Monte Carlo simulations of populations in Lambda and Vee qutrit configurations

A Python Monte Carlo simulation of qutrit dynamics built up from the fundamentals of quantum mechanics. This simulation demonstrates the differences of the dynamics of the commonly used Vee and Lambda configurations of qutrits. For the Lambda system it is shown how the continuous driving of the two laser probes results in the formation of a dark state and from this, electromagnetic induced transparency. For the Vee system the equilibrium state populations were found with a good precision of less than 2% of the total population of all 3 states using 300 runs of the simulation and reduced chi-squared values between 1 and 3 showing that the simulation models the physics reasonably well. At equilibrium, half the population ends up trapped and is shared between the two excited states as predicted by the theoretical models [REF8].

I. INTRODUCTION AND THEORY

In 1980 Yuri Manin proposed the idea of quantum computing in his paper 'Computable and Uncomputable' which formed the basis for this type of technology. Soon after, in 1981, Feynman presented his own quantum computing model, which influenced many others to begin research in this field after realising it's potential. Later, algorithms such as Shor's quantum computer algorithm [REF1] and adiabatic computation [REF2] were shown to be capable of rapidly breaking many of the modern encryption methods due to how they can handle much larger calculations compared to regular computers. This demonstrates the superiority of these computers for certain calculations.

The most basic set-up for a quantum computer is an arrangement of qubits, the quantum equivalent to bits. A classical bit is the smallest unit of data used to represent information in a computer - it will either be in state 0 or state 1. Similarly to a light switch being either on or off, a classical bit cannot be in a superposition of both states like a quantum bit (qubit) can.

Any quantum system with two states can be represented by a qubit, which is represented by a wave function of the form:

$$\Psi = a\,|0\rangle \;+\; b\,|1\rangle \tag{1}$$

The square of the coefficients a or b tell us the probability of finding the qubit in state 0 or 1 respectively. These coefficients need not be real, but the sum of their squares must add up to one. The coefficients can be fine-tuned by altering the proportion of the population in each state. For an atomic qubit, a laser can be used to drive the population of the ground and excited states so that they oscillate sinusoidally. These oscillations are known as Rabi oscillations. The excited state decays over time and the average time for decay is called the excited state lifetime. This decay of the excited state can be measured when the photon released hits a detector.

Building up on qubits, quantum information can be generalised to 3 or more level systems that can be represented in a similar way to the qubit with a wave-function given by:

$$\Psi = \sum_{i=0}^{n-1} C_i\,|i\rangle \tag{2}$$

for a n-level system. However, this report will focus on qutrits, the 3-level system and the different configurations. Not every 3-level quantum system is a qutrit;

each transition between energy levels needs to be independent and the transition between two of the states will be electrically dipole forbidden; forbidden due to angular momentum conservation. The two main configurations are the Lambda and Vee qutrit in which there are either two ground states and one excited state or one ground and two excited states. When using a

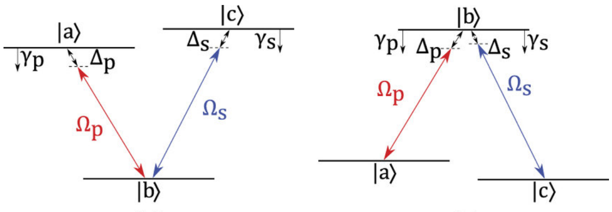

FIG. 1: diagram (a) – VEE (b) – Lambda configurations shown.[REF8]

frequency resonant to state $|g\rangle$ and $|a\rangle$ it will be absorbed. Then, if you take another laser and radiate on the state $|e\rangle$, the original frequency of light will be able to pass through and the gas will become transparent to that light. It becomes transparent because the original resonant field is no longer absorbed, causing the population to be trapped in the ground state. This effect is known as electromagnetically induced transparency (EIT) [REF3]. A common and easily-made confusion in quantum computing is the difference between EIT and coherent population trapping (CPT) [REF4]. CPT is the experimental setup involving a Lambda configuration with one of the ground states as a meta-stable state, meaning the state lifetime is very large. When two lasers are used, over time the atoms can be trapped in a desired state, this process is seen as a generalisation on of the optical pumping process. This process has many applications such as CPT magnetometers and atomic clocks [REF5]. When EIT occurs, the probe absorption vanishes at the correct frequency making the material transparent to a small range of light. This phenomenon was first observed in 1990. It can be explained by the result of two dressed states destructively interfering with their energy split induced by the oscillatory nature of the AC electromagnetic field interacting with the atom. This energy split can be controlled to give a desired quantity by changing the rabi frequency and detuning of the lasers used. Alternatives to EIT such as Raman Resonances for quantum memory applications have been used with success where Raman resonances are known as the narrow absorption resonances in a qutrit where 2 lasers are detuned. It is now known that EIT is a subset of 3-level Raman processes. [REF6] We can track the population of the states by looking at the density matrix at each point, which is given by:

$$\begin{pmatrix} aa* & ab* & ac* \\ ba* & bb* & cc* \\ ca* & cb* & cc* \end{pmatrix} \tag{3}$$

where the state population is analogous to the corresponding diagonal matrix element. This density matrix and its time evolution can be used to find an analytical solution under certain assumptions and approximations and is used throughout quantum mechanics [REF8]. Given that the system is isolated we can see this matrix is trace-preserving due to the total population of the three states being constant (set to 1).

II. METHODS

By representing the 3 states of the qutrit as 3 linearly independent vectors:

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{4}$$

we can find the Hamiltonians in the co-rotating frame [REF8] that describes the interaction of the Vee and Lambda qutrits and the EM fields driving them, which are given by:

$$H_{Eff,Vee} = \begin{pmatrix} 2\Delta_p & -\Omega_p & 0 \\ -\Omega_p - \gamma i & 0 & -\Omega_s \\ 0 & -\Omega_s & 2\Delta - \gamma i \end{pmatrix} \quad (5)$$

$$H_{Eff,Lambda} = \begin{pmatrix} -2\Delta_p & -\Omega_p & -\gamma i \\ -\Omega_p - \gamma i & 0 & -\Omega_s \\ 0 & -\Omega_s & -2\Delta \end{pmatrix} \quad (6)$$

For take sake of simplicity, at $t = 0$ state $|b\rangle$ was assumed to be full and no other states occupied. The decoherence which is the detuning of the lasers from the resonant frequency, Δ , was set to 0, the rabi fequencies, $\Omega_p = \Omega_s = 10$ was used and a decay rate, $\gamma \equiv 1$ was used for all transitions. The different positions of the decay terms are found by inspecting how the different states can decay in the different configuration. However, in both set ups the $|a\rangle$ to $|c\rangle$ transition is still dipole forbidden. Due to the Hamiltonian being non-hermitian, after each Monte Carlo step the wavefunction needs to renormalised back to a norm of 1 [REF 9, 10]. By using Schrodinger's equation [REF13]:

$$i\hbar\frac{\partial\Psi}{\partial t} = H_{eff}\Psi \quad (7)$$

we can find how the wavefunction propagates through time and by using dt to be very small (0.001 was used; smaller dt caused the kernel to crash as too many values were being calculated), we can approximate the exponential to first order in dt:

$$\Psi(t+dt) \approx (1-\frac{i}{\hbar}H_{eff}dt)\Psi(t) \quad (8)$$

as the other higher order terms will be negligible. We use this to know how the wave propagates and also construct a jump operator for when we want to simulate the quantum jumps.At each step we generate a random number between 0 and 1, if the new norm squared of the wavefunction after propagation is less than this number then we assume there are quantum jumps occurring so we apply the jump operator and re-normalise to repeat this process for the next step. If the norm squared is greater than the number generated then we assume no jumps occur at this step and then we just renormalise the wavefunction. Originally a unification of two, 2-dimensional vectors were used to represent the wavefunction with their second entries being the same and a constant proportion of the excited state in the lambda configuration was assumed to decay evenly into both ground states at each step in the Monte Carlo process. From this method it is clear how populations can be trapped when the laser driving is much smaller for the $|b\rangle$ and $|c\rangle$ transition. From this method it is clear how populations can be trapped but this led to problems when re-normalising and the results did not agree with the analytical solution showing there are quantum effects which are unique to the 3 level systems that cannot be described using only the knowledge of qubits.

III. RESULTS

Equilibrium values			
	P_{aa}	P_{cc}	P_{bb}
Vee	0.2507	0.2492	0.5001
Vee standard error	0.0004	0.0004	0.0070
Vee χ^2	1.4900	-	2.9400
Lambda	0.4971	0.5017	0.0011
Lambda standard error	0.0133	0.0136	0.0185
Lambda χ^2	2.3700	-	3.2650
Theoretical Vee	0.2500	0.2500	0.5000
Theoretical Lambda	0.5000	0.5000	0.0000

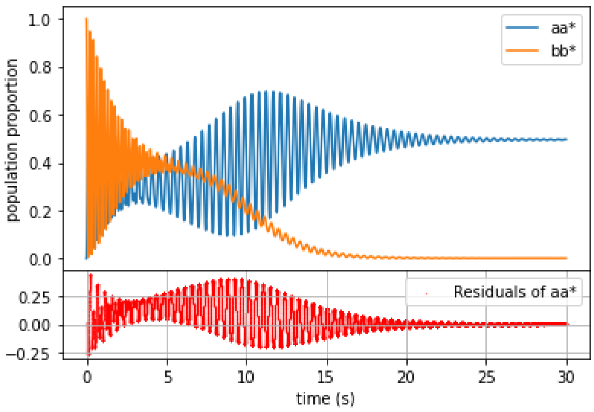

FIG. 2: 300 simulation cycles average of the Lambda qutrit

The analytical equations for the state populations were very complex and have been omitted but can be found in the references. [REF8] A Standard error of each value from 300 runs was calculated but were not plotted as error bars due to the graph being hard to read when added; however, the standard error of the values that the three states converge too are given in the results table. In the Vee configuration, looking at the population of state $|a\rangle$ residuals, we can see how the sig-

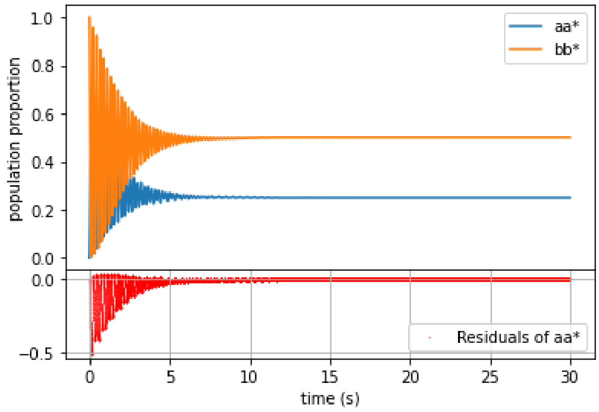

FIG. 3: 300 simulation cycles average of the Vee qutrit

nificant residuals are bunched towards the start of the simulation with a high magnitude of almost half the whole system population near the very start. As time increases the residues get smaller, showing some sort of systematic error for very low times. A possible source may be due to the small dt approximation used for the exponential function as it was found that the residuals greatly decrease when using a smaller step size. This may be because of randomness is more prevalent when less iterations of the algorithm cycle have occurred. In the Lambda configuration, we can see the residuals are smaller in magnitude but the time for convergence to the equilibrium values is longer than the theoretical model predicts causing the simulation to fit worse for this set-up.

IV. DISCUSSION

A result that may seem unexpected is that the analytical solution shows that for large values of time, the ratio of populations of state $|a\rangle$ and state $|c\rangle$ in the Lambda configuration are equivalent to: $\frac{\rho_{aa}}{\rho_{cc}} = \frac{\Omega_s^2}{\Omega_p^2}$ [REF8] This shows that a larger driving EM field on the $|c\rangle$ state transition leads to a larger final population of state $|a\rangle$. However, a possible explanation for this is that a larger field intensity will cause a higher proportion to be excited from state $|c\rangle$ then decay back to state $|a\rangle$. From the above we can see that the final state of the lambda qutrit is a multiple of $\frac{\Omega_s|a\rangle-\Omega_p|c\rangle}{\sqrt{\Omega_p^2+\Omega_s^2}}$ which is a dark state. This simulated dark state, of course, has the populations trapped and EIT occurs by the definition of a dark state, giving the desired result of the simulation's goal [REF14]. Looking at single runs of the Monte Carlo algorithm of the Lambda system shows that, for some reason it can become chaotic on rare occasions, possibly due to the random nature of the first number generation. However the final convergence of state populations was always consistent. The random simulation errors were reduced by using 300 runs and taking the average for each step. The standard error which was not plotted due to being barely visible on the graph in the last portion and making the initial section of the simulations very unclear. The initial oscillatory section of both qutrit configurations is the cause of the main deviation from the theoretical models, and each run of the simulation mainly differed in the initial section due to the random number generated having an effect of a possible chaotic start. However, the overall trend of decay and growth of the state populations line up with the analytical models and the agreement of the equilibrium values was always achieved over time. The randomness of the Monte Carlo simulation was reduced by taking an average of 300 runs and from this standard errors were found for each step in the algorithm. The lambda system had greater errors on the final equilibrium values due to the simulation being more chaotic and random in the beginning portion. Using chi-squared analysis it was found that the simulated results agreed well for the Vee qutrit; however, the Lambda results all have reduced chi-squared values above 2, suggesting the simulation does not fit the theoretical model quite well. This can be seen from the fact that the Lambda simulation does not decay fast enough, as seen by the residuals. The main source of contributions to the larger chi squared is the mid region where the oscillations begin to become larger again, which cannot be explained by the physics of the system and must be caused by some kind of systematic error. The small dt approximation may play a role in the large chi-squared value, however it seems unlikely that this approximation caused the 'regrowth' of the oscillations in the Lambda configuration simulation. From figures 2 and 3, it can seen that all populations end up constant and remain unchanged. This suggests some form of transparency which was confirmed for the Lambda configuration being proportional to a dark state.

V. CONCLUSIONS

In this report a Monte Carlo method that predicted the correct equilibrium state populations with very small standard errors by building upon the fundamentals of quantum mechanics was shown. This simulation may be useful applied to future research given how reproducible and easy to adapt it is. Many applications are already known so this simulation can be used to help predict and monitor the behaviour of various qutrit set ups when a full experiment may not be viable due to quantum systems in starting pure states being hard and expensive to produce. Other methods were found and attempted that demonstrate population trapping but problems arise due to the order of re-normalisation and were not as successful as the main method explained. Future work that needs to be done includes modelling the ladder configuration however I have found that this seems to be the least used configuration in research. Scenarios in which the decay of the excited states are not equal can be modelled using my Monte Carlo code however there is no known analytical solution for different decay rates to compare to. [REF15]

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SCIENTIFIC SUMMARY FOR A GENERAL AUDIENCE

In this paper a computational method was used to model 3 level quantum systems that were driven by 2 separate lasers in an attempt to show Electromagnetic induced transparency, a feature of 3 level or more systems where lasers can be used to turn a material transparent to certain frequencies. The simulation struggled to model the systems for times just after the lasers are switched on, however the end results always agreed to 4 decimal places or better. The simulation can be improved by using smaller step sizes in-between calculations due to the linear approximation of the exponential function. On the bright side, the simulation managed to come to a results of a dark state; specific conditions where the system no longer absorbs or emits light regardless whether the lasers are still on. This is an example of complete transparency which can only occur in certain 3 level system configurations.