 \mid 1\rangle\langle 1| + |1\rangle\langle 1 \mid 0\rangle\langle 0| + |1\rangle\langle 1 \mid 1\rangle\langle 1|) \\
&= \tfrac{1}{4}(|0\rangle\langle 0| + |1\rangle\langle 1|) \\
&= \tfrac{1}{2}\hat{\rho}_B
\end{aligned} \tag{4.5}$$

Thus $\hat{\rho}_B^2 \neq \hat{\rho}_B$.

The interpretation is as follows: If $\hat{\rho}_B^2 \neq \hat{\rho}_B$, Bob cannot tell from his density matrix $\hat{\rho}_B$ for his state $|b\rangle_B$ if it is a mixed state because of uncertainty, or if it is entangled with another state $|a\rangle_A$. If he could do this, then this would make possible instantaneous communication between Alice and Bob even if they are far away from each other, because he could then use his density matrix $\hat{\rho}_B$ to determine immediately if Alice performed a measurement on her subsystem A or not.

4.2 Time Evolution Entanglement

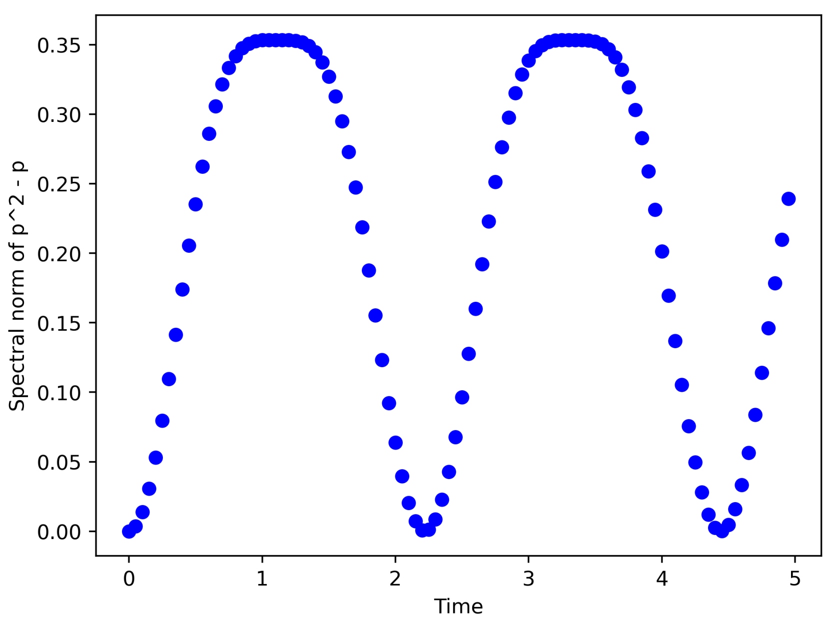

Figure 4.1: Photon spectral norm (using Qiskit)

We should be able to calculate an entanglement value as our circuit evolves in time (3.6) by calculating the spectral norm (L^2) , $\left\|\hat{p}_i^2 - \hat{p}_i,\right\|$ where i is either Atom 1, Atom 2, or the photon, (See Figure 4.1) for L^2 plot with respect of time for the photon ($i = p$).

In Figure 4.2, we plot the L^2 of all the differences for all three initial states (all i's) as time progresses, opening the door for the generation of two-qubit gates as proposed in [5].

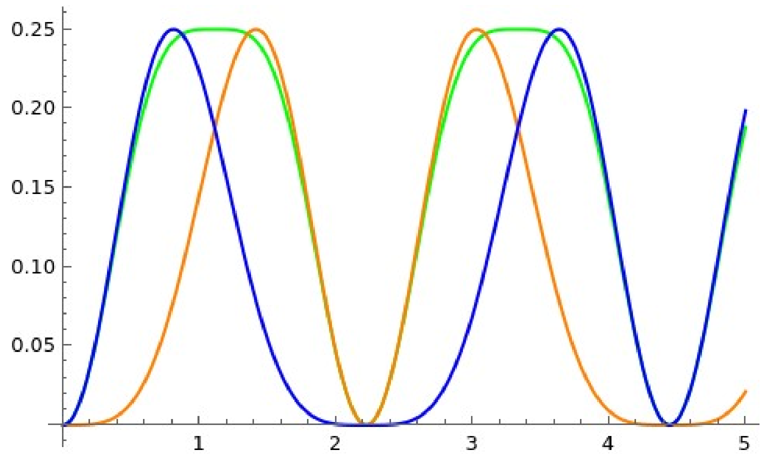

Figure 4.2: Spectral norm for all i values. Where photon, Atom 1, Atom 2

.

4.3 Conclusion

We were able to derive a Quantum Circuit for the Jaynes Cummings Hamiltonian successfully along with a new circuit that is able to model the Rydberg Blockade, allowing for a further examination of the latter.

We were also able to run the circuits both in simulation and in a real device, showing the real time limitation of the computer on the still on going NISQ era. Usually the problem is truncated to be an engineering one, yet there are several fields of research such as Quantum Error Correction trying to tackle the issue of decoherence from different angles theoretically. Lastly, we were able to show the existence of entanglement as time evolves for all initial states, which is crucial for the generation of Rydberg atom Multi-qubit gates which is an undergoing research in QuEra and research institutions like Harvard and MIT [1].

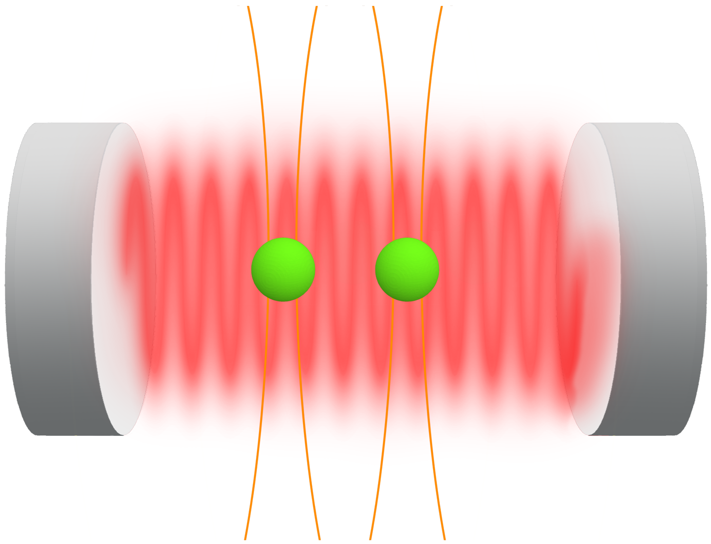

Figure 4.3: Rydberg Atoms in a Cavity Model. Two Rydberg atoms in a cavity, depicting the light as the red waves.

"Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy." - Richard P. Feynman

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APPENDIX A

APPENDIX A

INTRODUCTION TO QUANTUM COMPUTING

Quantum Computing (QC) has been a developing field since the 1980s. Richard Feynman first mentioned the idea in a keynote speech in Caltech in 1981. Since then, the field has been evolving from Shor's Algorithm, Simon's algorithm all the way to Quantum Simulation schemes and Quantum error correction codes. Generally speaking we are still far away from using Quantum Computers (QCrs) in a practical application if there even exists such use, and for that fault tolerant QCrs are needed; researchers and the private industry call this the fault tolerant era, an era in which the coherence of quantum devices will be fully controlled allowing for the usage of these devices effectively. We are still far away from that time; nevertheless, we encounter ourselves today in the NISQ era (Noisy Intermidiate Scale Quantum), an era in which we do not yet have noiseless devices but instead noisy devices that are still capable of being of use combined with classical devices, a hybrid approach if you will; variational algorithms are an example of an application of this. And so how do we measure the coherence then you may be asking? By using the value of Quantum Volume. Quantum Volume is a metric that takes into account the number of qubits, capabilities and error rates; for simplicity, usually the road to coherence is measured by the amount of physical qubits that the Quantum Computer (QCr) has.

The qubit is a fundamental unit in a QCr, think of it as analogous to the bit, except that its Quantum Mechanical and instead of being fixed on a single state its state is represented by the Bloch sphere. As of today that I am writing this, 1180 physical qubits are the maximum amount that has been achieved, done by the company Atom Computing, but the curve is exponentially increasing. An important fact is that, there is a big distinction between physical qubits and logical qubits. Logical qubits are used for application in the circuits, as we will we see, we will focus on

Figure A.1: IBM Quantum Computer. Credits to IBM

these; physical qubits on the other hand, are those qubits that are used to build on logical qubits, coherence and other applications (for more read...). For now I will be referring logical qubits as just qubits keeping in mind that important distinction.

A quantum bit or better known as qubit, is the most fundamental part of a QCr. Experimentally speaking, qubits can take a lot of shapes and forms depending on the implementation of the QCr. For example, in the SQUID implementation (Superconducting Quantum Interference Device) (Check Figure A.1) a superconducting loop in Josephson Junctions can perform as flux qubits; in neutral atoms, qubits are coded in the energy levels of atoms; in photonics, photons are used to encode qubits, and so forth. Ideally speaking, I will work with qubits in the most general way possible. In other words, I will not care about the implementation, but the most general interpretation which can be used for any of the implementations, at the end of the day, logical qubits are the ones that work with the algorithms.

The qubit is better represented in literature as a vector pointing in the surface of a *Bloch Sphere*. In Figure A.2, every point in the surface of the sphere has a value, whether its 0 and 1 in the north and south pole respectively or any value in between when pointing in any other direction. For example, if the arrow where to point in the equator, it would have an equal superposition of both 1 and 0. This only works when qubits are not measured though, when quantum information is measured then it becomes classical information, qubits become bits and the qubit will collapse to either the south or north pole respectively. The probability of collapsing to either one depends on the direction of the vector pointing to the surface.

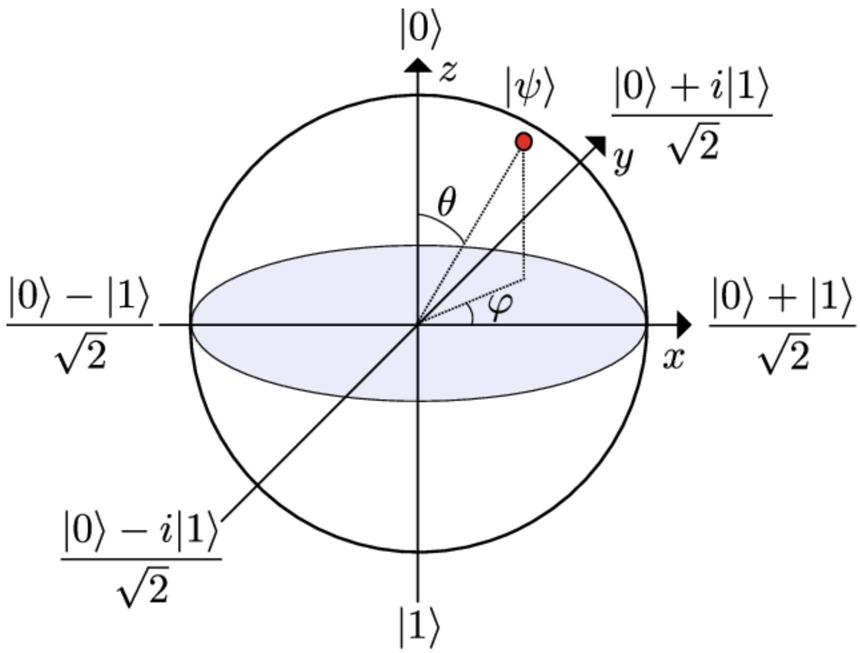


Figure A.2: Bloch Sphere. Taken from ResearchGate

It is important to know that the computational basis of qubits can be represented by column vectors. Generally speaking, a qubit can be represented by a linear superposition of both computational basis, such that:

$$|q\rangle = \alpha\,|0\rangle + \beta\,|1\rangle = \alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{1.1}$$

Here α and β represent the complex amplitudes of the given states, note that as in Quantum Mechanics, $|\alpha|^2 + |\beta|^2 = 1$ meaning that each complex amplitude squared gives the probability of collapsing to its appropriate state,

Furthermore,

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{1.2}$$

$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{1.3}$$

The general 1 qubit operator is represented by,

$$\hat{A} = \sum_{i,j} A_{ij} |i\rangle \langle j| \quad \text{with} \quad i,j = 0,1 \rightarrow \quad A = \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix} \tag{1.4}$$

For 2 qubit basis elements,

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \tag{1.5}$$

[1]

Given two 1-qubit operators:

$$\hat{A} = \sum_{i,j} A_{ij} |i\rangle \langle j| \tag{1.6}$$

$$\hat{B} = \sum_{k,l} B_{kl} |k\rangle \langle l| \tag{1.7}$$

Then

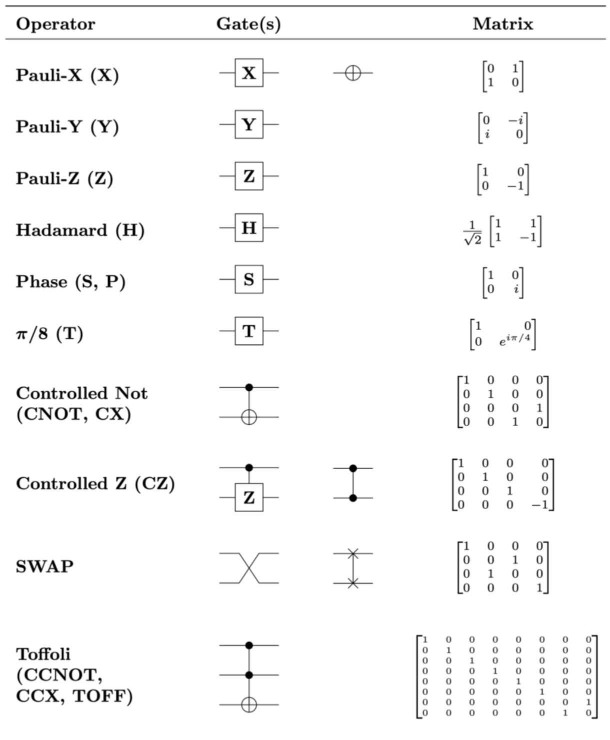
$$\hat{A} \otimes \hat{B} = \sum_{i,j,k,l} A_{ij} B_{kl} |ik\rangle \langle jl| \rightarrow \begin{pmatrix} A_{00}B & A_{01}B \\ A_{10}B & A_{11}B \end{pmatrix} \tag{1.8}$$

Equation (1.8) provides the tensor product of two operators in Matrix form.

[1] As the number of qubits increases so does the column matrix, allowing for 2^n scaling, where n is the number of qubits

The tensor product $\otimes$ not only provides necessary machinery for operator resolution, but a means to represent the different composition of qubits (more on that later).

To manipulate the arrow in the Bloch Sphere, it is necessary to introduce Quantum Logic Gates (See Figure 1.3) each one of them moves the arrow of the qubit and introduces a matrix definition.



Operator	Gate(s)	Matrix
Pauli-X (X)	X	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	S	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	T	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)	Z	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)		$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$

Figure A.3: List of Quantum Logic Gates. Taken from Wikipedia

The Hadamard Gate (H) for example, takes the qubit into the state of superposition. Pauli Z Gate rotates the qubit around the z-axis.

Quantum Gates can also be written as matrices as well, hence when applied to a state, the Matrix is multiplied to a column matrix representing the initial state such as (1.2), (1.3), and (1.5).

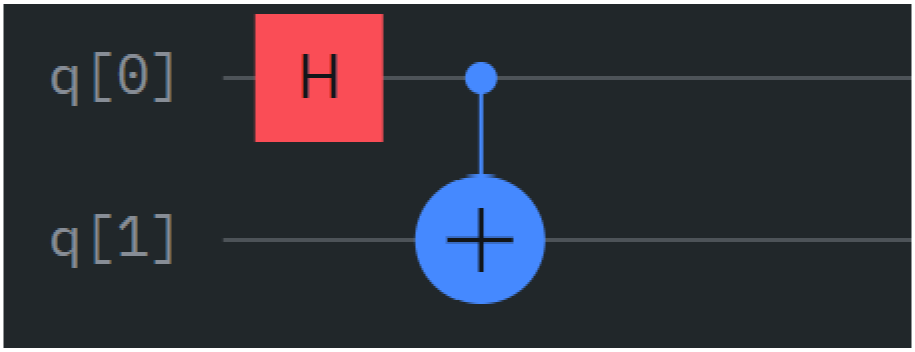


Figure A.4: Bell State Example

Quantum Circuits start from left to right and the number of qubits goes from top to bottom. In the case of Figure A.4 we have two qubits, the Hadamard (H) Gate applied to the first qubit followed by a $CNOT$ Gate taking the first qubit as control and the second one as target. This circuit is the well known Bell state, better known as an entangled state, and its written like this,

$$|\Phi^{+}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \tag{1.9}$$

Lets walk through the process, first we an initial state

$$|00\rangle \tag{1.10}$$

we apply the Hadamard Gate to the first qubit resulting in

$$\frac{1}{\sqrt{2}}(|00\rangle + |01\rangle) \tag{1.11}$$

The CNOT gate acts as on the first qubit as control and so for state $|0\rangle$ the target does not switch, yet for state $|1\rangle$ the target switches yielding,

$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \tag{1.12}$$

which is equation (1.9)

The state $|00\rangle$ can also be written as $|0\rangle \otimes |0\rangle$, the tensor product in quantum circuits is used to compose independent qubits, so if we go back to the basis states in (1.5), $|000\rangle$ can also be written as $|0\rangle \otimes |0\rangle \otimes |0\rangle$ now not all states can be decomposed to tensor products, one such example is the bell state and that is because its entangled, (Look up Chapter 4). Another way to work with the circuits is by doing matrix multiplication, you need to be really careful though, because Matrix Multiplication starts from right to left, in other words $CNOT$ multiplies H and I, this is shown here:

$$\begin{aligned}
&\text{CNOT} \cdot (H \otimes I) \cdot |00\rangle = \\
&\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)
\end{aligned} \tag{1.13}$$

Notice how the identity matrix only applies when qubits have no gates, and so if there is no gate it acts as an invisible gate that does nothing just like the identity matrix multiplies times one.

APPENDIX B

APPENDIX B

FREE FIELD HAMILTONIAN DERIVATION

The following are Maxwell Equations with no sources of radiation:

$$\nabla \cdot \mathbf{E} = 0 \tag{2.1}$$

$$\nabla \cdot \mathbf{B} = 0 \tag{2.2}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{2.3}$$

$$\nabla \times \mathbf{B} = \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \tag{2.4}$$

By having a one dimensional cavity such as in Figure (1.2), and the boundaries at z = 0 and z= L, we have an Electric Field assumed to be polarized along the x-direction,

$$\frac{\partial^2 E_x}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2 E_x}{\partial t^2} = 0 \tag{2.5}$$

We solve the following wave equation with separation of variables to get:

$$E_x(z,t) = \left(\frac{2\omega^2}{V\varepsilon_0}\right)^{1/2} q(t)\sin(kz) \tag{2.6}$$

where if $E_0 = \left(\frac{2\omega^2}{V\varepsilon_0}\right)^{1/2}$

$$E_x(z,t) = Z(z)\cdot q(t) = E_0 q(t)\sin(kz) \tag{2.7}$$

If we now focus our attention into the magnetic field, we can use Ampere's law (2.4):

$$\nabla \times \mathbf{B} = \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} \tag{2.8}$$

$$B_y = -\frac{1}{c^2}\int \frac{\partial E_x}{\partial t}\,dz = \frac{\mu_0 \varepsilon_0}{k} E_0 \dot{q}(t)\cos(kz) \tag{2.9}$$

Converting classical operators to quantum operators, ($q(t) \rightarrow \hat{q}$ and $\dot{q}(t) \rightarrow \hat{p}$), we will follow by using the well-known formula for the hamiltonian:

$$\hat{H} = \frac{1}{2}\int dV \left[\varepsilon_0 E_x^2(z,t) + \frac{1}{\mu_0} B_y^2(z,t)\right]. \tag{2.10}$$

which results in,

$$\hat{H} = \frac{1}{2}(p^2 + \omega^2 q^2), \tag{2.11}$$

By applying the well known non-hermitian bosonic operators,

$$\hat{a} = \frac{1}{\sqrt{2\hbar\omega}}(\omega\hat{q} + i\hat{p}) \tag{2.12}$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2\hbar\omega}}(\omega\hat{q} - i\hat{p}) \tag{2.13}$$

By solving for $\hat{p}$ and $\hat{q}$ by adding and subtracting the operators we get Eq (2.6) and (2.9) in terms of these operators, plugging everything into (2.11) yields,

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right). \tag{2.14}$$

where $\hat{a}^\dagger\hat{a}$ represents the number operator and the term $\frac{1}{2}$ represents the zero point energy of the system. For now we neglect the former and approximate to get us the Free Field Hamiltonian:

$$\hat{H} = \hbar\omega\hat{a}^\dagger\hat{a} \tag{2.15}$$

APPENDIX C

APPENDIX C

TROTTER DECOMPOSITION

Let us consider two commuting operators A and B (Pauli terms are Hermitian Operators). If we have H =A+B $e^{i(A+B)t} = e^{iAt}e^{iBt}$, then the Taylor series expansion of e^{iAt} is given by:

$$e^{iAt} = \sum_{n=0}^{\infty} \frac{(iAt)^n}{n!} \tag{3.1}$$

Expanding this, we get:

$$e^{iAt} \approx 1 + iAt - \frac{(At)^2}{2!} - i\frac{(At)^3}{3!} + \cdots \tag{3.2}$$

Where:

$$1 = \frac{(iAt)^0}{0!}, \quad iAt = \frac{(iAt)^1}{1!}, \quad -\frac{A^2t^2}{2} = \frac{(iAt)^2}{2!}, \quad \text{and} \quad -i\frac{A^3t^3}{6} = \frac{(iAt)^3}{3!}.$$

Similarly for:

$$e^{iBt} = \sum_{n=0}^{\infty} \frac{(iBt)^n}{n!} \tag{3.3}$$

and

$$e^{iBt} \approx 1 + iBt - \frac{(Bt)^2}{2!} - i\frac{(Bt)^3}{3!} + \cdots \tag{3.4}$$

The Taylor series expansion of $e^{i(A+B)t}$ is:

$$e^{i(A+B)t} = \sum_{n=0}^{\infty} \frac{(i(A+B)t)^n}{n!} \tag{3.5}$$

Expanding this, we get:

$$
\begin{aligned}
e^{i(A+B)t} &\approx 1 + i(A+B)t + \frac{(i(A+B)t)^2}{2!} + \frac{(i(A+B)t)^3}{3!} + \cdots \\
&= 1 + i(A+B)t - \frac{(A+B)^2 t^2}{2} - i\frac{(A+B)^3 t^3}{6} + \cdots
\end{aligned} \tag{3.6}
$$

This only works if $A = B$ or $AB = BA$.

Otherwise, the exponential of the sum of matrices A and B can be expressed as:

$$
\exp(\hat{A} + \hat{B}) = \lim_{n\to\infty} \left(\exp\left(\frac{\hat{A}}{n}\right) \exp\left(\frac{\hat{B}}{n}\right) \right)^n \tag{3.7}
$$

where

$$
\exp(\delta(\hat{A} + \hat{B})) = \exp(\delta\hat{A}) \exp(\delta\hat{B}) + O(\delta^2) \tag{3.8}
$$

and n is the trotter number, which as it approaches infinity makes δ go to zero.

VITA

Francisco D. Santillan was born in Matamoros, Mexico. He completed his Bachelor of Science in Physics in 2019 and graduated with a Master of Science in Engineering in Electrical Engineering in 2022. Along with his passion for Quantum Computing and Quantum Engineering, he enjoys building robotics projects with the hope that one day he can find a way to join both fields. He graduated with an Master of Sceince in Physics from The University of Texas Rio Grande Valley in August 2024. He can be reached at his personal email address: francisco.dsantillan@outlook.com.