Unitary Integration of Open Atomic Systems

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A Project Report Submitted in Partial Fulfillment of the Requirements for the Degree of
Master's in Physics

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ACKNOWLEDGEMENTS

I am able to achieve this feat because of unwavering support from various guides and would like to thank them here. Especially, I would like to thank Professor Sai Vinjanampathy who has been very generous, insightful and patient. I have deeply enjoyed the weekly discussions with him. Also, I would like to thank my colleagues Naman Kesharwani and Gourang Singh Padihar for their help throughout the journey.

ABSTRACT

To control the dynamics of a quantum system, the first thing to know is to learn how it reacts or evolves in various situations. But the long-withstanding problem with applying quantum mechanics is that the von-Neumann Equation for the most realistic systems is not solvable easily. This problem becomes impossible for (except for very few cases) time-dependent Hamiltonians. Hence, we opt for approximate methods that present two main difficulties. The number of unknowns increases exponentially as you increase the dimensions of your system and hence the number of differential equations associated with those. Next is more dangerous as due to accumulation of errors in your approximate solutions can make it nonphysical. It is of prime importance for these integration algorithms to preserve what we call constraints for the stability of the solution. One such algorithm is unitary integration which preserves the norm of the state vector during its evolution by its mere construction. Since in the end, our main aim is solving real-world problems that are essentially open quantum systems, we extend this to solving the Lindblad master equation (LvNL) for Markovian open quantum systems. These dynamics have to follow a constraint of trace preservation of the density matrix. This constraint, just like unitarity comes out from its governing LvNL equation naturally. In demonstrating so, we have described two famous problems in atomic physics; Avoided Level Crossing in both closed and open dynamics and Spin Relaxation. Solving these textbook problems using Unitary Integration may expose the reader to the subtleties of the method with all its limitations and advantages.

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Chapter 1

A BRIEF INTRODUCTION TO OPEN QUANTUM SYSTEM

Schrodinger equation describes the dynamics of a closed system's state vector whose dynamics are governed by the system's Hamiltonian. One can include the external interactions by bringing time-dependence in the Hamiltonian but that is still a limited portion of the vast ocean of systems. To incorporate this idea of mimicking the real world by considering an open quantum system we begin with defining **density operator**. The idea is based on the fact that any open system is a sub-part of a larger closed system. Since we are not concerned with this larger system, we ignore its dynamics, only considering its interactions with our system.

Density Operator

The most general quantum state is represented as a matrix called density matrix which contains all the **known** information about that system. It is called this because it behaves as if it is a probability density in expectation value expressions. [1.1]

The density operator needs to be a

1. Hermitian matrix: $\rho^\dagger = \rho$
2. Positive matrix (all non-negative eigenvalues): $\rho \geq 0 \equiv \langle\Psi|\,\rho\,|\Psi\rangle \geq 0$
3. and with unit trace: $\mathbf{Tr}\{\rho\} = 1$

A composite system can be thought of as made up of different correlated subsystems. Let's, for the time being, divide our system into two parts (could be of arbitrary dimensions) and call the parent Hilbert Space $\mathcal{H}_{AB}$ such that

$$\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$$

Now, if we would like to *operate* only our subsystem **A** (out of composite A and B), we operate on this composite system with $M_A \otimes \mathbb{I}$.

The expectation value of observable in a general composite state $|\psi\rangle = \sum_{ij} \psi_{ij}\,|A_i\rangle \otimes |B_j\rangle$ (where it is expanded in their orthonormal product bases set) is

$$\begin{aligned}
\langle M_A \rangle &= \langle \psi | \, M_A \otimes \mathbb{I} \, | \psi \rangle \qquad (1.1) \\
&= \Big(\sum_{i'j'} \psi^*_{i'j'} \, \langle A_{i'} | \otimes \langle B_{j'} | \Big) \big(M_A \otimes \mathbb{I} \big) \\
&\quad \sum_{ij} \psi_{ij} \, | A_i \rangle \otimes | B_j \rangle \\
&= \sum_{i,j,i',j'} \psi^*_{i'j'} \psi_{ij} \, \langle A_{i'} | \, M_A \, | A_i \rangle \otimes \langle B_{j'} | B_j \rangle \\
&= \sum_{i,j,i',j'} \psi^*_{i'j'} \psi_{ij} \, \langle A_{i'} | \, M_A \, | A_i \rangle \otimes \delta_{j'j} \\
&= \sum_{i,i',j} \psi^*_{i'j} \psi_{ij} \, \langle A_{i'} | \, M_A \, | A_i \rangle \\
&= Tr\{\rho_A M_A\} \qquad (1.2)
\end{aligned}$$

where $\rho_A = Tr_B\{\langle\psi|\psi\rangle\} = \sum_{i,i',j} \psi^*_{i'j} \psi_{ij} \, |A_i\rangle \langle A_{i'}|$[1] is called the Local Density Operator (LDO) of subsystem A. Similarly, we may find the evolution (could be non-unitary) and measurement (could be non-orthogonal) of the density matrix in accordance with the unitary evolution and orthogonal measurement of the parent system. This is the ensemble interpretation of the density matrix which represents a classical mixture (as there is no superposition in this summation) of pure states (need not be orthonormal). It is consistent and convenient to interpret ρ_A as representing an ensemble of possible quantum states, each occurring with a specified *classical* probability.

We will call the operation which we used to get the LDO from the pure density operator as **partial tracing** over subsystem B. Since, diagonal entries of the density matrix contain probabilities, we can interpret this tracing as averaging out. This act of averaging out over degrees of freedom of subsystem B is what could be thought of as losing the information about B. This slides classical probabilities into the description of the state and we get a mixed state, *incoherent* mixture of all possible pure states.

Summarising what is happening, we can say that A and B become *entangled*, that is, correlated. [2] The entanglement destroys the coherence of a superposition of states

[1] The operation $Tr_B\{\}$ is called partial trace and defined by the above equation

[2] It is not correlation always. Strictly, an entangled system is defined to be "one whose quantum state cannot be factored as a product of states of its local constituents; that is to say, they are not individual particles but are an inseparable whole." [1]

of A so that some of the phases in the superposition become inaccessible if we look at A alone.

It is noteworthy that you can represent an LDO as a sum of other density operators weighted by positive coefficients.

$$\rho(\lambda) = \lambda\rho_1 + (1-\lambda)\rho_2$$

where $0 \leq \lambda \leq 1$ is imposed, making it a *convex* linear combination. The term convex is due to mathematical definition as each linear combination has to be weighted positively, making the set of this ρ of convex shape. On the surface of these convex shapes lies the **extremal points** in the language of Convex vector spaces. If we look at the shape of the Bloch sphere of a general state of a qubit, we'd found that all extremal points are pure states. This means that you have a unique density operator for a pure state in particular bases. A more important version of this statement is "mixed states are not uniquely defined".

Schmidt Decomposition

It proposes to decompose a pure state vector in terms of a particular orthonormal basis of both $\mathcal{H}_A$ and $\mathcal{H}_B$.

$$|\psi\rangle_{AB} = \sum_{a,b} \psi_{a,b} \, |a\rangle_A \otimes |b\rangle_B = \sum_i \sqrt{p_i} \, |i\rangle_A \otimes |i'\rangle_B$$

where $|i\rangle$ and $|i'\rangle$ are orthonormal bases of their respective Hilbert space. This is very similar to the Singular Value Decomposition of a matrix ψ_{ab} which diagonalizes the matrix with non-negative values. The bottom line is to transform (rotate and stretch) the basis vectors of B subspace such that the number of new bases in B equals the number of bases used in A subspace. Therefore, for a particular state of subsystem A, you get a particular Schmidt decomposition.

This form is particularly helpful in calculating the partial trace easily. As we can take $|i\rangle_A$ to be the bases vectors in which ρ_A is diagonalised. It gives a spectral decomposition of a mixed state

$$\rho_A = Tr_B\{|\psi\rangle \langle\psi|\} = \sum_i p_i \, |i\rangle \langle i|$$

where p_i are the probabilities associated to each of the pure state $|i\rangle\langle i|$. This decomposition gives out the orthonormal basis set of both systems. Therefore, if suppose ρ_A has degenerate non-zero eigenvalues, then you can't construct Schmidt decomposition only through the eigenspectra of both density matrices. Hence, you can only predetermine your decomposition up to a unitary.

Kraus Operators

The evolution of pure states is described by Unitary operators. Since every observable is a hermitian matrix (according to the postulates of QM) and their exponential (which comes from the generator of that observable) is Unitary, hence every evolution is unitary. This seemingly cyclic argument is based on fundamental symmetries which say that for every observable, you would have an evolutionary operator and vice-versa. But if we look at a part of the system and call the other its environment, we may not get a unitary evolution of LDO.

An evolution of LDO is given by a map (called **super-operator** as it operates on density operator) which maps one LDO to another LDO. This map should be

1. Linear and
2. Preserves Hermiticity
3. Preserves Positivity (complete*)
4. Preserves Trace

This is called the Completely Positive Trace Preserving (**CPTP**) map. These requirements ensure that at the end of the map, we get a valid LDO. That is, a map of the following form

$$\varepsilon(\rho) = \sum_a M_a \rho M_a^\dagger$$

should give out a matrix (LDO essentially) which is a semi-definite Hermitian matrix with a unity trace. Here M_a, also known as Kraus operators, follow a completeness relation

$$\sum_a M_a^\dagger M_a = \mathbb{I} \tag{1.3}$$

This channel goes through a more constraint condition of **complete positivity*** that means that any map of the form $\varepsilon \otimes \mathbb{I}_d(\rho)$, where the dimension of latter subsystem d is arbitrary, should also be positive. Physically, this means that any channel acting on only a sub-part of a complete density matrix should give a valid global density matrix *even* if the environment is just an audience, completely detached.

Now, just like before let's write out a general evolution of a composite system's mixed state $\rho_{AB} = |\psi\rangle\langle\psi|_{AB} = \rho_A \otimes |0\rangle\langle 0|$ belonging to Hilbert space $\mathcal{H}_{AB}$ with a unitary U_{AB}. If we would like to know only about system A, we would trace B out from the final pure state of the composite system and would get ρ'_A

$$\begin{aligned}\rho'_A &= \varepsilon(\rho_A) = Tr_B\{U_{AB}|\psi\rangle\langle\psi|U^\dagger_{AB}\} \qquad (1.4)\\ &= Tr_B\{U_{AB}\rho_A \otimes |0\rangle\langle 0|U^\dagger_{AB}\}\\ &= \sum_b \langle b|_B \left(U_{AB}\rho_A \otimes |0\rangle\langle 0|U^\dagger_{AB}\right)|b\rangle_B\\ &= \sum_b \left(\langle b|_B U_{AB}|0\rangle\right)\rho_A\left(\langle 0|U^\dagger_{AB}|b\rangle_B\right)\\ &= \sum_b M_b\rho_A M_b^\dagger \qquad (1.5)\end{aligned}$$

where these Kraus operators follow equation (1). These maps are **linear** therefore, also follow concatenation. That is, a map $1 \longrightarrow 3$ can be written as $1 \longrightarrow 2 \longrightarrow 3$. These maps are irreversible, unlike their closed system counterparts unitaries. This also makes intuitive sense as throughout the process you are ignoring the effects which are being done on the environment through partial traces.

Liouvillian super-operator

Differentiating the density operator and plugging Schrödinger equation $i\hbar\partial_t|\psi\rangle = H|\psi\rangle$ would give us [3]

$$\begin{aligned}\partial_t\rho =&(\partial_t|\psi\rangle)\langle\psi| + |\psi\rangle\partial_t\langle psi|\\ =&-\frac{i}{\hbar}H\rho + \frac{i}{\hbar}H\rho\\ =&-\frac{i}{\hbar}[H,\rho] \qquad (1.6)\end{aligned}$$

[3] we have omitted $\hbar$ where ever required

This derivation of the so-called Schrödinger-von Neumann equation is given for pure state but it is readily extended to a general density state. One may rewrite this in a more compact form

$$\partial_t \rho = \mathcal{L}\rho \tag{1.7}$$

where $\mathcal{L}$ is the **Liouvillian Super-operator** where $\mathcal{L}$ can contain more than just H terms, like **Lindbladians** from equation (1.8).

Lindblad Master Equation

Just like Schrödinger equation can describe the continuous-time dynamics of a closed system, a master equation can describe the continuous-time dynamics of a density operator, at least to a good approximation. The main feature of the equation is that it evolves the system locally in time. The state $\rho(t + dt)$ would only depend on the state $\rho(t)$.

For an open quantum system, completely dissipative dynamics (Markovian dynamics) are not exactly possible but they are a good approximation if the time scales of the evolution of the concerned system are far larger than the correlation time of non-Markovian fluctuations. This is best reproduced while interacting with 'heat baths'. Because we can assume that the system and baths interact weakly (Born Approximation) and baths evolve quickly to their equilibrium state due to their large degree of freedom (typical nature of memoryless Markovian evolution).

Hence, we discard the state of the environment after each infinitesimal time step in the joint evolution of the system and environment and replaced it with the same unentangled state.

Encoding this idea in (1.5) gives us Lindblad master equation [2] of the density matrix:

$$\dot{\rho} = i[\rho, H] + \sum_i \Gamma(L_i \rho L_i^\dagger - \frac{1}{2}\{L_i L_i^\dagger, \rho\}) = \mathcal{L}\rho \tag{1.8}$$

The first term in $\mathcal{L}(\rho)$ is the familiar Hamiltonian term responsible for unitary evolution. The latter terms describe the possible transitions a system can take while interacting with the environment. The operators L_i are called *Lindblad operators or quantum jump operators*. The importance of this master equation can be felt from its widespread use in fields like quantum optics, condensed matter, atomic physics and quantum information [3, 4, 5, 6, 7, 8].

Representation for N-Qubit Subsystem

If considered $\sigma_\mu : \{\mu \in \{0,1,2,3\}\}$ as the basis set of one qubit LDO, where $\sigma_0 = \mathit{I}_2,\ \sigma_1 = \sigma_x,\ \sigma_2 = \sigma_y,\ \sigma_3 = \sigma_z$. You can define the basis set for N-Qubit System LDO as

$$\{\sigma_\mu^N\} = \bigotimes_{\{i\}}^{N} \sigma_{\mu_i} \tag{1.9}$$

Therefore, a general LDO for an N-qubit system looks like

$$\rho = \sum_{\mu}^{2^{2N}} r_\mu \sigma_\mu^N \ = \sum_{i,j,k,l\cdots\varsigma} r_{i,j,k,l\cdots\varsigma}\ \sigma_i^1 \otimes \sigma_j^2 \otimes \sigma_k^3 \otimes \sigma_l^4 \otimes \cdots \sigma_\varsigma^n \tag{1.10}$$

where $r_{000\ldots}$ needs to be $\frac{1}{N}$ and $i, j, k, l \cdots \in \{0,1,2,3\}$. If we vectorise this tensor $\mathbf{r}$ by parameterising it by μ (removing $r_{000\ldots}$), we can extend the notion of Bloch Vector by this $2^{2N} - 1$ dimensional vector whose **Euclidean** norm will give us an idea of how far is it from the maximally mixed state. For any density matrix ρ of $N \times N$ dimension, we can easily find these coefficients using the following

$$r_{i,j,k,l\cdots} = Tr\left[\rho(\sigma_i \otimes \sigma_j \otimes \sigma_k \otimes \sigma_l \otimes \cdots)\right]$$

SU(N): Digression

We can't press enough how often you see rotations or rotations-like operations in Quantum mechanics. Unitary integration (UI) is also loosely based on the easiness they bring to computations.

What are rotations? One can define them to be movements in a circle around a central point. The matrix associated with them is called **orthogonal matrices** with a determinant equal to 1. That is, an orthogonal matrix can be defined as

$$R^T R = \mathbb{I}$$

as it follows the basic property of any rotation operation of $R(\theta_1 + \theta_2) = R(\theta_1)R(\theta_2)$ and $R(-\theta) = R^T(\theta)$. You can write these together as $|R^T R| = 1$. For infinitesimal rotation, we write

$$R = \mathbb{I} + A \qquad where \quad A^T = -A \tag{1.11}$$

$$\implies R = \mathbb{I} + i\vec{\theta} \,.\, \vec{\mathbf{J}} \tag{1.12}$$

where **J** are called generators of rotation group because they capture all the information of the group. Now, based on the insight that rotation is a continuous operation, one can write

$$\mathbb{R}(\Theta) = \lim_{N->\infty} \left(\mathbb{I} + i\frac{\vec{\Theta}}{N} \,.\, \vec{\mathbf{J}}\right) = e^{i\vec{\Theta} \,.\, \vec{\mathbf{J}}} \tag{1.13}$$

Just for the sake of completeness, one should know that this formalism comes from a general theory of Lie Groups where equation (1.13) gives the definition of Lie Algebra of a Lie Group [9].

The connection of Algebra with the group is made clearer with the Baker–Campbell –Hausdorff formula:

$$Z = X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}([X, [X, Y]] + [Y, [Y, X]]) + \ldots \tag{1.14}$$

where (1.15)

$$e^Z = e^X e^Y \tag{1.16}$$

The generators Z, Y, and X are related by the relation (1.14) when their rotation operators are related by (1.16). The higher order in terms of commutators is omitted from the above expression. This expression highlights the non-commutativity of the SO(N) operations[4]. The importance of this relation can't be overemphasized for us as it is going to make the foundations of the method of unitary integration.

Closed Under Commutation

The above definition can be generalised. These groups are called Special Unitary Groups containing unitary operators with their absolute determinant equal one. For instance, the elements of $SU(2)$ of the group have the following zero-trace generators which are closed under commutation. This means that $[\sigma_i, \sigma_k] = \sigma_j$ where all three operators $\sigma_{i,j,k}$ belong to the same algebra.

[4]This is followed by other elements from Lie Algebra

$$\tau_1 = \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix}, \qquad \tau_2 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \qquad \tau_3 = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} \tag{1.17}$$

These are related to Pauli matrices as $\tau_1{=}i\sigma_1$, $\tau_2{=}{-}i\sigma_2$, $\tau_3{=}i\sigma_3$. The *Complexified* Lie algebra of $SU(2)$ also closed under commutation property: $[\sigma_+, \sigma_-] = 2\sigma_3$ and $[\sigma_\pm, \sigma_3] = \mp\sigma_\pm$. [1, 9, 10, 11]

Summary of Open/Noisy Quantum System

First of all, a connection of Open Quantum System to Probability Theory[11] is illuminating which is presented in the next table 1.1.

Scalar Probability Theory	**Noisy Quantum Theory**
Random Variable: X	χ
Ensemble: $\{p_X(x); x\}$	$\{p_\chi(x); \lvert x\rangle \langle x\rvert\}$
Mean: $\mathcal{E}[X] = \sum_x x p_X(x)$	$\mathcal{E}[\chi] = Tr[\chi\rho]$
Unions: $p(x_1 \cup x_2)$ $= p(x_1) + p(x_2)$	$p(x_1 \cup x_2) = Tr\{\sum_{x_1} \lvert x\rangle \langle x\rvert \rho\}$ $+Tr\{\sum_{x_2} \lvert x\rangle \langle x\rvert \rho\}$

Table 1.1: where $X = \sum_x x \lvert x\rangle \langle x\rvert$ & $\rho = \sum_x p_\chi \lvert x\rangle \langle x\rvert$ only when both variables are uncorrelated. Here the random variables belonged to two different subsets, i.e. $x_i \in X_i$. Therefore, noisy quantum theory contains most of the elements from probability theory. For an ensemble of random variables (could be scalar or vector) the form of mean and combination of the mean of disjoint variables follow the same rule.

One can generalise this notion of evolution and measurement through the concept of the TPCP map. Both give you incoherent mixtures of states **(decoherence)**. It is just that you don't have to average out other possibilities in the case of measurements.

We have now **three postulates of Quantum Mechanics** that

1. A state is defined by a semi-definite positive hermitian matrix with unit trace.
2. A measurement is defined by a positive operator-valued measure in which operators are a partition of identity.
3. A time evolution is defined by a trace-preserving a completely positive map.

Chapter 2

THE MOST GENERAL SCHRODINGER EQUATION

Consider the von-Neumann Liouville equation,

$$i\dot{U}(t) = H(t)U(t) \qquad \text{with} \quad U(0) = \mathcal{I} \tag{2.1}$$

where U is unitary, following $UU^\dagger = U^\dagger U = \mathcal{I}$.

This is equivalent to Schrodinger equation $i\dot{\rho} = [H(t), \rho]$ together with $\rho(t) = U(t)\rho(0)U^\dagger(t)$. in the following way. For the most general time-dependent Hamiltonian, U cannot be written by simple exponentiation of (2.1) except for infinitesimal steps in the time since H(t') at one time does not commute with the same operator at a different time H(t"). One of the possible solutions includes a series of nested *time-ordered integrating* terms called Dyson Expansion [1], for finite time [10]. Hence, it is impossible to solve these equations exactly. Hence, we look for techniques like **perturbation theory**, and numerical methods of integration for the nearest solutions of the nearest problem. This two-fold approximation may discourage the reader and present them with the idea that all is in vain. But these solutions have been remarkably useful in describing physics rather well. We will focus on a special type of Hamiltonian in this thesis, where the time dependence is only from the coefficients of *non-commuting time independent operators.* This includes a big portion of quantum mechanical problems from various fields of quantum optics and atomic and molecular physics. We will describe two approaches briefly in the upcoming sections.

2.1 Perturbation Theory

The biggest difference when solving a time-dependent Hamiltonian in contrast to a time-independent one is that separable solutions no longer exist, hence we can no longer find stationary states. So, we try to solve the following Schrödinger equation.

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = \left(H^0 + \delta H(t)\right)\left|\Psi(t)\right\rangle \tag{2.2}$$

[1] A time-ordered series of unitary operator for a time-dependent perturbation H'(t) to a time-independent Hamiltonian H_o

Consider a scenario of a hydrogen atom sitting idle. Hence, it is in its eigenstate. Now, it interacts with a time-dependent electromagnetic field which changes your state from one eigenstate to a superposition of many eigenstates, possibly infinite. So, our aim is to go in **interaction picture** to find the $|\Psi(t)\rangle$. Interaction picture takes a part from both Heisenberg's and Schrodinger's pictures.

We **define** a new wave function

$$|\Psi(t)\rangle = exp(-\iota H^0 t/\hbar)\,|\Psi(t)'\rangle$$

where $|\Psi(t)\rangle$ is the total wave function of H(t). Putting this in (2.5)

The time evolution can be written as

$$i\hbar\frac{\partial\,|\Psi(t)'\rangle}{\partial t} = \left(exp(iH^0 t/\hbar)\;\delta H(t)\;exp(-iH^0 t/\hbar)\right)\;|\Psi(t)'\rangle \tag{2.3}$$

which we can denote as $\delta H'(t)\;\;|\Psi(t)'\rangle$.

In any orthogonal basis set of this system's Hilbert space, our state can be readily expanded. Now, since the choice is upon us and we obviously will take energy eigenstates of H^0 as our basis ($|n\rangle$). Taking $|\Psi(t)'\rangle = \sum_n c_n(t)\,|n\rangle$, $|\Psi(t)\rangle$ would become

$$|\Psi(t)\rangle = \sum_n c_n(t) e^{(-iE_n t)/\hbar}\,|n\rangle \tag{2.4}$$

Now, plugging $|\Psi(t)'\rangle$ in equation (2.3)

$$\begin{aligned} i\sum_n \dot{c}(t)\,|n\rangle &= \sum_m |m\rangle\,\langle m|\;\;\delta H'(t)\;\;\sum_n c_n(t)\,|n\rangle \\ \implies c_n(t) &= -\frac{i}{\hbar}\int_0^t dt'\,\langle n|\,\delta H(t')\,|m\rangle\,e^{-i(E_m-E_n)t'} \end{aligned} \tag{2.5}$$

where we have assumed that the system used to be in some eigenstate of unperturbed Hamiltonian $c_n(0) = \delta_{nm}$. This expression makes an intuitive sense that the coefficients of other eigenstates depend on the coupling term with the initial state in perturbing Hamiltonian. In principle, using (2.5) one can find out the solution at all times.

In many cases when the time-dependent part is comparable to the free Hamiltonian, we look out for other methods among which, one is Unitary Integration (3). In the next chapter, we will use Unitary Integration to closely look at the limitations of this theory.

2.2 Numerical Integration: Runge Kutta 4

A matrix differential equation can be converted to scalar differential equations using ansatz. One example is covered in section (**??**). These differential equations are generally unsolvable analytically hence numerical techniques are needed. In any numerical technique, the basic step is to approximate differentials as finite differences: $df \approx \triangle f$

We are going to briefly describe the industrial standard algorithm called Runge-Kutta 4 that gives an expression to solve Linear Differential Equations. Taylor expanding a general function $y(t)$

$$y(t+\triangle t)y(t) + \triangle t\ y'(y,t) + \frac{1}{2}\triangle t^2 y''(y',\ y,\ t) + \bigcirc(\triangle t^3),$$

To best estimate the value of a function at some interval later, we have to compute the slopes wisely as given in Fig (2.1).[2]

$$y(t+\triangle t) = y(t) + \triangle t\ .[\ y'(t) + \frac{1}{2}\triangle t\ y'']$$

The term $[y'(t) + \frac{1}{2}\triangle t\ y''(y,t)]$ can be thought of as the slope of the function at half an interval later. Let, $g(t) = y'(t) \implies g(t+\frac{1}{2}\triangle t) = g(t) + \frac{1}{2}\triangle t\ g'(t)$ which is exactly the expression as above. Therefore, the second equation can be written as

$$y(t+\triangle t) = y(t) + \triangle t y'(y + \frac{1}{2}\triangle t y',\ t + \frac{1}{2}\triangle t)$$

Similarly, one extends this to four intermediate slopes to carry out the increment [13] in the function which is demonstrated in fig (2.1).

$$y(t+\triangle t) = y(t) + \frac{1}{6}[k_1 + 2k_2 + 2k_3 + k_4] + \bigcirc(\triangle t^5) \quad \text{where} \tag{2.6}$$

[2]The reason behind not going up to higher order terms is the stability of the algorithm. The numerical techniques have to deal with a trade-off between the rounding error and local truncation error [12]

$$
\begin{aligned}
k_1 &= \triangle t.\ y'(y, t), \\
k_2 &= \triangle t.\ y'(y + \frac{1}{2}k_1, t + \frac{1}{2}\triangle t) \\
k_3 &= \triangle t.\ y'(y + \frac{1}{2}k_2,\ t + \frac{1}{2}\triangle t)), \\
k_4 &= \triangle t.\ y'(y + k_3,\ t + \triangle t)
\end{aligned}
$$

For stiff [3] differential equations, RK-4 doesn't work at all. In this project, we will be dealing with stiff equations because of which we have to use smarter *adaptive algorithms* provided in MATHEMATICA notebooks.

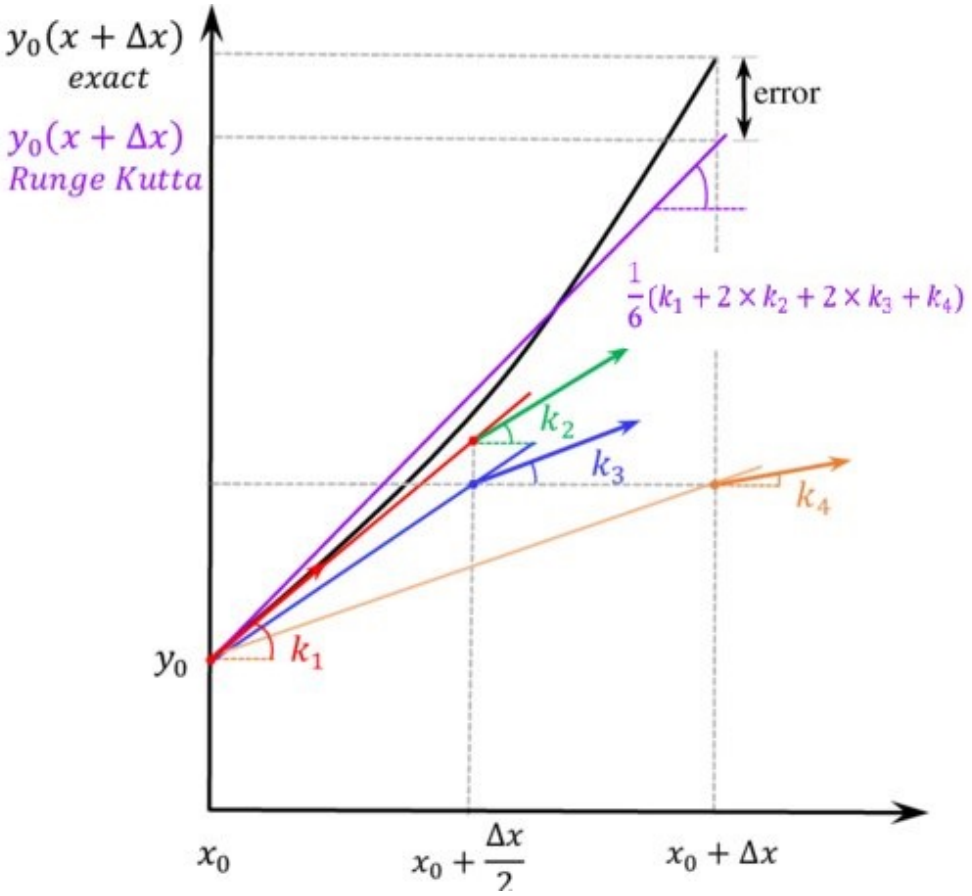


Figure 2.1: **Slopes used by the classical Runge-Kutta method:** Basically, it solves the problem with smaller time steps by simply by-passing it through taking intermediary slopes of function (2.6). The better you can mimic your real function, the better you can find the area under the curve. Image Courtesy [19]

[3] Stiff equations are the ones where you see a lot of variation, that is, the large higher order derivatives. These variations can be captured only when step size is taken to be very small making the procedure very inefficient

Chapter 3

UNITARY INTEGRATION

In the previous sections, we discussed how one could go about solving some limited time-dependent Hamiltonian. As mentioned previously, we will study other types of Hamiltonian where time dependence lies only in the scalar coefficients of non-commuting operators. For these, if we choose our set of time-independent generators to be of compact closed form, we can constrain the nested integration to very few terms. We have discussed such sets in the chapter (1) for finite-dimensional problems.

We shall describe this by putting a two-level general Hamiltonian in equation (2.1)

$$i\dot{U}(t) = [a(t)A + b(t)B]U(t) \tag{3.1}$$

where $[A, B] \neq 0$ *and* $U(0) = \mathcal{I}$.

A general solution would involve the product of infinite exponential terms of exponents A, B, [A,B], [A,[A,B]] and so on, which comes according to the dual of BCH (Zassenhaus formula) [15].

One choice of exponents could be J_+, J_-, J_z as they close under commutation (1). Here, $J_+ = \sigma_+/2 = (\sigma_x + i\sigma_y)/2$, $J_+ = \sigma_+/2 = (\sigma_x + i\sigma_y)/2$ & $J_z = \sigma_z/2$ Equation (3.1) will become $i\dot{U}(t) = [(X_-(t)J_- + X_+(t)J_+)/2 + X_z(t)J_z]U(t)$ in this basis. Setting $U(t)$ as

$$U(t) = e^{-i\mu_+(t)J_+} e^{-i\mu_-(t)J_-} e^{-i\mu_z(t)J_z} \tag{3.2}$$

and evaluating $i\dot{U}(t)$ to be

$$\begin{aligned} &\dot{\mu_+}(t)J_+ \;\; e^{-i\mu_+(t)J_+} e^{-i\mu_-(t)J_-} e^{-i\mu_z(t)J_z} + \;\dot{\mu_-}(t) \;\; e^{-i\mu_+(t)J_+} \; J_- \; e^{-i\mu_-(t)J_-} e^{-i\mu_z(t)J_z} \\ &+ \dot{\mu_z}(t) \;\; e^{-i\mu_+(t)J_+} e^{-i\mu_-(t)J_-} \; J_z \; e^{-i\mu_z(t)J_z} \end{aligned} \tag{3.3}$$

The second term and third term can be rearranged using the BCH lemma [14] for transformations like $e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \frac{1}{3!}[X, [X, [X, Y]]] + \ldots$

where X and Y don't commute with each other. This equation can help us a great deal for closed group algebra as now we can compare the equation (3.3) with the RHS of equation (3.1).

Finally, we compare the terms to get these three classical first-order non-linear coupled differential equations.

$$\dot{\mu_+} + i\mu_+ X_z - \frac{1}{2}\mu_+^2 X_+ = \frac{1}{2}X_-, \tag{3.4}$$

$$\dot{\mu_-} - i\mu_- \dot{\mu_z} = \frac{1}{2}X_+, \tag{3.5}$$

$$\dot{\mu_z} - i\mu_+ X_+ = X_z \tag{3.6}$$

with $\mu_i(0) = 0,\ i \in \{+, -, z\}$. The first equation (Riccati equation) turned out to be independent of the other two and can be solved independently increasing the efficiency of the algorithm. The other two can be solved using the solution of (3.4). Hence, the entire problem is reduced to solving these first-order coupled differential equations.

This algorithm has been repeatedly employed to solve various problems from different fields of physics in a series of articles [22, 23, 24, 25, 26, 27]. [30, 28, 29] uses these techniques in engineering quantum dynamics. We will further discuss the advantage of the algorithm in depicting the dynamics of the system accurately as well as preserving the norm of the wave function.

Landau Zener Stuckleberg Majorana (LZSM) Transition: A Demonstration of Unitary Integration for two-level system

Imagine an atom experiencing a time-dependent magnetic field. For simplicity, we will consider the atom to be free so that no other interactions are there. This magnetic field will split the concerned degenerate atomic state into two states (Zeeman Splitting), making one state higher in energy than the other, depending on the orientation of the Angular Momentum. On decreasing the magnetic field linearly with time, there will be a change of the energy of two states with respect to time as can be in figure (3.1) and since they are uncoupled, to a first approximation, they will cross each other at time 0.

But if we turn the interaction between two levels on, the degeneracy at the crossing is broken and levels seem to repel each other. This gives a very interesting behaviour

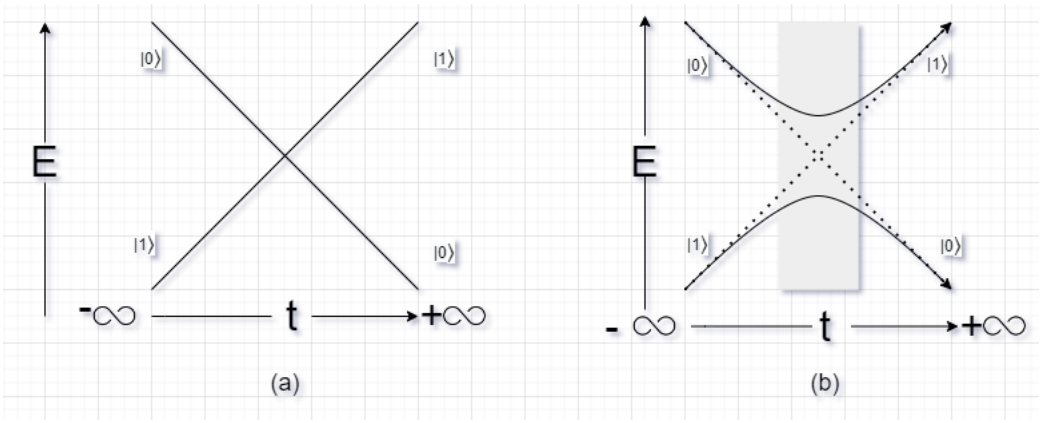


Figure 3.1: **(a)** When there is no coupling between the states, the states cross each other without 'noticing'. Similar behaviour can be captured by using adiabatic approximation. **(b)** When there is a coupling term present, we see **avoided energy level crossing** depending on the speed of inversion v. The shaded region is called the non-adiabatic transition region and the unshaded region is called the adiabatic region as it can be approximated by adiabatic evolution.

that a system starting in, let's say $|0\rangle$ state would emerge in state $|0\rangle$ or $|1\rangle$ after the crossing. This problem was tackled and solved by LZSM in the early days of Quantum Mechanics where it was famously proposed as a model for inelastic **molecular collisions** moving freely. This transition is called **Non-adiabatic transitions** at avoided crossings and can describe many other phenomena in atomic and molecular physics [16]. Here, we are going to solve the time-dependent Hamiltonian using the unitary integration technique for all time and demonstrate how the UI algorithm performs.

The phenomenological Hamiltonian is $H = -\frac{1}{2}\left(\Delta\sigma_x + vt\sigma_z\right)$ that can be rewritten in terms of our closed-algebra basis as $H = -\frac{\Delta}{2}J_+ - \frac{\Delta}{2}J_- - vtJ_z$.

Equations (3.4, 3.5, 3.6) transform for our system as

$$\begin{aligned} \dot{\mu_+} - iv\,t\,X_z + \frac{\Delta}{2}\mu_+^2 + \frac{\Delta}{2} &= 0, \\ \dot{\mu_-} - i\mu_-\dot{\mu_z} + \frac{\Delta}{2} &= 0, \\ \dot{\mu_z} + i\Delta\mu_+ + v\,t &= 0 \end{aligned}$$

with $\mu_- = \mu_+ = \mu_z = 0$. All the non-linearity in the exponentials of unitary operators transforms to the non-linear (quadratic) terms in the equation. It is instructive to know that the transformation depends on the type of ansatz one is taking, which maps one problem to another. Non-linear mapping is thus a very handy tool in

reducing the complexity of problems if used mindfully. One can generalise this to an N-level system and still gets quadratic coupled equations [17].

For the follow the evolution of the state, we just have operated our initial wave function with the propagator once we have the μ_i:

$$\psi(t) = U(t)\psi(0) \tag{3.7}$$

Solving these coupled equations using RK-4 (2.6) turns out to be numerically difficult due to their stiffness. They don't converge readily unless you apply the Unitarity constraint explicitly. Hence, writing equation (3.2) in matrix form explicitly for our system and putting it in $U^\dagger U = \mathcal{I}$ will give

$$\begin{pmatrix} \exp(i\mu_z^*/2) & 0 \\ 0 & \exp(-i\mu_z^*/2) \end{pmatrix} \begin{pmatrix} 1 & i\mu_-^* \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ i\mu_+^* & 1 \end{pmatrix} \begin{pmatrix} 1 & -i\mu_+ \\ 0 & 1 \end{pmatrix}$$
$$\begin{pmatrix} 1 & 0 \\ -i\mu_- & 1 \end{pmatrix} \begin{pmatrix} \exp(-i\mu_z^*/2) & 0 \\ 0 & \exp(i\mu_z^*/2) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The following equations satisfy the above equation.

$$\mu_- = \mu_+^*/(1 + |\mu_+|^2) \tag{3.8}$$
$$e^{\mathbb{I}(\mu_z)} = 1 + |\mu_+|^2 \tag{3.9}$$

As a result, we have to calculate just two independent coefficients, $\mu_+(t), \mathbb{R}(\mu_z(t))$. The solution would give us U(t) which can give us wave function at all times by $|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$ where initial state can be parameterised by

$$|\psi(0)\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Results Comparison: Majorana's Solution and Unitary Integration's Solution

As given in [20], we will briefly discuss how Italian theoretical physicist, Ettore Majorana solved the problem. He considered the case of an atomic beam passing a point of a varying magnetic field and reduced the problem to a two-level system.

Using the ansatz

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} f\,\exp(i\tau^2/2) \\ g\,\exp(-i\tau^2/2) \end{pmatrix}$$

where f & g are a function of scaled time τ. One obtains the following homogeneous differential equations. These are solved in **Laplace Space** using the *method of steepest decent* [21] for large times only.

$$\frac{d^2 f}{d\tau^2} + 2i\tau\frac{df}{d\tau} + 2\delta f = 0 \tag{3.10}$$

$$\frac{d^2 g}{d\tau^2} - 2i\tau\frac{dg}{d\tau} + 2\delta g = 0 \tag{3.11}$$

The authors of [20] concluded that Majorana's asymptotic solution describes the dynamics correctly far from avoided level crossing and also the transient dynamics. But only in the vicinity of τ=0 when $\tau < 1$, the solution diverges.

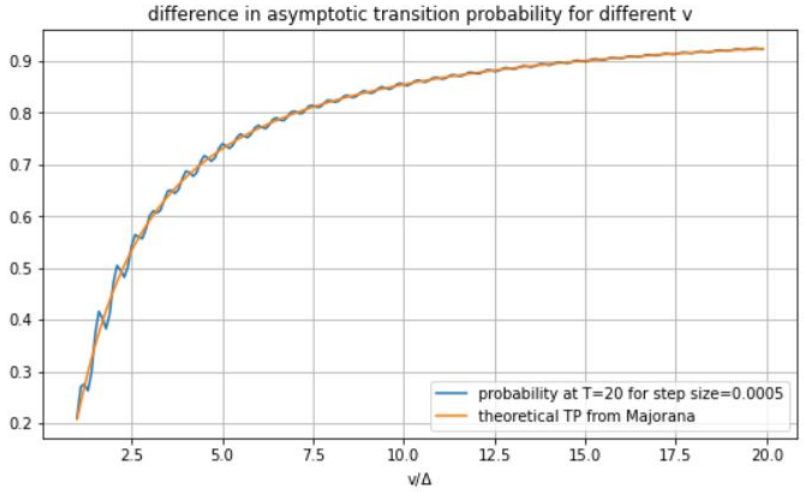


Figure 3.2: Comparison of asymptotic transition probability using Unitary Integration and derived **LZSM** formula. For the given initial condition, $\mathcal{P} = |\beta(t \to \infty)|^2 = \exp(-2\pi\delta)$ [20]

Comparison of the dynamics of the occupation probabilities versus time t is given in figures (3.3, 3.4, 3.5, 3.6, 3.7, 3.8) obtained by Majorana's Method and Unitary Integration Method for three increasing values of v and a fixed value of $\Delta = 1$. The initial state $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ was chosen for all cases. The coloured region represents the adiabatic transition region where Majorana's solution fails but Unitary works perfectly. Both approaches' results converge to the same limit far from the transition region. One can also notice the conservation of norm in all cases for the UI's solution.

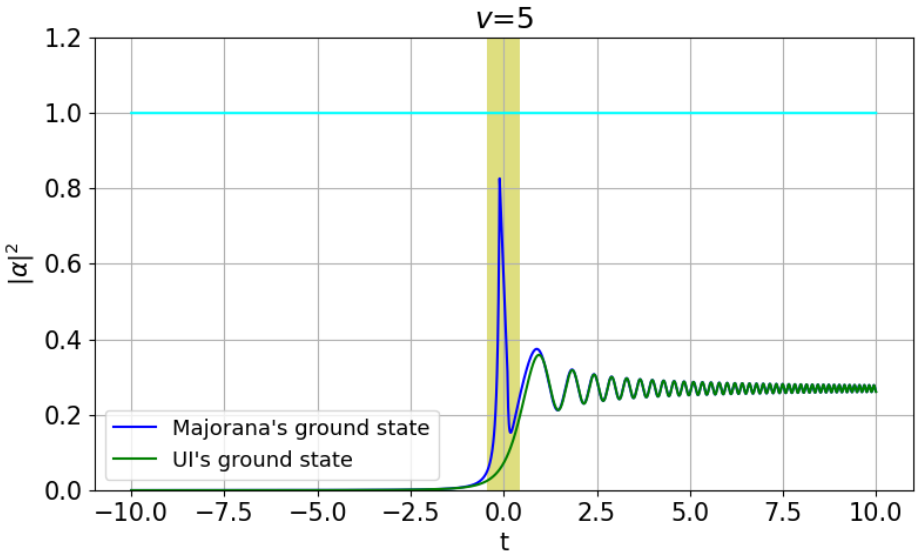


Figure 3.3: Occupation Probabilities $|\alpha(t)|^2$ for $v = 5$

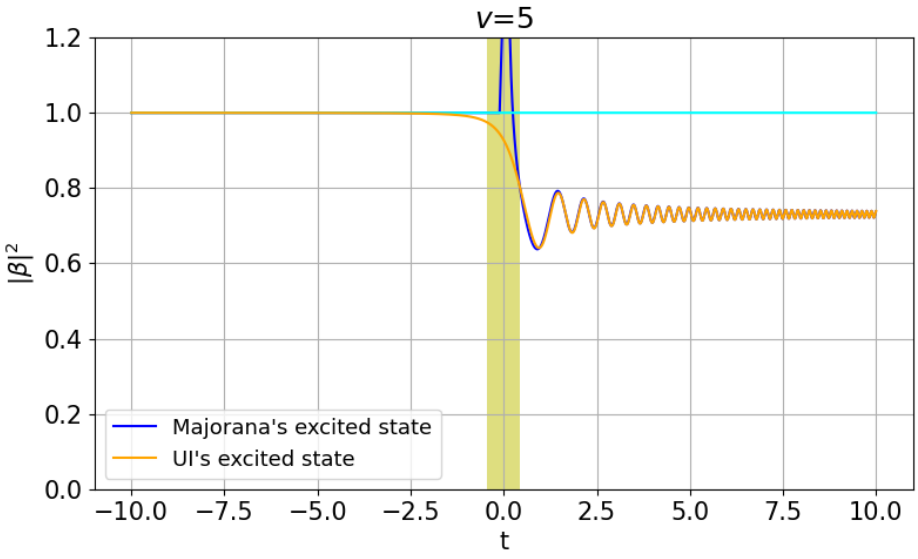


Figure 3.4: Occupation Probabilities $|\beta(t)|^2$ for $v = 5$

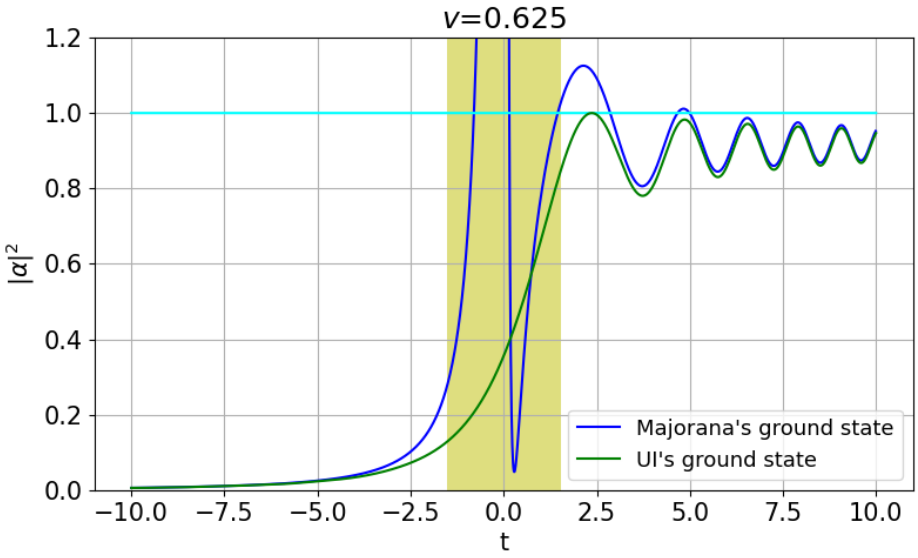


Figure 3.5: Occupation Probabilities $|\alpha(t)|^2$ for $v = 0.625$

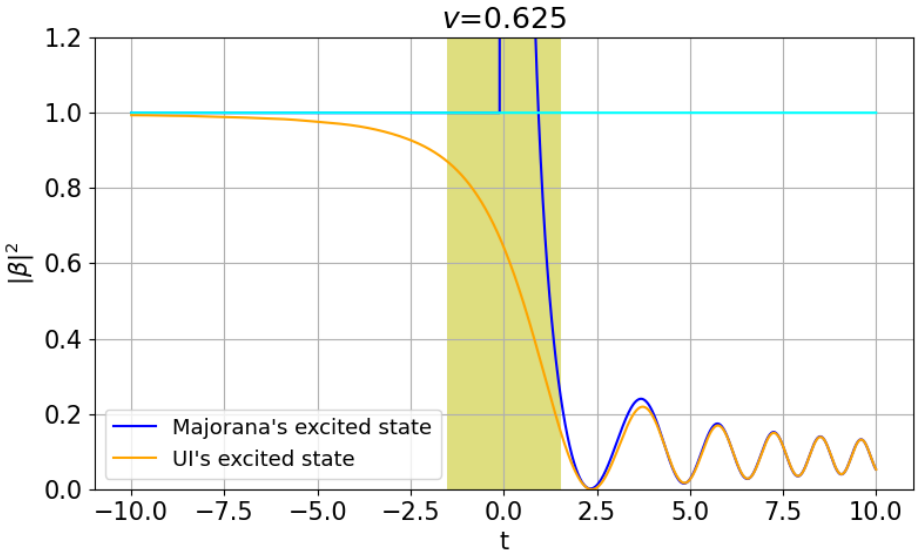


Figure 3.6: Occupation Probabilities $|\beta(t)|^2$ for $v = 0.625$

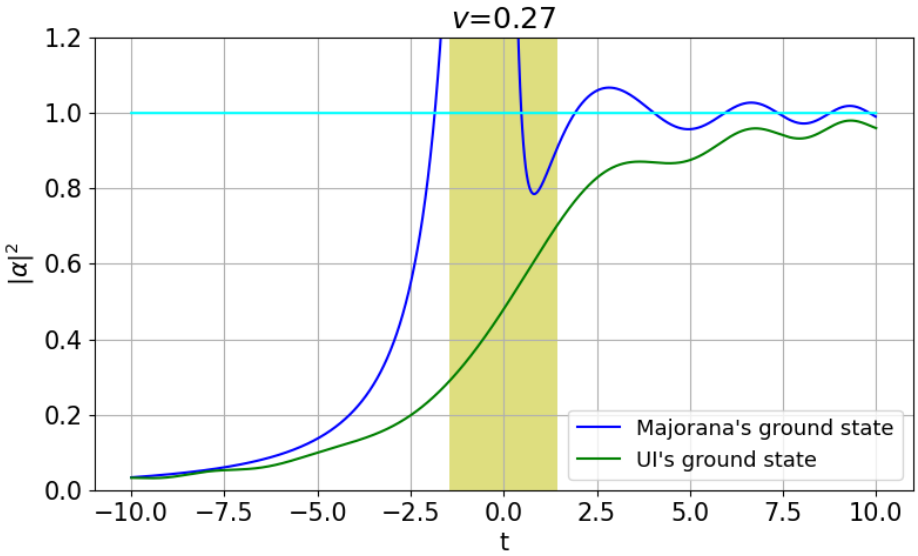


Figure 3.7: Occupation Probabilities $|\alpha(t)|^2$ for $v = 2.7$

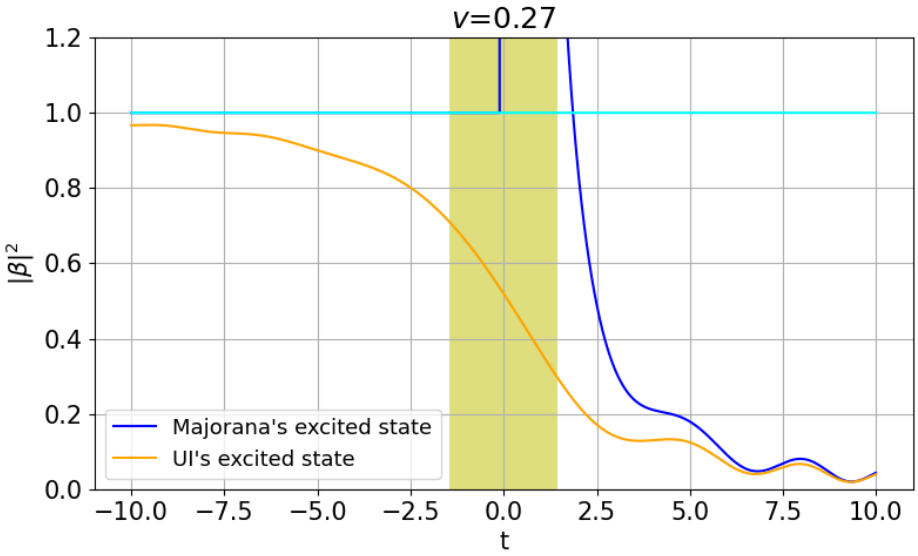


Figure 3.8: Occupation Probabilities $|\beta(t)|^2$ for $v = 0.27$

Chapter 4

DRIVEN DISSIPATION TWO LEVEL SYSTEM

We can describe the dynamics of open systems attached to *Markovian baths* by the Liouville-von Neumann-Lindblad (LvNL) equation

$$i\dot{\rho} = [H(t), \rho] - \frac{i}{2}\sum_k \Gamma_k (L_k^\dagger L_k \rho + \rho L_k^\dagger L_k - 2L_k \rho L_k^\dagger]) \tag{4.1}$$

where L_k are called Lindblad or Jump operators and coefficients $\Gamma > 0$. It is a generalisation of the Schrödinger equation in the sense that the exact coherent time dynamics are determined by the Hamiltonian of the system, and on top of it, averaged decoherent interactions (quantum jumps) with a bath are modelled through these Lindblad operators.

4.1 Periodically Driven Two-Level System

We will take a simple case of Hamiltonian for a periodically driven two-level system, generalising the previous Hamiltonian.

$$H = \frac{\epsilon(t)}{2}\sigma_z + J\sigma_x, \qquad L_k = \sqrt{\frac{\Gamma}{2}}\sigma_k \tag{4.2}$$

Hence, your system is coupled to a bath with the rate of decoherence Γ. To solve the system in the form of equation (1.7), we would have four levels which introduce us to the major problem with quantum mechanics; the problem of dimensionality. We have to deal with fifteen 4X4 matrices to model the dynamics completely in general.

$$\frac{d}{dt}\begin{bmatrix}\rho_{11}\\ \rho_{12}\\ \rho_{21}\\ \rho_{22}\end{bmatrix} = \begin{bmatrix} i\Gamma & -J & J & i\Gamma \\ -J & (\epsilon - 2i\Gamma) & 0 & J \\ J & 0 & -(\epsilon + 2i\Gamma) & -J \\ i\Gamma & J & -J & -i\Gamma \end{bmatrix}\begin{bmatrix}\rho_{11}\\ \rho_{12}\\ \rho_{21}\\ \rho_{22}\end{bmatrix} \tag{4.3}$$

This would lead to lengthy calculations and large computational power (so as to solve all the corresponding coupled differential equations). Hence, to simplify the problem a bit, we recall from (4.1) that the evolution governed by equation (4.2) is

trace-preserving. Hence, $\rho_{11} + \rho_{22} = 1$ for all times. Therefore, transforming ρ to η such that the LvNL equation reduces in form of Liouville-Bloch as

$$i\dot{\eta} = \mathcal{L}(t)\eta(t) \tag{4.4}$$

$$\iota\frac{d}{dt}\begin{bmatrix}\rho_{12}+\rho_{21}\\ \rho_{21}-\rho_{12}\\ \rho_{11}-\rho_{22}\end{bmatrix} = \begin{bmatrix}-i\Gamma & -\epsilon(t) & 0\\ -\epsilon(t) & -i\Gamma & 2J\\ 0 & 2J & -i\Gamma\end{bmatrix}\begin{bmatrix}\rho_{12}+\rho_{21}\\ \rho_{21}-\rho_{12}\\ \rho_{11}-\rho_{22}\end{bmatrix} \tag{4.5}$$

Our effective "Hamiltonian" (4.4) can be written as

$$\mathcal{L} = -i\Gamma\mathbb{I} - a\epsilon(t)A_z + 2JA_x \tag{4.6}$$

Now, we use the recipe of UI given in the last chapter even though "Hamiltonian" is no longer Hermitian. Considering the coefficients (like μ_-, μ_+, μ_z) to be complex and linearly independent, we can extend the method to accommodate the above case. Remember, it was the equation (2.1) which essentially forces U to be unitary, making these coefficients real and linearly dependent. But (4.1) poses no such constraints.

We need eight operators that are closed under $SU(3)$ algebra in general. But as $\mathcal{L}$ involves only the elements of its sub-algebra $\{A_x,\ A_y,\ A_z\}$, it is sufficient to write just three exponential operators from the Gell-Mann set:

$$A_x = \begin{bmatrix}0&0&0\\0&0&1\\0&1&0\end{bmatrix}, \qquad A_y = \begin{bmatrix}0&0&-i\\0&0&0\\i&0&0\end{bmatrix}, \qquad A_z = \begin{bmatrix}0&1&0\\1&0&0\\0&0&0\end{bmatrix}$$

Our choice of operators are A_+, A_-, A_z where $A_\pm = A_x \pm iA_y$ and follow $[A_+, A_-] = 2A_z$ and $[A_\pm, A_z] = \mp iA_\pm$. Just like previously, these operators reduce the non-linearity in the coupled equation as the infinite series gets truncated due to $A_\pm^2 = 0$.

The first term in (4.6) leads to a scalar in front of the remaining Hermitian part of $\mathcal{L}$

$$\eta(t) = \exp(-\Gamma t)\exp(-i\mu_+(t)A_+)\exp(-i\mu_-(t)A_-)\exp(-i\mu(t)A_z)\eta(0) \tag{4.7}$$

where the initial state is $\eta(0) = (0, 0, 1)$.

Using (4.7) in equation (4.4) we get a set of differential equations after comparing them as

$$0 = \dot{\mu}_+ - i\epsilon(t)\mu_+ - J(1+\mu_+^2) \tag{4.8}$$

$$0 = \dot{\mu}_- - i\mu_-\dot{\mu} - J \tag{4.9}$$

$$0 = \dot{\mu} - 2iJ\mu_+ + \epsilon(t), \qquad \mu_i(0) = 0 \tag{4.10}$$

Here we are taking more interesting behaviour of external drive than in LZSM, $\epsilon(t) = a\cos\omega t$. After solving the above equations numerically, we calculate $\eta(t)$ with the initial state being pure; $\rho_{11}(0) = 1$.

4.2 Results

One can build the unitary from the solutions of the differential equation using direct exponentiation. But in our case, we also can have the complete solution in terms of the element of the density matrix. Using equation (4.7), we get

$$\begin{aligned}
\rho_{11(t)} &= \frac{1}{2} + \frac{1}{2}e^{-\Gamma t}[1 - 2\mu_+\mu_-], \\
\rho_{22(t)} &= \frac{1}{2}[1 - e^{-\Gamma t}] + \mu_+\mu_- e^{-\Gamma t}, \\
\rho_{12(t)} &= i\mu_- e^{-\Gamma t}, \\
\rho_{21(t)} &= i\mu_+[\mu_+\mu_- - 1]e^{-\Gamma t}
\end{aligned} \tag{4.11}$$

From the expressions, one can make the following observations:

- The state is reaching a maximally mixed state as the coherence, which is depicted by off-diagonal terms in density matrices, is vanishing.
- In turn, $\lim_{t\to\infty}$ both ρ_{11} and $\rho_{22} \to \frac{1}{2}$.
- Adding the first two equations will give us the trace that is equal to 1 at all times.
- Any other choice of initial condition will lead to the same qualitative behaviour.

These observations can be made from the Figures (4.1, 4.2, 4.3).

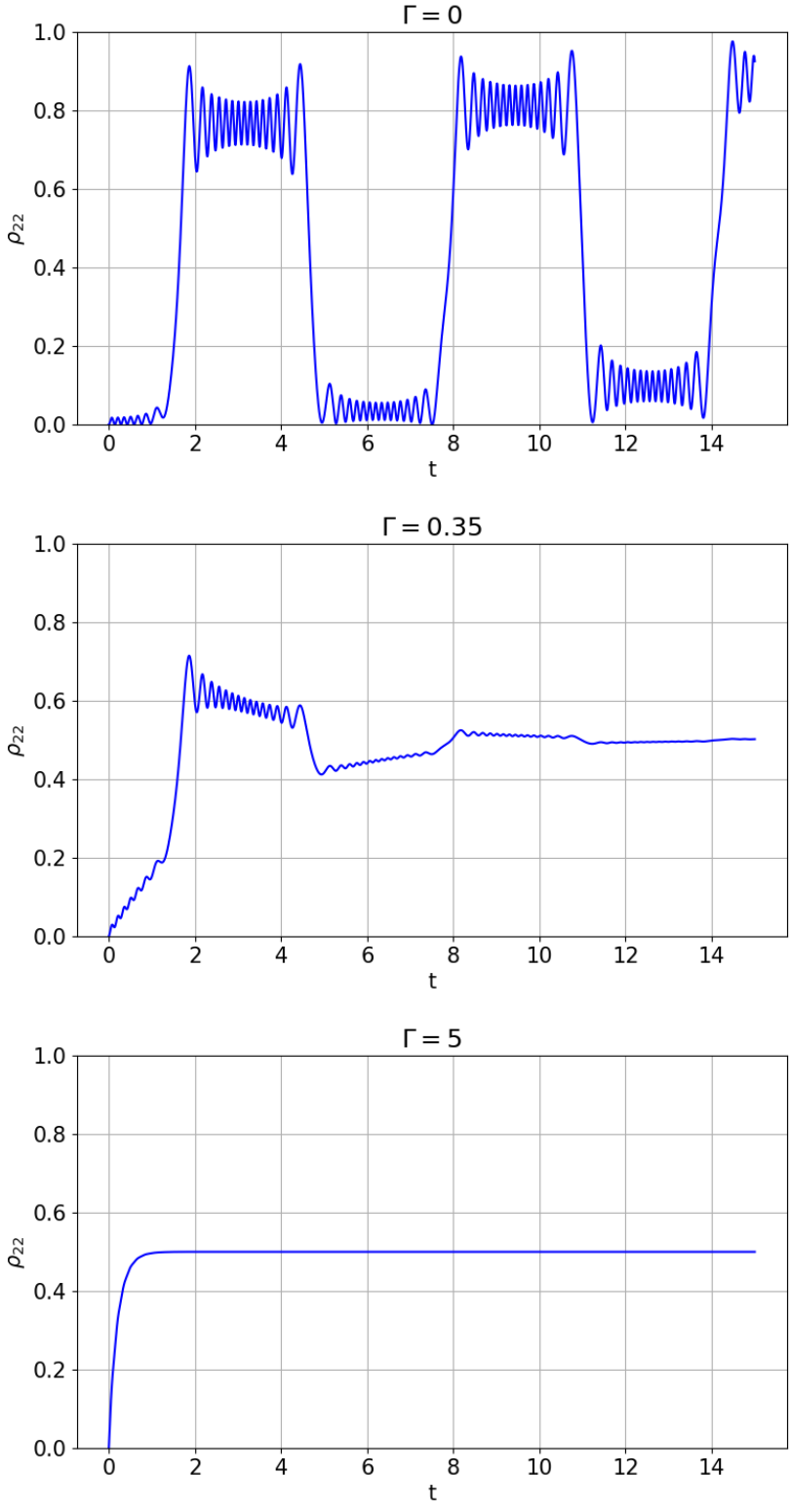
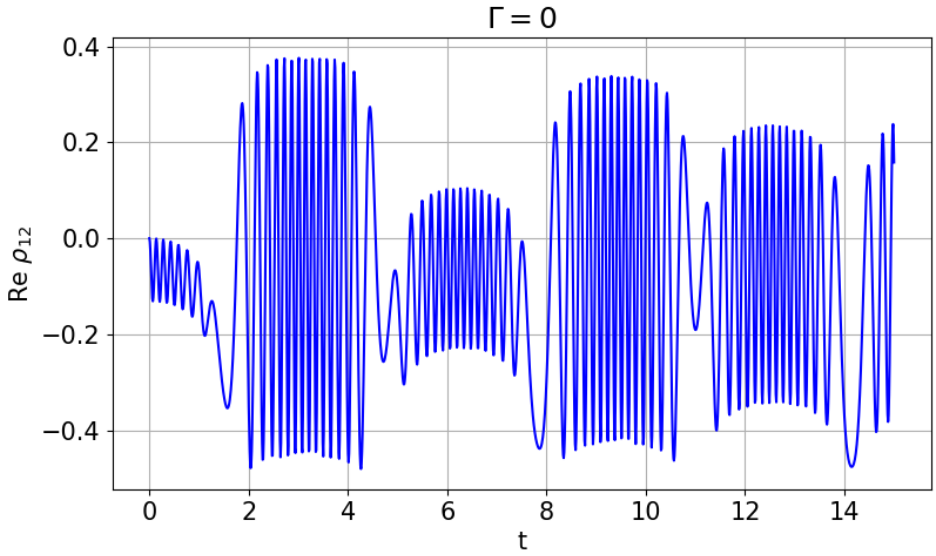
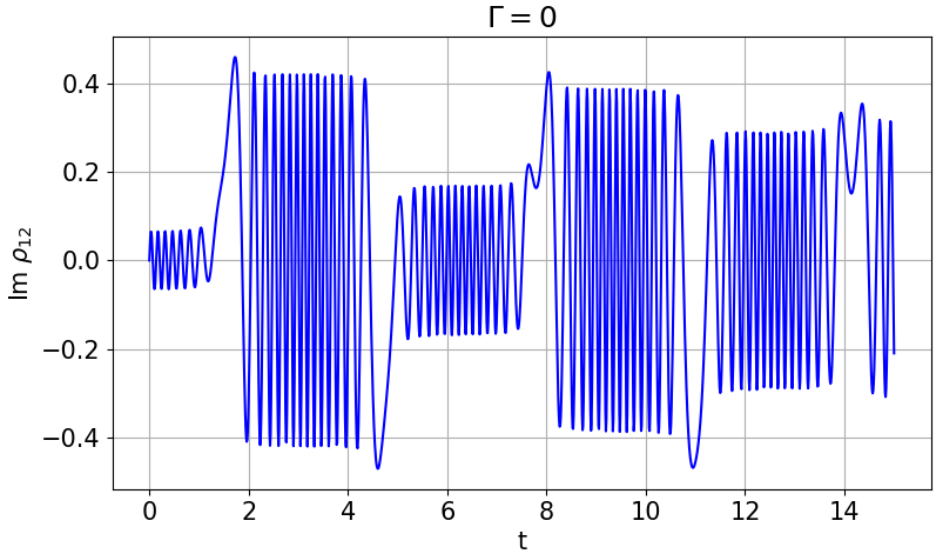


Figure 4.1: $\rho_{22}(t)$ for an oscillating driving field with $\omega = 1$, $J = 3$, $A = 45$ and different values of rate Γ=0, .35, 5

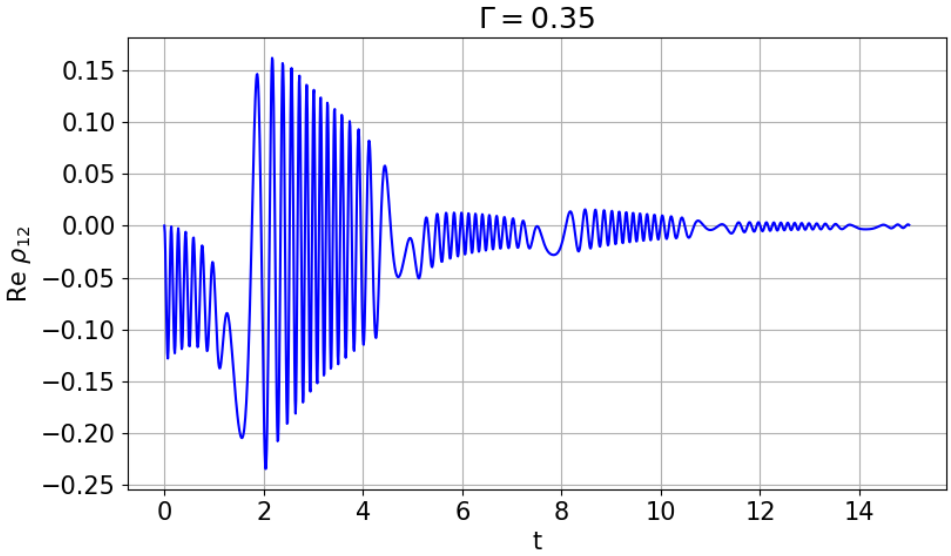


(a)

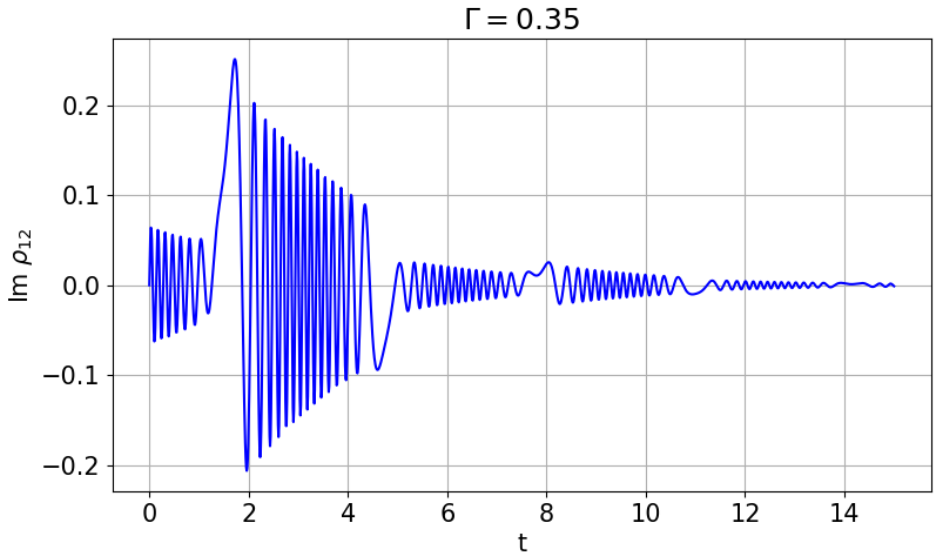


(b)

Figure 4.2: For $\rho_{12}(t)$ with $\omega = 1$, $J = 3$, $A = 45$ and rate Γ=0



(a)



(b)

Figure 4.3: For $\rho_{12}(t)$ with $\omega = 1$, $J = 3$, $A = 45$ and rate Γ= 0.35

Chapter 5

FORWARD

5.1 Nuclear Magnetic Resonance Relaxations

In the previous chapter, we presented the method for solving certain restrictive time-dependent operator equations where the rate of coupling Γ was equal for all the Jump Operators. Here, we extend our system with two different coupling rates Γ_1 & Γ_2. This relates to the situation either when you are coupled to two different kinds of baths or when your system can interact with the same bath in two different ways. Both of these situations are mathematically equivalent. We are going to consider the following system

$$H = \frac{\epsilon(t)}{2}\sigma_z + J\sigma_x, \qquad L_{\pm} = \sqrt{\frac{\Gamma_1}{2}}\sigma_{\pm}, \qquad L_3 = \sqrt{\frac{\Gamma_2}{2}}\sigma_z \tag{5.1}$$

Following the same procedure as in the last chapter that will consist of inserting equation (5.2) into equation (4.4) at which point the derivative on the left-hand side can be rearranged to have the same structure as the right-hand side through repeated application of the BCH lemma and choosing the $\mu_i(t)$ suitably. The system in equation (5.1) requires only eight operators rather than fifteen as it can be written in the form of (4.4) from the raw form of LvNL equation (4.3). But unlike in the previous problem, it can't be represented by a sub-algebra of three or five operators.

Hence, the eight linearly traceless independent matrices from standard $SU(3)$ description are chosen [31] for the unitary integration basis set. It was further simplified by choosing the linear combination of operators, that are, $a_{\pm} = 1/2(\lambda_6 \pm i\lambda_7)$, $b_{\pm} = 1/2(\lambda_1 \mp i\lambda_2)$, $c_{\pm} = 1/2(\lambda_4 \pm i\lambda_5)$, & $a_3 = 1/2(\sqrt{3}\lambda_8 - \lambda_3)$, $c_3 = 1/2(\sqrt{3}\lambda_8 - \lambda_3)$, where λ are full set of eight operators of $SU(3)$ algebra [31].

We want to emphasize that not only is the choice of basis matter now but also the order of the operations in the time evolution operator is of prime importance. This flexibility is provided by the method itself. The trade-off with this flexibility is simply that now we can't put a constraint on these coefficients as we did in (3.8).

We chose the following order according to [22] following form

$$U(t) = e^{-i\delta} e^{-i\mu_8 b_+} e^{-i\mu_7 b_-} e^{-i\mu_6 c_+} e^{-i\mu_5 c_-} e^{-i\mu_4 a_+} e^{-i\mu_3 a_-} e^{-i\mu_2 a_3} e^{-i\mu_1 a_3} \tag{5.2}$$

Finally, we obtain the following eight equations for the eight coefficients after a very tedious algebra, following the procedure stated above.

$$\dot{\mu_8} = -\epsilon(t) - iS\mu_5 - \epsilon\mu_8^2 \tag{5.3}$$

$$\dot{\mu_7} = -\epsilon(t) + i\mu_6 R + i\mu_5\mu_7^2 S + 2\epsilon(t)\mu_7\mu_8 \tag{5.4}$$

$$\dot{\mu_6} = 2iJ\mu_7 - 2iJ\mu_8\mu_6^2 + \epsilon(t)\mu_6\mu_8 + iS\mu_5\mu_6\mu_7 + \mu_6(\Gamma_2 - \Gamma_1) \tag{5.5}$$

$$\dot{\mu_5} = -2iJ\mu_8 - \epsilon(t)\mu_5\mu_8 + 4iJ\mu_5\mu_8\mu_6 - iS\mu_5^2\mu_7 - \mu_5(\Gamma_2 - \Gamma_1) \tag{5.6}$$

$$\dot{\mu_4} = i\epsilon(t)\mu_8 + 2J\mu_6\mu_8 - S\mu_5\mu_7 + \frac{i}{3}(\Gamma_2 - \Gamma_1) \tag{5.7}$$

$$\dot{\mu_3} = S + R\mu_3^2 - i\mu_3\big(-i\epsilon(t)\mu_8 + 2J\mu_6\mu_8 + S\mu_5\mu_7 + i(\Gamma_2 - \Gamma_1)\big) \tag{5.8}$$

$$\dot{\mu_2} = 2J(1 - \mu_8\mu_7) + i\mu_2\big(i\epsilon(t)\mu_8 + 2iR\mu_3 + 2J\mu_6\mu_8 + S\mu_5\mu_7 + i(\Gamma_2 - \Gamma_1)\big) \tag{5.9}$$

$$\dot{\mu_1} = -i\epsilon(t)\mu_8 + S\mu_5\mu_7 + iR\mu_3 + \frac{i}{3}(\Gamma_2 - \Gamma_1) \tag{5.10}$$

where

$$R = 2J(1 - \mu_7\mu_8) \tag{5.11}$$

$$S = \frac{2J}{1 - \mu_5\mu_6} \tag{5.12}$$

These coupled equations can be solved in MATHEMATICA easily in two iterations. One can solve the first four equations independently from what follows and use the solution from these in the latter four equations. This feature is simply due to the choice of $U(t)$ that relieves us from solving eight stiff-coupled nonlinear differential equations.

This situation arises in the case of Nuclear Magnetic Resonance (NMR) where there are two mechanisms with which a spin interacts with its environment. In NMR, the nuclei in a strong constant magnetic field ($J >> |\epsilon(t)|$) are perturbed by a weak oscillating magnetic field. They respond by producing an electromagnetic wave with a characteristic frequency. But since they are not completely decoupled from the environment, there is a *spin relaxation* mechanism responsible for its equilibration. They are termed as **spin lattice relaxation** (T_1) and **spin spin relaxation** (T_2) [32]. Typically due to their underlying mechanism, T_1 is usually longer than T_2. Finally, it

has been proved that such phenomena can be captured by stochastic approximations of a Lindblad equation [32, 33]. Hence, we have different coupling rates (Γ_1 & Γ_2) for each of the processes that can be modelled by the above system.

5.2 Conclusion

Unitary integration can solve our difficulty with a time-dependent Hamiltonian for small systems extensively. Primarily, it helps in decoupling the time dependence of operator equations from the non-commuting nature of the operators. The time dependence is further dealt with in time-dependent classical differential equations. A large number of interacting and non-interacting models come under the regime of Unitary Integration due to their same underlying Lie Algebra. We have explicitly solved for LZSM problem which illustrates the advantage of the algorithm in comparison to another totally analytical approach taken by Majorana. It has proved vital for solving open quantum systems' LvNL equation. With the main focus on these problems, we have illustrated this for two different cases. One is for engineering the dynamics and controlling small atomic systems with the external time-dependent drive where only a finite number of states are accessible. Second, a more general and widespread problem of spin relaxation in NMR using the most general three-level recipe. The exactness of the solutions only depends on the method one is using to solve a differential equation. The Riccati and other following equations obtained are exact. The exactness of the solution from differential equations, in turn, depends on the external drives and heat baths associated with the system.

But this method is not extendable to many-particle systems. Due to the dimensionality of the system, the algorithm is just near impossible to solve as, for instance, one would obtain fifteen coupled non-linear differential equations for the most general four-level closed system. In this too, we would have to consider the various choices in the ordering of exponentials. But we can still use this to collective atomic systems due to the similar underlying algebra. In the future, we would like to employ the method in these famous scenarios from quantum optics and molecular physics relevant to quantum control.

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