

QUANTUM DYNAMICS OF QUBITS

An Undergraduate Research Scholars Thesis

by

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ABSTRACT

Quantum Dynamics of Qubits

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The basic unit of information within quantum mechanics can be modeled through two-level systems to provide a foundational understanding of quantum information theory. These quantum systems, which can be represented by qubits, can be transformed and manipulated when strongly coupled to an applied electromagnetic field. I study the quantum dynamics of two-level systems strongly coupled to a classical electromagnetic field, with the inclusion of dissipation and decoherence, to understand the method of using state transitions to transmit information. Furthermore, I characterize physical properties of Al(III) and Silicon based molecules that can serve as possible candidates for a qubit. Using the advantages of π pulses, I solve for analytical solutions of differing electromagnetic pulses that would create transitions within the variety of candidate molecules. The stochastic Schrodinger equation approach for the Lindbald approximation is used to provide insight into including dissipation of the states and decoherence of the electromagnetic field within the quantum systems. The electromagnetic effects of a qubit-cavity system are observed to establish a realistic understanding of the scenario and provide the experimental requirements to create transitions through the use of pulsed light. Additionally, I study the coupled interaction of elec-

tromagnetic pulses between multiple qubits to determine the conditions for interchanging states between them. The combination of classical and quantum electromagnetic effects are considered to fulfill a scheme for a CNOT quantum gate. The goal of these theoretical topics is to create a quantum system of qubits that can be used to function as a possible experimental basis of a quantum gate for computation.

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The data analyzed/used for Qubit Candidate Molecules were provided by Dr. Matthew Pelton group, University of Maryland, Baltimore County, and these data are unpublished.

All other work conducted for the thesis was completed by the student independently.

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1. INTRODUCTION

Quantum information is a growing field that provides technological innovation as well as creates a more efficient method of computation and storage of memory. Solid-state quantum systems such as circuit quantum electrodynamics and cavity quantum electrodynamics offer a technologically attractive monolithic solution as compared to other approaches such as ions in a vacuum trap [1, 2]. In this project, we consider the qubits, i.e. two level systems, that are strongly coupled to an electromagnetic field in a dielectric or plasmonic nanocavity [3]. By understanding how qubits transition between states due to the interaction with the common cavity field or direct coupling, quantum logic gates, which are necessary for computing, can be created. Furthermore, the superposition of states within a qubit can lead to an exponential potential in the amount of information such a system can hold [4] and a manipulation of this system is necessary to be able to push the boundaries of computing power. Multi-qubit systems that include the interaction of the coupled qubits should consider both quantum and classical electromagnetic field contributions to best approach this topic [5, 1]. As such, this project initially explores the feasibility of the coherent control of coupled qubit systems through the use of a classical electromagnetic field, then the scheme of a quantum gate is determined through the use of the quantum electromagnetic interaction of the qubit system with a probing photon.

The behavior of a simple setup of a classical electromagnetic field applied on a two level system [6] will first be considered to understand the requirements in controlling the transitions of the qubit. Candidate molecules for the role as the qubit will be used for the numerical solutions. In order to use these molecules, specific physical characteristics such as their decay lifetime and wavelength emission will have to be measured. Then, their individual dipole moments will be determined in order to numerically solve their dipole interaction with the classical external electromagnetic pulse and cavity electromagnetic field. Once the foundation for manipulation of qubits' energy states has been built, the effects of introducing a cavity will be considered in both the field

experienced by the two level system that undergoes transitions as well as emissions that are released. A more realistic cavity geometry will then be considered and the effects of dissipation and decoherence, through interaction with an environment, will be included [6, 5] to apply realism in the system. A solution to this system will provide an understanding on how changing the applied field can manipulate the transitions within a qubit and communicate what observables could be used to allow storage and retrieval of information. Once a solution has been found, applications of the system into a model of a quantum logic gate will be discussed. In order to create a gate, multiple qubits will have to be introduced and their interaction between each other will be considered. While there are ideas for a single qubit quantum gate through the use of a multi-level system within the qubit, this project will focus on the coupling of two qubits to the cavity field and their possible entangled "dark" state to provide functionality of a CNOT gate. The design of the multi-qubit scheme is shown in Fig. 1. The logic operations for the gate will be determined by the polarization of probing photons [7]. Therefore, single photon interactions with the cavity of coupled qubits will be discussed.

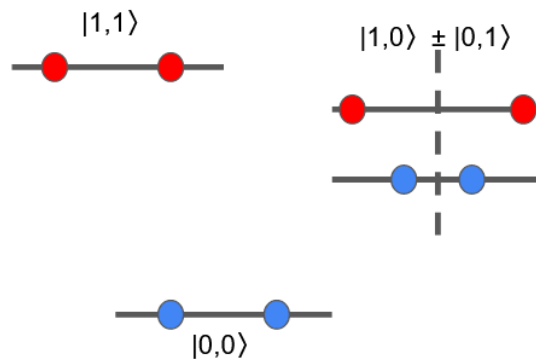


Figure 1: The scheme for a multi-qubit cavity system with entangled states.

Overall, the goal of this project is to find a solution of a practical qubit scenario with can-

didate molecules that stems from the usage of a classical electromagnetic field. Quantum electrodynamical effects will need to be considered for the later steps, however the semiclassical system, one that describes the behavior of the particle quantum mechanically within a classical electromagnetic field, can bring insight into further research on the topic and possible functionality for a quantum gate.

2. TWO-LEVEL SYSTEMS AND THEIR TRANSITIONS

2.1 Finding Transition Probabilities from Applied Electric Field

Qubits are two-level quantum mechanical systems, typically the energy levels of particles, that are able to undergo energy transitions. These transitions populate different states which determine the information of a system, such as the particle being in the ground state versus an excited state. Energy transitions can be manipulated through the electric-dipole interaction between the strong coupling of the particle and applied external electromagnetic field. With the correct field amplitude applied onto the system, the probability is guaranteed and an energy transition occurs. The transition probability between states in a basic two level system can be calculated through the probability amplitude coefficients of the given particle's eigenstates within a system. The probability amplitude coefficients are found by solving the Schrodinger differential equation using the proper eigenstates of the two-level system's Hamiltonian and correct wave function of the particle.

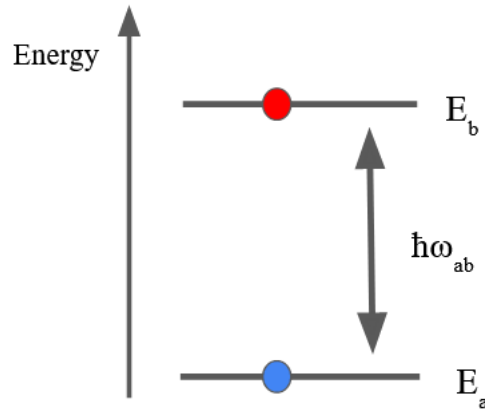


Figure 2: Two-level system with ground state $|0\rangle$ energy E_a and excited state $|1\rangle$ energy E_b .

In the case where there is a two-level system with discrete states 0 and 1, where 0 is the lower energy state shown in Fig. 2., the wave function of the system can be written as

$$|\Psi(t)\rangle = c_0(t) |0\rangle + c_1(t) |1\rangle. \quad (1)$$

The atomic Hamiltonian H_o is the following, and we can apply it to its eigenstates to get each state's energy value

$$H_o |0\rangle = E_a |0\rangle, \quad H_o |1\rangle = E_b |1\rangle. \quad (2)$$

A coupling potential component V can be included to give the full Hamiltonian $H = H_o + V$. The Hamiltonian becomes

$$H = \begin{pmatrix} E_1 & V_{12} \\ V_{21} & E_2 \end{pmatrix}. \quad (3)$$

In this case, the coupling potential is due to the coupling of the electric dipole d_{12} to the applied electric field $\epsilon(t)$. This determines the transition between states.

$$V_{12}(t) = -\mathbf{d}_{12} \cdot \boldsymbol{\epsilon}(t) = -d_{12} |1\rangle \langle 2| \epsilon(t) \cos \nu t. \quad (4)$$

Here, ϵ represents the time dependent amplitude of the electric field with a frequency of ν . The probability amplitude coefficients $c_1(t)$ and $c_2(t)$ can be solved for by applying the previous Hamiltonian into the Schrodinger differential equation.

In addition, the rotating wave approximation will be taken to simplify the equations where the contribution of higher frequencies will be excluded. This is an appropriate approximation when considering that the applied electric frequency is near resonance with the energy frequency between the states.

$$\dot{c}_1(t) = i \frac{d_{12}\epsilon(t)}{2\hbar} c_2(t) e^{i(w-\nu)t}, \quad (5)$$

$$\dot{c}_2(t) = i \frac{d_{21}\epsilon(t)^*}{2\hbar} c_1(t) e^{-i(w-\nu)t} \quad (6)$$

One can find numerical solutions of the coupled differential equations depending on the shape of the electric field, however a general analytical solution assuming a constant electric field amplitude

can be found to be

$$c_1(t) = A_1 e^{\frac{i}{2}(\Delta + \sqrt{\Delta^2 + \Omega_R^2})t} + A_2 e^{\frac{i}{2}(\Delta - \sqrt{\Delta^2 + \Omega_R^2})t}, \quad (7)$$

$$c_2(t) = B_1 e^{-\frac{i}{2}(\Delta + \sqrt{\Delta^2 + \Omega_R^2})t} + B_2 e^{-\frac{i}{2}(\Delta - \sqrt{\Delta^2 + \Omega_R^2})t}. \quad (8)$$

Here A and B represent coefficients that can be solved for using initial conditions of the system. Additionally, $\Delta = w - \nu$ is defined as the difference in the field and energy frequencies and $\Omega_R = \frac{d_{12}\epsilon}{\hbar}$ is the Rabi frequency of the particle. The Rabi frequency is the characteristic atomic transition frequency of a particle when influenced by an oscillating electromagnetic field, the previously mentioned electric-dipole interaction of primary focus.

Finally, using the following equation along with the correct wave function of the two-level system and previously solved probability coefficients the transition probabilities can be determined.

$$P_{1 \rightarrow 2} = |\langle 2 | \Psi(t) \rangle|^2. \quad (9)$$

$$P_{1 \rightarrow 2} = |\langle 2 | \Psi(t) \rangle|^2. \quad (10)$$

Specifically, this gives the probability of transition to the excited state. Initial conditions of the particle being in the ground state $c_1(0) = 1$ and $c_2(0) = 0$ can be substituted in to produce the final excited state transition probability,

$$P_{1 \rightarrow 2}(t) = \frac{\Omega_R^2}{\Delta^2 + \Omega_R^2} \sin^2 \left(\frac{\sqrt{\Delta^2 + \Omega_R^2} t}{2} \right). \quad (11)$$

In theory, an appropriate electromagnetic square pulse determined by the relation of the Rabi frequency and probability amplitude coefficients of the particle could then be applied to the two-level system to flip its energy state. The pulse would be a component of experiment that could be chosen and controlled within the lab. The controlled energy transitions could then be read in and interpreted as a form of quantum information. π pulses are popular choices due to the dependence of the area of an electromagnetic pulse on the Rabi frequency. The pulse can be set

at an appropriate electric field amplitude where, with its relation to the Rabi frequency, can equal to π in order to flip the state. In the case of a constant square pulse, the π pulse is the integral of a short electric square pulse due to its constant amplitude over time. Moreover, differing realistic pulses can be applied to the scenario and through a numerical solution of the specific differential equation, estimated values of the electric pulse amplitudes and pulse widths can also be found for the purpose of experiment.

2.2 Including Dissipation and Decoherence

Dissipation of information and decoherence of energy states is a major limitation to quantum computing and is an important factor to consider when implementing such a scheme. One method of including dissipation into the picture is through the use of the Lindblad operator of the stochastic equation from Markovian models of relaxation [5]. For the current system, the Lindblad operator adds a noise reservoir that can be connected to the field and energy values of the qubits. The inclusion of dissipation and decoherence consequently forms a new effective Hamiltonian experienced by the system and a noise vector $|R\rangle$ that is a stochastic Langevin source. This source is included due to the relaxation operator necessary in keeping the equation balanced. Overall, the Langevin equation is a preferred method of combining random aspects of the environment, such as dissipation and decoherence, along with deterministic values, such as our transition probabilities, into a single understood and solvable scheme. The stochastic differential equation becomes

$$\frac{d}{dt} |\Psi\rangle = -\frac{i}{\hbar} \hat{H}_{eff} |\Psi\rangle - \frac{i}{\hbar} |R\rangle \quad (12)$$

where the new effective Hamiltonian becomes

$$\hat{H}_{eff} = \hat{H} - \frac{i\hbar}{2} \hat{L} \quad (13)$$

$$\hat{L} = \sum_{j=1} \gamma_j \sigma_j^\dagger \sigma_j. \quad (14)$$

Here, γ can represent the inelastic and elastic relaxation that represent the dissipation and decoherence of the states within the qubits, respectively. Within the summation, each j th component represents a single qubit and thus the summation of all qubits' contributions to the system. Inelastic relaxation is the reason for dissipation within the qubits; the quantum electromagnetic contribution can be considered when introducing individual photon states by using the Q-factor of the system, which includes the build up of diffraction and ohmic losses within the cavity. Elastic relaxation, the reason for decoherence, considers the collision that lead to dephasing within the system. Therefore, the γ_{tot} that will consider the dissipation and decoherence within the effective Hamiltonian becomes

$$\gamma_{tot} = \frac{\gamma^d}{2} + \gamma^{el}. \quad (15)$$

The R term within the stochastic differential equation is a random white noise term that helps conserve the norm of the wave function when averaging the state vector. However, its contribution within this system is minimal, as thermal fluctuations do not have much effect yet and therefore can be ignored when solving for solutions of the equations. γ^d represents the dissipation factor and γ^{el} represents the decoherence factor. The full stochastic differential equation with the inclusion of the γ_{tot} factor leads to

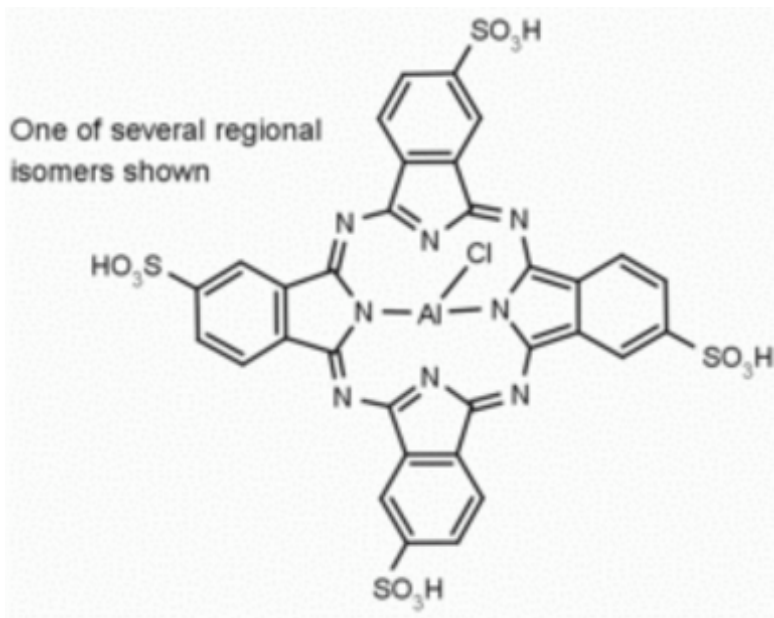
$$\dot{c}_1(t) = i \frac{d_{12}\epsilon(t)}{2\hbar} c_2(t) e^{i(w-\nu)t}, \quad (16)$$

$$\dot{c}_2(t) = i \frac{d_{21}\epsilon(t)^*}{2\hbar} c_1(t) e^{-i(w-\nu)t} - \left(\frac{1}{2}\gamma^d + \gamma^{el}\right) c_2(t). \quad (17)$$

Numerical solutions will be found of the previous differential equations to solve the probability amplitude coefficients of the qubits. This will give information on how to create transitions between energy states of the specific candidate molecules through the use of a pulsed electromagnetic field when including the proper dissipation and decoherence.

3. CANDIDATE MOLECULES AS QUBITS

For an experimentally feasible quantum gate, there needs to be specific particles that can fulfill the role of the qubit. These particles need to be able to undergo energy transitions with a specific electromagnetic pulse. That function requires an understanding the properties of the particle and how it behaves within the qubit cavity system. The two potential molecules tested were Al(III) Phthalocyanine Chloride Tetrasulfonic Acid Fig. 3, and Silicon Phthalocyanine Dichloride Fig. 3. These two molecules are a mixture of a non-organic metal like inner structure with an organic outer coating shell, a key component for candidacy. The inner core is more susceptible to undergoing an energy transition due to an electromagnetic pulse, while the outer layer is able to act as a shield to other electromagnetic sources.



Al(III) Phthalocyanine Chloride Tetrasulfonic Acid
(AIPc)

Figure 3: Al(III) Phthalocyanine Chloride Tetrasulfonic Acid molecule structure.

3.1 Decay Lifetime and Wavelength of Emission

When exciting particles in general, they will rise to a higher energy state, then whether by the probe of an electromagnetic field or natural decay by the universe, the particle will decay back into the lower energy state and emit a photon in stimulated emission or spontaneous emission, respectively. Stimulation of the molecule is what we aim to do through an applied electromagnetic pulse, however what is important to consider is the uncontrollable spontaneous decay that the molecules will naturally undergo. This spontaneous decay will determine, on average, how long the molecule can last in the excited state before it inevitably loses energy and decays. Furthermore, the wavelength of its emission will inform us what energy of a photon would be needed to excite the molecule initially, thus its photon emission from its decay is an important property to measure. Fig. 4 and Fig. 6 show the emission values of AlPc and SiPc and Fig 5 and Fig. 7 show their decay lifetimes as well, respectively.

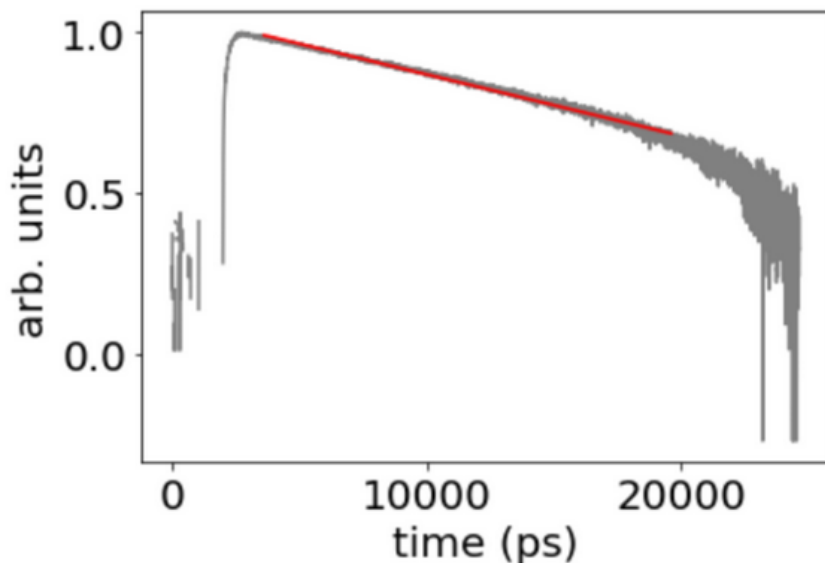


Figure 4: Lifetime decay of the AlPc molecule.

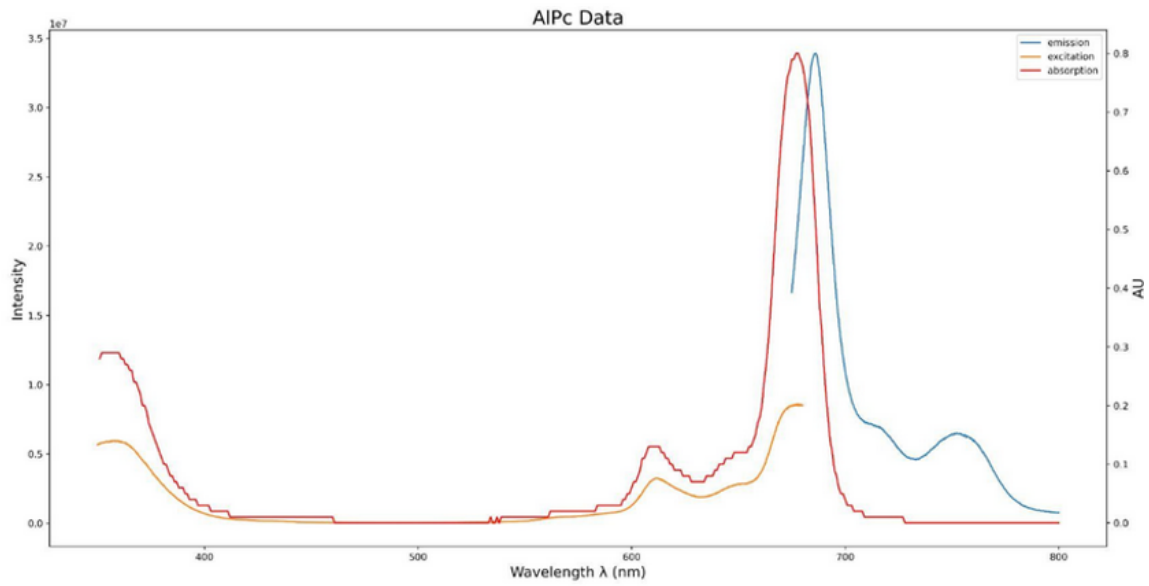


Figure 5: Wavelength emissions of the excited AlPc molecule.

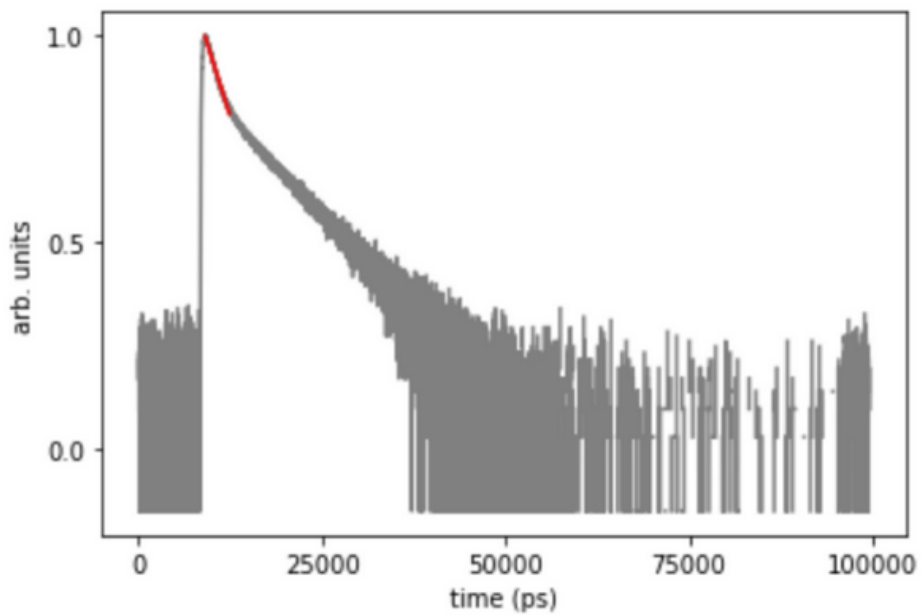


Figure 6: Lifetime decay of the SiPc molecule.

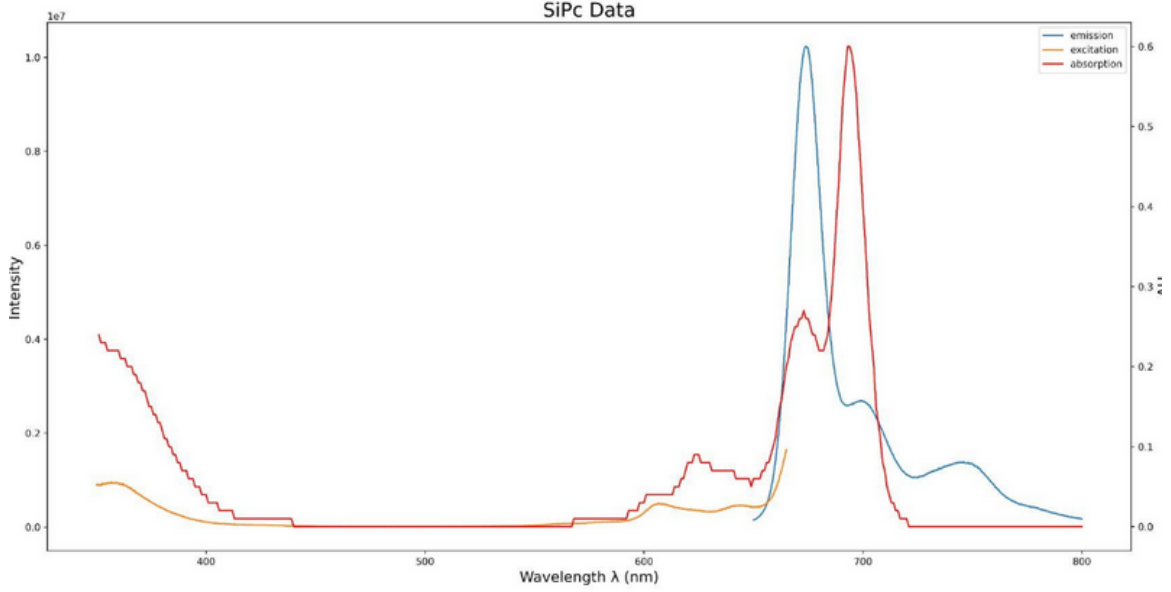


Figure 7: Wavelength emissions of the excited SiPc molecule.

The lifetime and emission wavelength will also be useful in calculating the dipole moment of each molecule. The dipole moment is an important factor, as the dipole of a particle will interact with the external electromagnetic field, as well as the dipole interactions between each of the qubits. These dipole considerations are included within the coupled differential equations shown earlier in Eq. 16 and Eq. 17 and thus will be needed to solve for the probability amplitude coefficients. The dipole moments will also help determine what value of electromagnetic field amplitude and pulse width will be needed to apply energy transitions. Thus, these dipole moments of the molecule are crucial to the development of the qubit cavity system.

3.2 Solving for the Dipole Moments

The solution for the dipole moments of a particle can originate from the derivation of the popular Einstein coefficients. The Einstein coefficients explain the relation between the rate of spontaneous and stimulated emissions of a particle. Each coefficient represents a rate value; A and B correspond to spontaneous emission and stimulated emission, respectively. Assuming a number of particles N, there will be a certain amount N_a in the ground state Ψ_a and a certain amount N_b in the excited state Ψ_b . Stimulated emission can transition a particle from ground to excited and vice

versa, where as spontaneous emission can only transition a particle from excited to ground. That gives the following equations

$$\frac{dN_b}{dt} = -N_b A - N_b B \rho(w_{ab}) + N_a B \rho(w_{ab}) \quad (18)$$

$$\frac{dN_a}{dt} = -\frac{dN_b}{dt} \quad (19)$$

where $\frac{dN_a}{dt}$ represents the rate at which particles transition into the ground state and $\frac{dN_b}{dt}$ represents the rate at which particles transition into the excited state. Additionally, $\rho(w_{ab})$ represents the spectral energy density of the isotropic radiation field at a specific frequency of transition that determines the energy splitting. In a closed system, the two rates equal the negative of each other. Furthermore, within thermal equilibrium, the rate of transitions will cease and the state populations will remain constant, meaning $\frac{dN_b}{dt} = 0$. We can solve for the spectral energy density of this system and then equate it to Placks's law for black body radiation at a specific temperature T . With the stimulated emission depending on the dipole moment of the electromagnetic fields we have

$$\rho(w_{ab}) = \frac{A}{\frac{N_a}{N_b} B - B}, \quad (20)$$

$$B = \frac{d_{1,0}^2 \pi \sqrt{\epsilon}}{3\hbar^2} \quad (21)$$

and setting the black body radiation equation to Eq. 20. we get the relation

$$A_{1,0} = \frac{4w_{1,0}^3 d_{1,0}^2 \sqrt{\epsilon}}{3c^3 \hbar}. \quad (22)$$

In the end, we end up with a smooth relation between the spontaneous coefficient of a particle, its dipole moment, and frequency of transition. The spontaneous coefficient is the efficiency of converting absorbed light into emitted light, or quantum yield, divided by the lifetime of the particle in its excited state. Thus, we finally have our needed dipole relation, in terms of spontaneous

emission wavelength, to be

$$d_{1,0} = \left(\frac{3\hbar \lambda_{spon}^3 Q}{32\pi^3 \epsilon^{1/2} t} \right)^{1/2} \quad (23)$$

Using Eq. 23, along with the experimentally measured lifetime and emission wavelength, the dipole moments of Al(III) Phthalocyanine Chloride Tetrasulfonic Acid (AlPc) and Silicon Phthalocyanine Dichloride (SiPc) are shown in (**Table 1**). These calculated dipole moments of the candidate molecules can now be used for a proper numerical solution of the coupled differential equations.

Table 1: Experimentally Measured Values of Molecules

Molecule	Quantum Yield	Lifetime (s)	λ_{spon} (nm)	Dipole Moment (cm StatC)
AlPc	0.45	8.5×10^{-9}	690	6.45×10^{-18}
SiPc	0.15	5.5×10^{-9}	675	4.48×10^{-18}

4. CLASSICAL ELECTROMAGNETIC EFFECTS ON CANDIDATE MOLECULES

The previous section focused on calculating the dipole moments of the molecules in an effort to use those values within the Hamiltonian of the proposed qubit cavity scheme. All that will be needed for the numerical solution are assumed values of electromagnetic pulse amplitudes and widths. With the lifetime being in the range of nanoseconds, the proposed pulse width would be in the range of picoseconds, leaving the electromagnetic field amplitude of the pulse to range in the tens of V/m. There are two types of electric field pulse shapes that will be applied to the system: a constant square pulse and a Gaussian shaped pulse. Using Eq. 16 and Eq. 17, the dipole moment of the molecule and the electric field values will be plugged in for d_{12} and $\epsilon(t)$, respectively. Both types of pulses are realistic classical electromagnetic pulses that can be experimentally applied to such a scenario, however the initial scenario will be an unrealistic system of a single qubit with no cavity floating in a vacuum. This scheme will simply aid in understanding how manipulation of the energy levels of the qubit can take place. The initial conditions for the differential equations will be such that the qubit is initially in the ground state and the goal will be to raise it so that its probability amplitude reaches a value of 1, meaning it is completely in the excited state after the length of the pulse. This will be done for both molecules.

The next step will be to introduce the previously mentioned dissipation and decoherence into the system. The decay of excited states will become much more important later on, but for now this introduction is simply to include the realistic conditions of a qubit within a cavity with a dissipative environment. It is important to note that since there is the consideration of dissipation, the numerical solution requires specific values for the environment. Specific values would require information on neighboring materials, dissipation of the specific experimental set up, and other factors that are not as easy to introduce in such a numerical state. Thus, in an effort to target this potential issue, dissipative values in ratio with the electromagnetic pulse width were considered in

these calculations. Values such as fractions of the pulse width $\gamma = \frac{\tau}{3}$ that should see no dissipative effect, versus $\gamma = 3\tau$, which should theoretically should give a much larger effect and skew with the excitations, were the determining boundaries of the numerical solution. The hope is that with a reference of the dissipation and decoherence with that excitation of the molecule, it can provide enough insight into the scenario and give a proper stance on the feasibility of the system. The effect of a square pulse can be seen in Fig. 8 and the effect of a Gaussian pulse can be seen in Fig. 9.

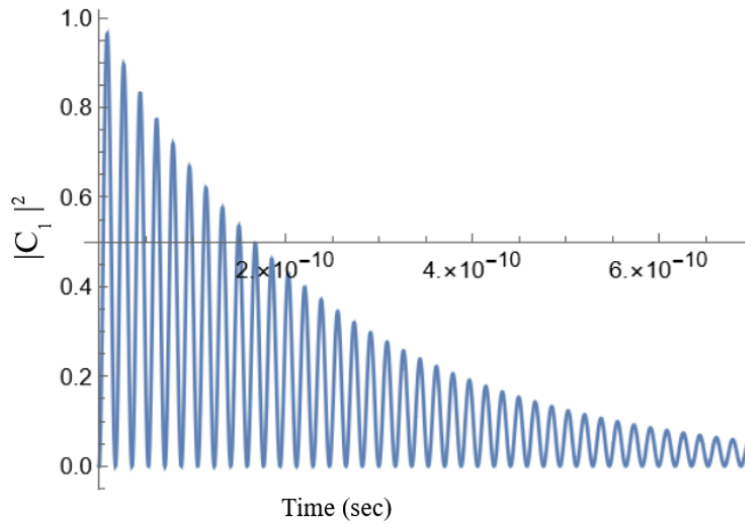


Figure 8: The effect of a square pulse on a qubit cavity system with the inclusion of dissipation and decoherence. It is important to note that the oscillations are due to a constant square pulse throughout. In reality, a single smaller square pulse and the decay is shown in the flow of the oscillations.

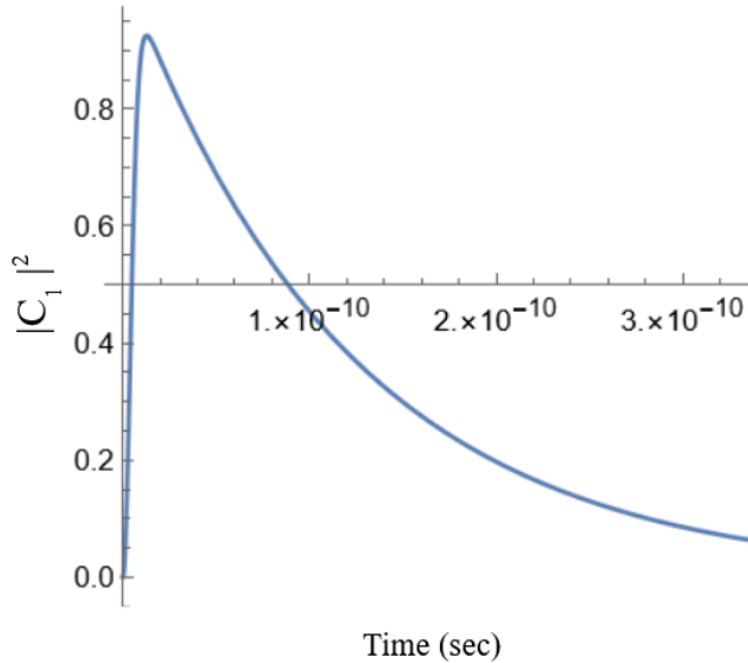


Figure 9: The effect of a Gaussian pulse on a qubit cavity system with the inclusion of dissipation and decoherence.

Overall, this is the main concept to focus on when using a classical electromagnetic pulse. The reason such a pulse would be useful in creating a gate is the ease the classical electromagnetic pulse method provides in effectively applying transitions on the system. The next step for a quantum gate will require the consideration of more qubits within the system, however the classical pulse will be the main component in transferring the system of qubits between different states that will function as the control and target aspects of the CNOT gate. Furthermore, this next step will need to consider the quantum electrodynamical properties of the qubits to initiate probing and reading of information of the system. The combination of classical and quantum aspects of electrodynamics is the key foundation of this scheme.

5. SCHEME FOR THE QUANTUM GATE

There have been multiple designs for a quantum gate, ranging from ion traps and coupled quantum dots to multi-level qubits. Normal logic gates serve many purposes in processing and sending information and the gate at hand transforming into a quantum gate is the previously mentioned CNOT gate. This type of gate has many forms but the general purpose is to flip that state of a signal; if an on signal is sent, then the signal is flipped and an off output is sent. Vice versa is true as well. Normally in modern electronics this is done through a transistor switch and through the flow of electrons, or current, the signal is either on or off. Quantum mechanically, the idea is typically to have some type of control bit that functions as that gate keeper of the operation and a target bit that will send the flipped or not flipped signal. For example, if the control bit is in a state $|0\rangle$, then regardless of the signal of the target, $|0\rangle$ or $|1\rangle$, the state of the target bit remains the same. Furthermore, if the control bit is instead in a state of $|1\rangle$, then the target will flip states. Mathematically, this can be shown through a four by four matrix that represents a CNOT gate, along with the state vectors of the qubits

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \\ \delta \\ \gamma \end{bmatrix}. \quad (24)$$

The scheme brought forward will have a control and target “bit”, where instead of a single qubit acting as the bit of information, the state of the coupled qubits will give the effect of a control bit. Moreover, the inclusion of quantum electromagnetic effects will be introduced to function as the signal of the target bit. The scenario will be a multi-qubit cavity system that will have two qubits coupled in a ground state that is coupled to the cavity electromagnetic field, these qubits being the previously tested molecules. The qubits will have a strongly coupled transition when a single photon, which acts as a probe, is sent to the system. With the qubits in their normal ground

state and unaffected by any other pulses, they will excite and decay as normal. The probe photon will have been sent with a specific electromagnetic polarization that would remain unaffected once it is absorbed and emitted by the system of qubits. This would function the same as if the control “bit” had been in a state of $|0\rangle$. The signal, or in this case the polarization, of the probe photon would remain unchanged and here the probe photon acts as the target “bit”. For the function of the control “bit” being in the state $|1\rangle$, the classical electromagnetic pulses and their effects would play a role. Previously, the coupled qubits had been untouched within their cavity, however a specific classical pulse can now be used to transition the qubits into an entangled state. This entangled state is the key component for this CNOT functionality and the reason for the need of multiple qubits. The entangled state would be such that it becomes a slowly decaying decoupled state from the strong cavity field, a state that can be labeled a “dark” state of the cavity field. Now, the probe of the photon would not read qubits in their ground state but instead what seemed to be an empty cavity. This electromagnetically empty cavity would in turn cause a polarization shift of the photon’s electromagnetic field. A reading of this shifted photon would serve as the flipping of a state and thus output the second function of the CNOT gate. The functionality can be seen in Fig. 10 and Fig. 11.

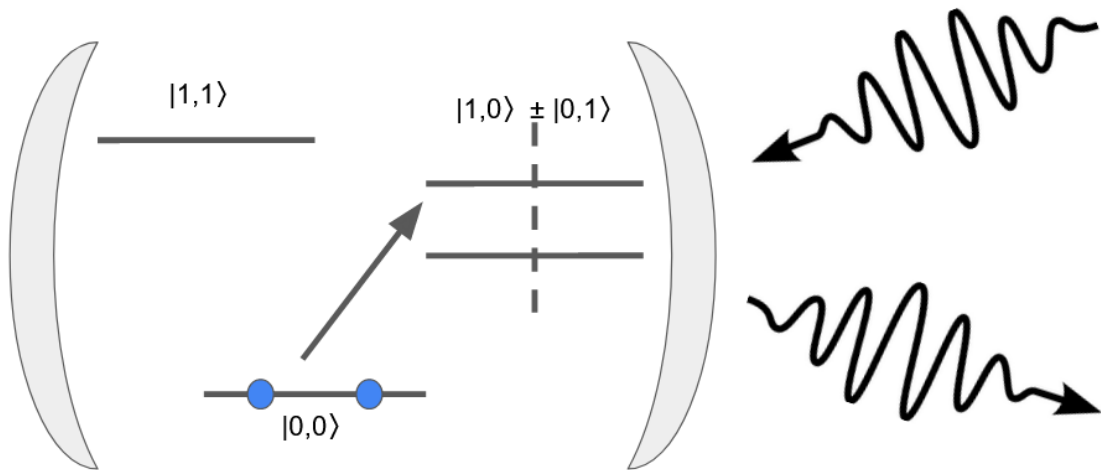


Figure 10: The multi-qubit cavity system set up in control $|0\rangle$ bit with probe of photon resulting in “bright” state.

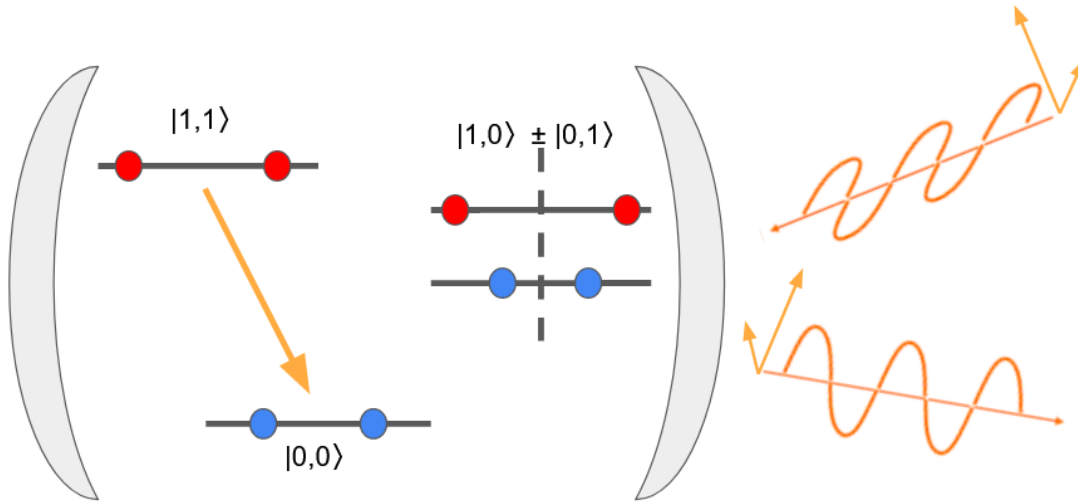


Figure 11: The multi-qubit cavity system set up in control $|1\rangle$ bit with probe of photon resulting in the entangled “dark” states as well as the “bright” state.

It is important to note a lingering flaw in this scheme. While the idea of a “dark” state is physically possible, there are also the unavoidable effects of “bright” states. These “bright” states function opposite to their counterpart; they are short lived transitions that remain coupled to the strong cavity field. The glaring flaw comes when attempting to transition the qubits into the desired entangled “dark” state. A classical field would be applied to the qubits in their ground state which will not only cause the qubits to become entangled but also have the chance to excite both states into a $|1, 1\rangle$ “bright” state. Then, due to the fast acting dissipation of the system, the qubits also have the probability of decaying back into the ground state once again. Thus, in reality, there is not just a solo entangled state when applying the classical electrical pulse, but in fact the wave function of the qubits can either be in the “dark” entangled state or the “bright” ground state. Thus, a probe photon aimed at the cavity can hit the system and if returned unaffected, or the outcome of a $|0\rangle$ control bit, there is difficulty determining whether that came from a true $|0\rangle$ control bit or the reminisce of a “bright” state within a supposed entangled “dark” state of a $|1\rangle$ control bit. The hope is that the presence of the entangled state can change the photon polarization just enough to be able to make a noticeable difference.

5.1 Equations for Coupled Qubits in a Cavity

The scheme for coupled qubits provides four possible eigenstates that the qubits can fall into: a ground state $|0, 0\rangle$, excited state $|1, 1\rangle$, and entangled states $|1, 0\rangle$ and $|0, 1\rangle$. Here, the first index represents the value of the first qubit, whether it individually is in the excited or ground state, and the second index represents the same individual value for the second qubit. This gives the wave function to be:

$$\Psi = C_{0,0} |0, 0\rangle + C_{0,1} |0, 1\rangle + C_{1,0} |1, 0\rangle + C_{1,1} |1, 1\rangle. \quad (25)$$

With this wave function, the goal is to solve for the values of the coefficients in order to get an understanding of the behavior of the coupled qubits in a cavity and what initial values would place the qubits in the entangled state. The Hamiltonian for this system now depends on how each molecules' dipole interacts with the cavity field. It will be assumed that each molecule has the same Rabi Frequency, meaning the values of the dipole moments and electromagnetic field experienced are the same. Furthermore, the same dissipation and decoherence methods for the cavity will be considered as previously mentioned through the Lindblad operator and effective Hamiltonian. The Hamiltonian will then be:

$$\begin{aligned} H_{int} &= -\hbar \sum_{j=1}^N (\Omega_j \sigma_j^\dagger e^{i\Delta t} + \Omega_j^* \sigma_j e^{-i\Delta t}) \\ \Omega &= \frac{d_j \cdot E}{\hbar} \\ d &= - \sum_{j=1}^N (d_j \sigma_j^\dagger + d_j^* \sigma_j) \end{aligned} \quad (26)$$

With a defined Hamiltonian and state wave function, an understanding of the interaction can be understood by solving for the Schrodinger Equation of these two components. The resulting coupled

differential equations become:

$$\begin{aligned}
\dot{c}_{00} &= i\Omega^* e^{-i\Delta t} c_{01} + i\Omega^* e^{-i\Delta t} c_{10}, \\
\dot{c}_{01} &= i\Omega^* e^{i\Delta t} c_{00} - \frac{1}{2}\gamma_2 c_{01} + i\Omega^* e^{-i\Delta t} c_{11}, \\
\dot{c}_{10} &= i\Omega^* e^{i\Delta t} c_{00} - \frac{1}{2}\gamma_1 c_{10} + i\Omega^* e^{-i\Delta t} c_{11}, \\
\dot{c}_{11} &= i\Omega^* e^{i\Delta t} (c_{01} + c_{10}) - \frac{1}{2}(\gamma_1 + \gamma_2) c_{11}.
\end{aligned} \tag{27}$$

The goal would be to find specific electromagnetic pulses that would result in purely entangled states of the qubits. However, as previously mentioned, this becomes a struggle as it is not clear how to solely get an entangled qubit dark state as the excitement and the decay of a classical electromagnetic pulse would result in a combined state of the desired entangled state and ground state. This would be a component of this scheme that would need to be later developed past the timeline of this project.

5.2 Understanding the Polarization of a Photon

At a fundamental level, a photon is a particle that is a quantum of light and the carrier of the electromagnetic field. Although it is a particle, it has wave-like properties that dictate the behavior of the particle. Under the properties of a sinusoidal wave, the photon can have polarization which provides a degree of freedom in the direction in which the wave oscillates in. The photon will propagate forward in a certain direction over time, but its polarization will be in some other direction. For example, a photon can propagate in the x direction, which leaves its polarization to fall into either the y or z direction or some linear combination of the two. Its polarization will determine how the photon interacts and is either affected or unchanged due to other electromagnetic fields, so it is crucial to understand this interaction. As previously mentioned, the scheme of the quantum gate will depend on probing a photon onto the cavity. Once the photon interacts with the cavity and is received, its polarization will determine the status of the cavity and information can then be processed.

5.3 How the Interaction with the Cavity Affects Photon Polarization

Within the scheme of a qubit cavity system, say the cavity holds a single mode in its electric field. Here, a mode represents the allowed frequency in system and since electromagnetic fields depend on a frequency, then there is only one frequency that propagates within the cavity. Outside the cavity, there is an external multi-mode field. We can also say for now that the polarization of the modes within the cavity and outside the cavity are in the same plane, so this is just pure interaction between the fields [8]. The positive frequency components of the quantum electromagnetic field for the external modes will be focused on excited modes centered on the resonant frequency of the cavity. Having the cavity in a resonant frequency is a key component to having the qubits undergo transitions for the quantum gate scheme, thus an understanding of the quantum electromagnetic field interaction with a resonant cavity frequency is also needed. The external electrical field can be described as

$$E(x, t) = i \left(\frac{\hbar\Omega}{2\epsilon AL} \right)^{1/2} \sum_{n=0}^{\infty} b_n e^{-i\omega_n(t-x/c)} \quad (28)$$

Here, b_n is the coefficients of the allowed modes A is the characteristic transverse area of the field. This is an operator of the quantum electromagnetic field, but for ease of use an operator of the field will be Fourier transformed into a dependency of propagating frequency modes and time rather than spatial components and time of the field.

$$b(x, t) = e^{-i\Omega(t-x/c)} \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega b(\omega) e^{-i\omega(t-x/c)} \quad (29)$$

When probing the cavity qubit system, we only care for the interaction of the photon with a single side, thus we can assume a single sided cavity. With this one sided cavity, the following can be written to describe the interaction between the interaction Hamiltonian of the cavity and the external electromagnetic field [8].

$$V(t) = i\hbar \int_{-\infty}^{\infty} d\omega g(\omega) [b(\omega)a^\dagger - ab^\dagger(\omega)] \quad (30)$$

Here, $g(\omega)$ represents the coupling strength between the two fields as a function of the frequency of the mode and a is the operator within the cavity interaction Hamiltonian. The Heisenberg equation of motion for the b operator $b(t, \omega)$ can give the relation between the a operator in the cavity interaction Hamiltonian and b operator of the external field. We can use initial conditions of an input field, which in our case would represent characteristics of the probing photon, to get a solution of the b operator. This b solution will be in terms of our cavity operator. Furthermore, the cavity operator has its own Heisenberg equations of motion to obey. When substituting in the previously mentioned solution of the external field operator, we get an equation for the cavity operator to be

$$\dot{a} = -\frac{i}{\hbar} [H_{sys}, a] - \int_{-\infty}^{\infty} d\omega g(\omega) b(t, \omega). \quad (31)$$

In terms of polarization, the input operator of the field polarization can be defined as [8]

$$a_{IN}(t) = \frac{-1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t_0)} b_o(\omega). \quad (32)$$

With the input field polarization operator defined, it can be substituted into the Heisenberg equation of motion of the cavity field operator to give the Quantum Stochastic Differential Equation

$$\dot{a} = -\frac{i}{\hbar} [a(t), H_{sys}] - \frac{\gamma}{2} a(t) + \sqrt{\gamma} a_{IN}(t). \quad (33)$$

Additionally, the output field polarization operator can similarly be defined in terms of time and frequency of mode as

$$a_{OUT}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t_0)} b_1(\omega). \quad (34)$$

Finally, using the Quantum Stochastic Differential Equation and defined values of the input and output field polarization, the following relation can be made [8]

$$a_{IN}(t) + a_{OUT}(t) = \sqrt{\gamma} a(t). \quad (35)$$

Understanding how the input and output field polarization operators of a photon interact with, the cavity can now establish the assumption on what to expect from the probing photon for the quantum gate scheme. With a now representing the input polarization operator of a photon and b representing the output polarization operator of a photon, the following assumption can be made [7]

$$b_x = a_x - \sqrt{\kappa}a \quad (36)$$

$$b_y = a_y \quad (37)$$

Same as before, the polarization of the cavity is in the x direction and none in the y, as the photon propagates in the z. Thus, with no polarization in the y the operator in that direction remains unaffected and the main change is the x component. This assumption [7, 8] leads to the following expectation values on the output operator depending on the initial state of the coupled qubits within the cavity.

As previously mentioned, if the qubits are initially in the ground state, they are in a bright state that is resonant with the field of the cavity. Therefore the probe photon would be absorbed and then emitted through decay, as it will also be at a frequency resonant with the cavity. While the polarization is not completely unchanged as initially stated within the scheme the polarization, it is instead shifted according to the following expectation values, which can be controlled through the characteristics of the cavity system

$$\langle b_x(\omega) \rangle = \frac{C - 1}{C + 1} \langle a_x(\omega) \rangle \quad (38)$$

where $C = \frac{2g^2}{\kappa\gamma}$ is the atomic cooperativity. Controversially, if the coupled qubits are initially set into the entangled state through the use of the classical field, the probing photon reads an empty cavity since the qubits would have been in the 'dark' state. Thus, the polarization of the probing

photon is shifted and gives the following expectation value

$$\langle b_x(\omega) \rangle = -\langle a_x(\omega) \rangle. \quad (39)$$

In the end, the output polarization of a probing photon differs depending on the state that the coupled qubits are placed into. This can develop further investigation into the experimental feasibility of this type of quantum gate scheme.

6. CONCLUSION

Overall, the scheme and functionality for a quantum gate through the use of qubits within a cavity has been attempted and holds promise for the future. A foundation for classical electromagnetic transitions through the use of classical laser pulses has been established, including the consideration of coupling dipole moments between multiple qubits with the cavity field and inclusion of dissipation and decoherence. Candidate particles have been experimentally tested and numerically characterized, showing potential in filling the role as the qubit. All results lead to a possible scheme for a CNOT gate that involves entanglement of multiple qubits within a cavity, using both quantum and classical electromagnetic fields, which has been established for further development and analysis. While there are flaws to the CNOT gate scenario, there are routes to consider as a probe photon can still differentiate the signal of a fully grounded state versus the mixture of an entangled and ground state through the use of photon polarization. Once that difference has been strongly established, this scheme holds strong promise, along with its potential candidates, to be the next stepping stone in the realm of quantum computing and overall quantum technologies.

REFERENCES

- [1] S. A. M. E. M. T. Q. Chen, Y. Wang and A. Belyanin., “Dynamics and control of entangled electron-photon states in nanophotonic systems with time-variable parameters,” *Phys. Rev. A*, vol. 103, 2021.
- [2] M. Malinowski., “Unitary and dissipative trapped-ion entanglement using integrated optics.” PhD Thesis; ETH thesis repository. 2021.
- [3] D. S. Dovzhenko, S. V. Ryabchuk, Y. P. Rakovich, and I. R. Nabiev, “Light–matter interaction in the strong coupling regime: configurations, conditions, and applications,” *Nanoscale*, vol. 10, pp. 3589–3605, 2018.
- [4] A. Z. D. Bouwmeester, A. Ekert, *The Physics of Quantum Information*. Springer-Verlag, Berlin, Heidelberg, 2000.
- [5] M. Tokman, A. Behne, B. Torres, M. Erukhimova, Y. Wang, and A. Belyanin, “Dissipation-driven formation of entangled dark states in strongly coupled inhomogeneous many-qubit systems in solid-state nanocavities,” *Phys. Rev. A*, vol. 107, p. 013721, Jan 2023.
- [6] M. O. Scully and M. S. Zubairy, *Quantum Optics*. Cambridge University Press, Cambridge, 1997.
- [7] T. C. S. G. S. S. Hyochul Kim, Ranojoy Bose and E. Waks, “A quantum logic gate between a solid-state quantum bit and a photon,” *Nature Photons*, vol. 7, p. 373–377, 2013.
- [8] D. F. Walls and G. J. Milburn, *Quantum Optics*. Springer-Verlag Berlin Heidelberg, 1994.