Summer Internship Project
Report

Simulations in Open Quantum Systems

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Chapter 1

Mathematical Formalism

It is assumed that the reader has an acquaintance with fundamental quantum mechanics and linear algebra, including specific familiarity with state vectors and the importance of eigenvectors in Hilbert space. In an open quantum system, we lack knowledge of the quantum state the system is in, and this leads us to use the Density Matrix formulation. I will only discuss the part which will be useful in Our Study of Master Eqautions.

A classic way of illustrating this concept is through the Stern-Gerlach experiment, where a beam of silver atoms is passed through an inhomogeneous magnetic field. The spin quantum number of a normal silver atom is $\frac{1}{2}$, so in trasversing the inhomogeneous magnetic field, the beam is split into two: one in which each silver atom has a spin magnetic moment of $+\frac{1}{2}$ (let us call it Beam 1) and another in which each atom has a spin magnetic moment of $-\frac{1}{2}$ (Beam 2). Beam 1 can be collected. The spin state of all the silver atoms in Beam 1 is completely known so the beam is in a pure (spin) state. And we can assign a single spin state vector $|\psi_1\rangle$ to Beam 1. The same applies to Beam 2. These states are known as pure states. When we cannot assign a single state vector to the system because there is classical uncertainty on the system's quantum state, we resort to (classical) statistics to describe the state. The result is what we call a mixed state. Density matrix formulation can handle both classical and quantum uncertainty present in the system. [2]

1.1 Density Matrix and Its Properties

1.1.1 Density Operator

Suppose, a system is in state $|\psi_1\rangle$ with probability p_1, or in state $|\psi_2\rangle$ with probability p_2 and so on. In other words, we have pure state ensemble $\{p_i, |\psi_i\rangle\}_{i=1}^{N}$ describing our system. We now define the

density operator as,

$$\rho = \sum_i p_i \left| \psi_i \right\rangle \left\langle \psi_i \right| \tag{1.1}$$

Note: This sum is not over the eigenvectors of the Hilbert space of the system. (1.1) expresses a classical mixture of states.

It is necessary to distinguish between pure and mixed states from the density matrix. Let's say we have a pure state $\{1, \left| \psi \right\rangle\}$ in d dimensional Hilbert space and so it follows that,

$$\rho = \left| \psi \right\rangle \left\langle \psi \right| \tag{1.2}$$

Now, from (1.2), you might get the illusion that pure states must have zero off-diagonal elements. What if we represent the density matrix on another orthonormal basis $\left| \phi_i \right\rangle$? For example, we get,

$$\rho = \mathbb{I}_d \left| \psi \right\rangle \left\langle \psi \right| \mathbb{I}_d \tag{1.3}$$

$$= \sum_n \sum_m \left| \phi \right\rangle \left\langle \phi_n | \psi \right\rangle \left\langle \psi | \phi_m \right\rangle \left\langle \phi_m \right| \tag{1.4}$$

$$= \sum_n \sum_m c_{nm} \left| \phi_n \right\rangle \left| \psi_m \right\rangle \tag{1.5}$$

with $c_{nm} = \left\langle \phi_n | \psi \right\rangle \left\langle \psi | \phi_m \right\rangle$. It's now evident that pure states can have nonzero off-diagonal or coherent terms on different basis. To check whether a density matrix represents a mixed or pure state, one has to put it in its diagonal form: if there is more than one nonzero p_i, then the state is mixed. Otherwise, it is pure. [3] Another way is to check the purity of the density matrix. We will discuss it in subsequent subsections.

1.1.2   Properties of Density Matrices

We will assume that state vectors all are normalized ($\left\langle \psi | \psi \right\rangle = 1$.

1. Unit Trace: The density operator ρ satisfies

$$\mathrm{Tr}[\rho] = \sum_i p_i \mathrm{Tr}[\left| \psi_i \right\rangle \left\langle \psi_i \right|] \tag{1.6}$$

$$= \sum_i p_i \sum_j \left\langle \phi_j | \psi_i \right\rangle \left\langle \psi_i | \phi_j \right\rangle \tag{1.7}$$

$$= \sum_i p_i \sum_j \left\langle \psi_i | \phi_j \right\rangle \left\langle \phi_j | \psi_i \right\rangle \tag{1.8}$$

$$= \sum_i p_i = 1 \tag{1.9}$$

where $0 \leq p_i \leq 1$ are the probabilities corresponding to states $|\phi_i\rangle$. Therefore, $\boxed{\text{Tr}[\rho] = 1}$ whether its pure or mixed state.

2. Purity: we observe that $\text{Tr}[\rho^2] = \sum_i p_i^2 \leq 1$. Only in case of pure state, $\text{Tr}[\rho^2] = 1$ where $p_i = 1$ and $p_{i \neq j} = 0$. But in Mixed state, $\text{Tr}[\rho^2] = \sum_i p_i^2 < 1$ because $0 < p_i < 1$. *Therefore, we define "pure" and "mixed" states above according to the value of the purity* $P = \text{Tr}[\rho^2]$ *being 1 or < 1.* You can be concerned about what will happen in case of a change of basis. Here, Linear algebra tells us that a trace is preserved over the change of basis under a unitary transformation. This ensures that checking purity on any basis of ρ can confirm the system's state.

   Caution: pure state is a projector $(|\psi\rangle\langle\psi||\psi\rangle\langle\psi| = |\psi\rangle\langle\psi|)$. If a state ρ is pure then $\rho^2 = \rho$. Converse is also true. The concepts of mixed state and entangled state are different. Let me give you examples. Consider a quantum system in a mixed state where the system has a 50% probability of being in state $|0\rangle$ and a 50% probability of being in state $|1\rangle$. The density matrix for the system is,

$$\rho_{mixed} = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| \tag{1.10}$$

This represents a classical probabilistic mixture of the states $|0\rangle$ and $|1\rangle$.

An entangled state cannot be written as a product of states of individual subsystems. It represents a quantum correlation between the subsystems. A well-known example of an entangled state is the Bell state:

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \tag{1.11}$$

$$\therefore \rho_{entangled} = |\Phi^+\rangle\langle\Phi^+| = \frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|) \tag{1.12}$$

where, $|ab\rangle\langle cd| = (|a\rangle \otimes |b\rangle)(|c\rangle \otimes |d\rangle) = |a\rangle\langle c| \otimes |b\rangle\langle d|$.

It is also possible that the density state is both mixed and entangled. Consider a mixed state that is a mixture of the Bell states $|\Phi^+\rangle$ and $|\Phi^-\rangle$. Assume that a state is in $|\Phi^+\rangle$ with probability p and in $|\Phi^-\rangle$ with probability (1-p). The density matrix for this mixed entangled state is:

$$\rho = p|\Phi^+\rangle\langle\Phi^+| + (1-p)|\Phi^-\rangle\langle\Phi^-| \tag{1.13}$$

3. Hermiticity: *Density matrices are hermitian,* $\rho^\dagger = \rho$. It follows from,

$$\rho^\dagger = \sum_i p_i^*(|\psi\rangle\langle\psi|)^\dagger = \sum_i p_i|\psi\rangle\langle\psi| = \rho \tag{1.14}$$

where we've used that probabilities p_i are real and outer-products are Hermitian.

4. Positive Definite: An operator is defined as positive when all its eigenvectors are positive. In the case of the density operator, for all $\Phi \in \mathcal{H}$,

$$\langle \Psi | \rho | \Psi \rangle = \sum_i p_i | \langle \psi_i | \Psi \rangle |^2 \geq 0 \tag{1.15}$$

Because probabilities are always semi-positive. All vectors include eigenvectors ϕ_i, so eigenvalues must be semi-positive ($0 \leq \langle \phi_i | \rho | \phi_i \rangle = \lambda_i \langle \phi_i | \phi_i \rangle = \lambda_i$). Considering $\text{Tr}[\rho] = 1$, One of the eigenvectors of the density matrix must be non-zero positive. *Therefore, density matrix ρ is always positive.*

5. Expectation Values as Traces of Density Operators: We have a useful theorem depending on the density matrix.

Consider a mixed state described by a density operator, $\rho = \sum_i p_i | \psi_i \rangle \langle \psi_i |$. Then for any observable A, we have,

$$\text{Tr}[\rho A] = \sum_j \langle j | \rho A | j \rangle \tag{1.16}$$

$$= \sum_j \langle j | (\sum_i p_i | \psi_i \rangle \langle \psi_i |) A | j \rangle \tag{1.17}$$

$$= \sum_i p_i (\sum_j \langle j | \psi_i \rangle \langle \psi_i | A | j \rangle) \tag{1.18}$$

$$= \sum_i p_i (\sum_j \langle \psi_i | A | j \rangle \langle j | \psi_i \rangle) \tag{1.19}$$

$$= \sum_i p_i \langle \psi_i | A | \psi_i \rangle \tag{1.20}$$

This is precisely the statistical ensemble average of observable A in this density matrix system. For pure state, consider $p_j = \delta_{ij}$ and then $\text{Tr}[\rho A] = \langle \psi_i | A | \psi_i \rangle$. Therefore, to find out the statistical average of any observable, we gonna use again and again $Tr[\rho A]$.

6. Unitary Evolution: **For a closed system,**, the dynamics of a quantum system are governed by these two completely equivalent equations,

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle \leftrightarrow |\dot{\psi}\rangle = -\iota H |\psi\rangle \tag{1.21}$$

Where $U(t) = e^{-\iota \mathbb{H} t}$. Similarly, we have two different governing descriptions for the density matrix.

Consider an ensemble $p_i, |\psi_i\rangle_i$ and the time evolution of the density matrix associated with the ensemble is,

$$\rho(t) = \sum_i p_i |\psi_i(t)\rangle \langle \psi_i(t)| \tag{1.22}$$

$$= \sum_i p_i U(t) |\psi_i\rangle \langle \psi_i| U^\dagger(t) \tag{1.23}$$

$$\therefore \boxed{\rho(t) = U(t)\rho(0)U^\dagger(t)} \tag{1.24}$$

(1.15) is one of our governing equations. Now, using the Schrodinger equations,

$$\dot{\rho}(t) = \sum_i q_i \left[\left(\frac{\partial}{\partial t} |\psi_i(t)\rangle \right) \langle \psi_i(t)| + |\psi_i(t)\rangle \left(\frac{\partial}{\partial t} \langle \psi_i(t)| \right) \right].$$

The Schrödinger equation for pure states, while noting that after obtaining $\langle \dot{\psi}_j | = \iota \langle \psi_j | H$. Thus:

$$\dot{\rho}(t) = \sum_i q_i \left(-iH|\psi_i(t)\rangle \langle \psi_i(t)| + i|\psi_i(t)\rangle \langle \psi_i(t)|H \right)$$

$$= -i \left[H \left(\sum_i q_i |\psi_i(t)\rangle \langle \psi_i(t)| \right) - \left(\sum_i q_i |\psi_i(t)\rangle \langle \psi_i(t)| \right) H \right]$$

$$= -i(H\rho - \rho H)$$

$$\boxed{\dot{\rho}(t) = -i[H, \rho]} \tag{1.25}$$

This is called the Schrodinger equation for the density operator. [3]

1.1.3 Partial Trace

The partial Trace over the **B** subsystem is a linear operator that maps from the combined Hilbert space to the Hilbert Space of **S**, i.e., $\mathcal{H} \to \mathcal{H}_\mathcal{S}$, defined as follows.

$$\text{Tr}_B[\rho_{SB}] = \sum_k (\mathbb{I}_S \otimes \langle k|_B) \rho_{SB} (\mathbb{I}_S \otimes |k\rangle_B) \tag{1.26}$$

We often write it as, $\rho_S = \text{Tr}_B[\rho_{SB}]$, the marginal on $\mathcal{H}_A$. **Ultimately, The reduced density operator ρ_S describes completely all the properties/outcomes of measurements of system**

1, given that system 2 is left unobserved ("tracing out" system 2) The partial trace can be generalized to composite systems of more than two parts, for example, ρ_{ABC} or ρ_{ABCD}. The idea is the same, however—act with identity on the system(s) you care about and trace out (sum over) the systems you don't care about. To build a partial trace, we need identity operators and orthonormal bases.

The partial trace has the following properties:

1. Hemitian: Any density state of a combined system can be written as,

$$\rho_{SB} = \sum_{jl;km} \lambda_{jl;km} \left| j \right\rangle_S \left\langle l \right| \otimes \left| k \right\rangle_B \left\langle m \right| \tag{1.27}$$

for some bases $\left| j \right\rangle_S$ and $\left| k \right\rangle$ of $\mathcal{H}_S$ and $\mathcal{H}_B$, respectively and $\lambda_{jl;km} = \lambda_{lj;mk}^{\dagger}$ is hermitian. The reduced density operator ρ_S is given by,

$$\rho_S = \mathrm{Tr}_B[\rho_{SB}] = \sum_{jl} \sum_{\mu} \lambda_{jl;\mu\mu} \left| j \right\rangle_S \left\langle l \right| \tag{1.28}$$

Hermeticity of ρ_S follows from

$$\rho_S^{\dagger} = \sum_{jl} \sum_{\mu} \lambda_{jl;\mu\mu}^{\dagger} (\left| j \right\rangle_S \left\langle l \right|)^{\dagger} = \sum_{jl} \sum_{\mu} \lambda_{lj;\mu\mu} \left| l \right\rangle_S \left\langle j \right| = \rho_S \tag{1.29}$$

1.29 stands because j and l are all dummy indices and could be interchanged.

2. Positive: Let $\left| \psi \right\rangle_S$ be an arbitrary pure state in $\mathcal{H}_S$ and define $\left| \Psi \right\rangle = \left| \psi \right\rangle_S \otimes \left| \mu \right\rangle_B$, a state on $\mathcal{H}_S \otimes \mathcal{H}_B$. Since, ρ_{SB} is positive (1.15),

$$0 < \sum_{m} \left\langle \Psi \right| \rho_{SB} \left| \Psi \right\rangle \tag{1.30}$$

$$= \sum_{\mu} \left\langle \psi \right|_S \otimes \left\langle \mu \right|_B \rho_{SB} \left| \psi \right\rangle_S \otimes \left| \mu \right\rangle_B \tag{1.31}$$

$$= \sum_{\mu} \sum_{jl;km} \lambda_{jl;km} (\left\langle \psi | j \right\rangle \left\langle l | \psi \right\rangle)_S (\left\langle \mu | k \right\rangle \left\langle m | \mu \right\rangle)_B \tag{1.32}$$

$$= \sum_{\mu} \sum_{jl} \lambda_{jl;\mu\mu} \left\langle \psi | j \right\rangle \left\langle l | \psi \right\rangle_S \tag{1.33}$$

$$= \left\langle \psi \right| \rho_S \left| \psi \right\rangle \text{ (follows from 1.28)} \tag{1.34}$$

Therefore, by definition of the positive operator, ρ_S is positive.

3. Trace-Preservation: Consider,

$$\text{Tr}[\rho_S] = \sum_{\mu,n} \sum_{jl} \lambda_{jl;\mu\mu} \langle n|j\rangle \langle l|n\rangle \tag{1.35}$$

$$= \sum_{\mu,n} \lambda_{nn;\mu\mu} \tag{1.36}$$

$$= \text{Tr}[\rho_{SB}] \tag{1.37}$$

In general, $\text{Tr}[\rho_{SB}] = 1$. Therefore, $\text{Tr}[\rho_S] = 1$ and it is preserved when $\text{Tr}[\rho_{SB}]$ remains constant.

4. Another two important properties I want to mention without proof, which will be useful in the upcoming discussion, are,

$$\text{Tr}[S_{AB}] = \text{Tr}_A[\text{Tr}_B[S_{AB}]] \text{ and} \tag{1.38}$$

$$\text{Tr}[S_{AB}(\mathbb{T}_S \otimes \mathbb{I}_B)] = \text{Tr}_B[\rho_{SB}]\mathbb{T}_A \tag{1.39}$$

Traces can be decomposed into partial traces, and partial trace commutes with multiplication with operators of the form $\mathbb{T}_S \otimes \mathbb{I}_B$.

1.1.4 Formal Justification of using Partial Trace

It's ok that we are not very concerned about the environment. But how do we ensure that the partial trace of the combined density matrix over the environment B offers the density matrix of the subsystem S?

Let's define the problems first clearly. In a composite system, the measurement is actually of the observable $O = O_S \otimes \mathbb{I}$ on the entire system ρ in $\mathcal{H}_S \otimes \mathcal{H}_B$. Thus,

$$\langle O \rangle := \text{Tr}[O\rho] \tag{1.40}$$

To be accepted as a defining mathematical tool, ρ_S must have the property that

$$\langle O_S \rangle := \text{Tr}[O_S \rho_S] = \text{Tr}[O\rho] \tag{1.41}$$

Let's prove it.

Proof: Let $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B = span|j\rangle_S \otimes |k\rangle_B$ (Using the postulate of Quantum Mechanics). Then

$$\langle O_S \rangle = \sum_j \langle j|\rho_S O_S|j\rangle \tag{1.42}$$

$$= \sum_j \langle j|\mathrm{Tr}_B[\rho_{SB}]O_S|j\rangle \tag{1.43}$$

$$= \sum_j \langle j| \sum_\mu \langle \mu|\rho_{SB}|\mu\rangle O_S|j\rangle \tag{1.44}$$

Now, to proceed further, we have to use our intuition and also the definition of partial trace here. Here, ρ_{SB} acts on the composite system, not just on A. To change O_A acting on the composite system, we must extend it to $O_A \otimes \mathbb{I}_B$. It's not changing anything physically but helping us to proceed analytically.

$$= \sum_{j,\mu} \langle j| \otimes \langle \mu| |[\rho_{SB}(O_A \otimes \mathbb{I}_B]| |j\rangle \otimes |\mu\rangle \tag{1.45}$$

$$= \mathrm{Tr}[\rho_{SB}O] \tag{1.46}$$

Therefore, if $\rho_S = \mathrm{Tr}_B[\rho_{SB}]$, then $\langle O \rangle = \langle O_A \rangle$. Having only knowledge of ρ_S can provide us with every interesting knowledge of the system.

Another mechanical way to prove this:

$$\langle O \rangle = \mathrm{Tr}[(O_S \otimes \mathbb{I}_B)\rho_{SB}] \tag{1.47}$$

$$= \mathrm{Tr}_S(\mathrm{Tr}_B[(O_S \otimes \mathbb{I}_B)\rho_{SB}]) \tag{1.48}$$

$$= \mathrm{Tr}_S(O_S Tr_B(\rho_{SB})) \tag{1.49}$$

$$= \mathrm{Tr}[O_S\rho_S] \tag{1.50}$$

1.38 and 1.39 helps us to reach the result. **Ultimately, The reduced density operator ρ_S describes completely all the properties/outcomes of measurements of subsystem S, given that subsystem B is left unobserved ("tracing out" system 2)**

1.1.5   How to Use Partial Trace

Let's illustrate with a general two-qubit system where each qubit can be in states $|0\rangle$ or $|1\rangle$. The basis states of the combined system are $|00\rangle, |01\rangle, |10\rangle$, and $|11\rangle$. Therefore, the density matrix ρ can be written as:

$$\rho = \begin{array}{c|cccc} & |00\rangle & |01\rangle & |10\rangle & |11\rangle \\ \hline |00\rangle & \rho_{00,00} & \rho_{00,01} & \rho_{00,10} & \rho_{00,11} \\ |01\rangle & \rho_{01,00} & \rho_{01,01} & \rho_{01,10} & \rho_{01,11} \\ |10\rangle & \rho_{10,00} & \rho_{10,01} & \rho_{10,10} & \rho_{10,11} \\ |11\rangle & \rho_{11,00} & \rho_{11,01} & \rho_{11,10} & \rho_{11,11} \end{array} = \sum_{ijkl} \rho_{ijkl}(|a_i b_j\rangle\langle a_k b_l|) \tag{1.51}$$

Note: An easy way to remember the form is to: Draw a 4×4 grid and label the rows and columns with $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$ and fill in the matrix with coefficients for each combination.

To find out the reduced density operator ρ_1, we will use some properties that,

1. $|a_i b_j\rangle\langle a_k b_l| = |a_i\rangle\langle a_k| \otimes |b_l\rangle\langle b_k|$

2. $Tr_B(A \otimes B) = A \cdot Tr[B]$

3. *For two eigenvectors i and j, $Tr(|i\rangle\langle j|) = \sum_n \langle n|i\rangle \langle j|n\rangle = \sum_n \langle j|n\rangle \langle n|i\rangle = \langle j|i\rangle = \delta_{ij}$.*

$$\therefore \rho_1 = Tr_2\left(\sum_{ijkl} \rho_{ijkl}|a_i\rangle\langle a_k| \otimes |b_l\rangle\langle b_k|\right) \tag{1.52}$$

$$= \sum_{i,k,\mu} \rho_{i\mu k\mu}|a_i\rangle\langle a_k| \tag{1.53}$$

Note that:

$$\rho_1 = \begin{pmatrix} \rho_{00,00} & & \rho_{00,10} & \\ & \rho_{01,01} & & \rho_{01,11} \\ \rho_{10,00} & & \rho_{10,10} & \\ & \rho_{11,01} & & \rho_{11,11} \end{pmatrix} = \begin{pmatrix} \rho_{00,00} & \rho_{00,10} \\ \rho_{10,00} & \rho_{10,10} \end{pmatrix} + \begin{pmatrix} \rho_{01,01} & \rho_{01,11} \\ \rho_{11,01} & \rho_{11,11} \end{pmatrix} \tag{1.54}$$

$$= \begin{pmatrix} \rho_{00,00} + \rho_{01,01} & \rho_{00,10} + \rho_{01,11} \\ \rho_{10,00} + \rho_{11,01} & \rho_{10,10} + \rho_{11,11} \end{pmatrix} \tag{1.55}$$

Elements can be interpreted as the trace of the Bloch matrix corresponding to the element's position derived from the generalized density matrix.

Example: To provide an intuition, we examine scenarios that represent the extremes of the interaction between the system and the bath: the simplest case of a separable density operator and the scenario where the system and bath are maximally entangled. These examples will also justify the taking of partial trace over the subsystems.

1. In a scenario where the bath and system states are entirely separate and thus form a tensor product, we anticipate that the density operator of A, obtained through partial trace, should correspond exactly to the component of A within the tensor product, $\rho = \rho_A \otimes \rho_B$. Both terms in the product are properly normalized. Then,

$$Tr_B(\rho) = Tr_B(\rho_A \otimes \rho_B) = \rho_A Tr(\rho_B) = \rho_A \tag{1.56}$$

2. Let's say we have the entangled density matrix just as 1.12. Here, qubits are maximally entangled. This is not in the form of $\rho_A \otimes \rho_B$. But, ρ can be written as,

$$\rho = \frac{1}{2}(|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |0\rangle\langle 1| \otimes |0\rangle\langle 1| + |1\rangle\langle 0| \otimes |1\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1|) \tag{1.57}$$

Now, we want to trace out the subsystem $\mathbb{B}$,

$$\text{Tr}_B[\rho] = \frac{1}{2}(|0\rangle\langle 0| \cdot Tr(|0\rangle\langle 0|) + |0\rangle\langle 1| \cdot Tr(|0\rangle\langle 1|) + |1\rangle\langle 0| \cdot Tr(|1\rangle\langle 0|) + |1\rangle\langle 1| \cdot Tr(|1\rangle\langle 1|)) \tag{1.58}$$

Therefore,

$$\rho_S = \text{Tr}_B[\rho] = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{\mathbb{I}}{2} \tag{1.59}$$

while we started in an EPR pair by tracing out one of the qubits, we effectively measured (and forgot the result) the one that was left.

1.2   Liouville Formalism of Density Matrices

While this section draws heavily from [2], I will focus exclusively on the aspects crucial to my research in Open Quantum Systems. For a comprehensive understanding of tensor products and detailed proofs, which I will skip mostly, I recommend reading [2].

1.2.1   Rule to Transform Matrices into Vectors

Operaors like density matrices become column vectors in Liouville formalism. We will use bra-flipper operator to transform matrices into column vectors. For example, let say

$$|\psi\rangle = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} \tag{1.60}$$

The density matrix $\rho(t)$ corresponding to this pure state is of the form

$$\rho(t) = |\psi\rangle\langle\psi| = \begin{pmatrix} |a(t)|^2 & a(t)b^*(t) \\ a^*(t)b(t) & |b(t)|^2 \end{pmatrix} \tag{1.61}$$

We choose the form dictated in [3],

$$|\rho\rangle\rangle = \text{vec}[\rho(t)] = \begin{pmatrix} |a(t)|^2 \\ a(t)b^*(t) \\ a^*(t)b(t) \\ |b(t)|^2 \end{pmatrix} = |\psi\rangle \otimes |\psi\rangle^* \tag{1.62}$$

So, the map is, $\mho : |a\rangle\langle b| \to |a\rangle \otimes |b\rangle^*$ where $|a\rangle\langle b| \in \mathcal{O}_d$, Hilbert space of Linear Operator on $\mathcal{H}_d$ and $|a\rangle \otimes |b\rangle^*$ is $d^2 \times 1$ dimensional column vector in Linear Vector space, $\mathcal{L}_d$. For any mixed state, we have

$$|\rho\rangle\rangle = \mho[\rho] = \sum_{n=1}^{d}\sum_{n'=1}^{2} \rho_{nn'}\mho[|\psi_n\rangle\langle\psi_{n'}|] = \sum_{n=1}^{d}\sum_{n'=1}^{2} \rho_{nn'} |\phi_n\rangle \otimes |\phi_{n'}\rangle \tag{1.63}$$

Superket Property: We will use this property the most in our report. Say A, B and C are operators on $\mathcal{H}_d$; The product ABC is also an operator on $\mathcal{H}_d$. The superket triple product identity says that,

$$|ABC\rangle\rangle = (A \otimes C^T) |B\rangle\rangle \tag{1.64}$$

where, $(A \otimes B^T) \in \mathcal{S}_d$, Hilbert space of Linear Operators on $\mathcal{L}_d$, acting on $|B\rangle\rangle \in \mathcal{L}_d$. From 1.64,

$$|ABC\rangle\rangle = (AB \otimes \mathbb{I}_d) |C\rangle\rangle \tag{1.65}$$

$$|ABC\rangle\rangle = (\mathbb{I}_d \otimes C^T B^T) |A\rangle\rangle \tag{1.66}$$

Now, for the superket of the commutation $[A, B]$,

$$|[A, B]\rangle\rangle = |AB - BA\rangle\rangle = (A \otimes \mathbb{I}_d - \mathbb{I}_d \otimes A^T) |B\rangle\rangle = [\![A, \mathbb{I}_d]\!] |B\rangle\rangle \tag{1.67}$$

$$\text{Similarly, } |[A, B]\rangle\rangle = [\![\mathbb{I}_d, B]\!] |A\rangle\rangle \tag{1.68}$$

Where, super-commutator, $[\![A, B]\!] |B\rangle\rangle = A \otimes B^T - B \otimes A^T$. Proof of this property is given in [3]. Analogusly, we have anti-super commutator, $[\![A, B]\!]_+ = A \otimes B^T + B \otimes A^T$.

1.2.2 Applications

For $\rho(t)$ defined on a finite-dimensional state space of dimension d, the lindblud equation reads,

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H, \rho(t)] + \sum_{k=1}^{d^2-1} \gamma_k \left(A_k\rho(t)A_k^\dagger - \frac{1}{2}A_k^\dagger A_k\rho(t) - \frac{1}{2}\rho(t)A_k^\dagger A_k \right) \tag{1.69}$$

where the first and second terms represent the unitary and the dissipative parts of the system's evolution, respectively. We can send this equation to Liouville space by applying $\mho$ operator on both sides of 1.69 and then use the superket triple product identity to factorize out $\rho(t)$ as $|\rho\rangle\rangle$. This leads us to the form,

$$\frac{d}{dt}\,|\rho\rangle\rangle(t) = \mathcal{L}(t)\,|\rho\rangle\rangle(t) \tag{1.70}$$

$$\text{where,} \mathcal{L}(t) = -\frac{i}{\hbar}[\![H,\rho(t)]\!] + \sum_{k=1}^{d^2-1} \gamma_k \left(A_k \otimes A_k^* - \frac{1}{2}[\![A_k^\dagger A_k, \mathbb{I}_d]\!]_+ \right) \tag{1.71}$$

Here, the generator $\mathcal{L}$ is not skew-Hermitian or Hermitian.

Chapter 2

Open Quantum Systems

2.1 Interaction Picture

We will express and evaluate the density matrix in interaction representation. So, we will use general notations used in quantum mechanics to represent the interaction picture.

Let us consider a system with a Hamiltonian,

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}' \tag{2.1}$$

H_0 is chosen to be exactly solvable, while it is much tougher to deal with $\mathcal{H}'$. In the Interaction representation, state vectors are written as,

$$|\psi\rangle_I = \mathcal{U}_0^\dagger(t) |\psi\rangle_S = e^{\frac{\iota \mathcal{H}_0 t}{\hbar}} |\psi\rangle_S \tag{2.2}$$

where subscripts I and S indicate the interaction and Schrodinger picture, respectively. For the observable operators we can define the corresponding interaction picture operators as:

$$A_I(t) = \mathcal{U}_0^\dagger(t) A_S \mathcal{U}_0(t) \tag{2.3}$$

Now The density matrix can be shown to transform to the interaction picture in the same way as any other operator. If there is probability p_n to be in the physical state ψ_n, then,

$$\rho_I = \sum_n p_n |\psi\rangle_I \langle\psi| \tag{2.4}$$

$$= \sum_n p_n e^{\iota \mathcal{H}_0 t} |\psi\rangle_S \langle\psi| e^{-\iota \mathcal{H}_0 t} \tag{2.5}$$

$$= e^{\iota \mathcal{H}_0 t} \rho_S e^{-\iota \mathcal{H}_0 t} \tag{2.6}$$

$$\boxed{\therefore \rho_I = \mathcal{U}^\dagger \rho_S \mathcal{U}} \tag{2.7}$$

Partial differentiating the last equation with time, we get,

$$\partial_t \rho_I = \iota H_0 \rho_I + e^{\iota H_0 t} \frac{\partial}{\partial t} \rho_S e^{\iota H_0 t} - \iota \rho_I H_0 \tag{2.8}$$

$$= \iota [H_0, \rho_I] - e^{\iota H_0 t} \iota [H_0 + \mathcal{H}'(t), \rho_S] e^{\iota H_0 t} \text{ (From 1.25)} \tag{2.9}$$

$$= \iota [H_0, \rho_I] - e^{\iota H_0 t} \iota [H_0, \rho_S] e^{\iota H_0 t} - e^{\iota H_0 t} \iota [\mathcal{H}', \rho_S] e^{\iota H_0 t} \tag{2.10}$$

$$= \iota [H_0, \rho_I] - \iota [H_0, \rho_I] - \mathcal{U}^\dagger (\iota [\mathcal{H}', \rho_S]) \mathcal{U} \tag{2.11}$$

Because, $e^{\iota H_0 t} H_0 \rho_s e^{-\iota H_0 t} = H_0 e^{\iota H_0 t} \rho_S e^{-\iota H_0 t} = H_0 \rho_I$. Now,

$$= -\iota (\mathcal{U}^\dagger \mathcal{H}' \rho_S \mathcal{U} - \mathcal{U}^\dagger \rho_S \mathcal{H}' \mathcal{U} \tag{2.12}$$

$$= -\iota (\mathcal{U}^\dagger \mathcal{H}' \mathcal{U} \mathcal{U}^\dagger \rho_S \mathcal{U} - \mathcal{U}^\dagger \rho_S \mathcal{U} \mathcal{U}^\dagger \mathcal{H}' \mathcal{U}) \tag{2.13}$$

$$= -\iota (\mathcal{H}'_I \rho_I - \rho_I \mathcal{H}'_I \rho_I) \tag{2.14}$$

From 2.7 and 2.3, we can write

$$\boxed{\frac{\partial \rho_I}{\partial t} = -\iota [\mathcal{H}'_I, \rho_I]} \tag{2.15}$$

This equation is consistent with the Schrodinger picture. Nevertheless, it is obvious to see that,

$$\langle A_I(t) \rangle = \langle \psi_I | A_I | \psi_I \rangle = \langle \psi_S | A_S | \psi_S \rangle = \langle A_S(t) \rangle \tag{2.16}$$

and using cyclic property of trace, we have

$$\boxed{\langle A_I \rangle = Tr[\rho_I A_I]} \tag{2.17}$$

2.16 and 2.17 shows us that the statistical average over some ensemble (ex: 1.1) have remained the same in both Schrodinger and interaction picture.

2.2   Open Quantum System

This portion is mainly taken from [3]. An open quantum theory concerns the composite system where we have a subsystem of our interest, S (often it's called 'System'), and another subsystem is a bath, B. If subsystems are coupled, then our subsystem S don't follow unitary dynamics as we discussed in (1.16). Though S + B is a closed system in our assumption, and so follows according to the Schrodinger equation (1.16). Mathematical treatment of non-unitary dynamics of subsystem S is discussed below.

Let say,

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B = span|i\rangle_S \otimes |j\rangle_B \tag{2.18}$$

be the corresponding S + B Hibert Space (Postulate of Quantum Mechanics) where $\mathcal{H}_{\mathcal{S}} = span|j\rangle_S$ and $\mathcal{H}_{\mathcal{B}} = span|k\rangle_B$. Here, j goes from 0 to $d_S - 1$, the dimension of Hilbert space of **S** and k goes from 0 to $d_B - 1$, the dimension of Hilbert space of **B**. Usually, the dimension of bath $d_B \to \infty$.

The Hamiltonian of the total closed $S + B$ system reads,

$$H = H_0 + H_{int} = H_S \otimes \mathbf{I}_B + \mathbf{I}_S \otimes H_B + H_{int} \tag{2.19}$$

Let, the initial state of our system "**S** + **B**" is,

$$\rho_{SB}(0) = \rho(0) \otimes \rho_B$$

Initially, **S** and **B** are not correlated, so $\rho(0)$ can be written as a factorized state. (1.15) tells us that

$$\rho_{SB}(t) = U(t)\rho_{SB}(0)U^\dagger(t) = U(t)(\rho(0) \otimes \rho_B)U^\dagger(t) \tag{2.20}$$

where $U = e^{-\iota Ht}$.

Generally, we are not concerned about the whole system but the only subsystem **S**. The state of **S** evolves according to

$$\rho_{\mathbf{S}} = \text{Tr}_{\mathbf{B}}[U(t)(\rho(0) \otimes \rho_B)U^\dagger(t)] \tag{2.21}$$

and it is called the **reduced evolution** of the **S**. But before going into that, I want to address some concerns.

- We might feel that $Tr_B[U(A \otimes B)U^\dagger] = Tr_B[(A \otimes B)U^\dagger U] = Tr_B[A \otimes B] = ATr[B]$. But this whole line of argument fails when the coupling is present in the system, and also Trace becomes non-commutative because $U(t)$, is of a different matrix size compared to $A \otimes B$. Therefore generally we observe that $\rho_S \neq \rho(0)Tr[\rho_B]$

- Simplest case rises when $H_{int} = 0$. Then subsystem **S** follows unitary dynamics. It is easy to show mathematically.

$$U(t) = exp(-\iota(H_S \otimes \mathbf{I}_B + \mathbf{I}_S \otimes H_B)t) \tag{2.22}$$
$$= exp(-\iota(H_S \otimes \mathbf{I}_B)t)exp(-\iota(\mathbf{I}_S \otimes H_B)) \tag{2.23}$$
$$= (exp(-\iota H_S) \otimes \mathbf{I}_B)(\mathbf{I}_S \otimes exp(-\iota H_B)) \tag{2.24}$$
$$U(t) = e^{-\iota H_S t} \otimes e^{-\iota H_B t} \tag{2.25}$$

2.23 followed from the logic that the system and bath operators commute with each other and $e^{A+B} = e^A e^B$. 2.24 can derived from Taylor expansion using e^x. Now,

$$\rho_{SB} = e^{-\iota H_S t} \otimes e^{-\iota H_B t}(\rho(0) \otimes \rho_B)e^{\iota H_S t} \otimes e^{\iota H_B t} \tag{2.26}$$
$$= (e^{-\iota H_S t}\rho(0)e^{\iota H_S t}) \otimes (e^{-\iota H_B t}\rho_B e^{\iota H_B t}) \tag{2.27}$$

2.27 can be written in the form of 2.34. Tracing out the bath(often we call this environment), we get,

$$\rho_S = Tr_B[(e^{-\iota H_S t}\rho(0)e^{\iota H_S t}) \otimes (e^{-\iota H_B t}\rho_B e^{\iota H_B t})] \tag{2.28}$$

$$= (e^{-\iota H_S t}\rho(0)e^{\iota H_S t})Tr[e^{-\iota H_B t}\rho_B e^{\iota H_B t}] \tag{2.29}$$

$$= (e^{-\iota H_S t}\rho(0)e^{\iota H_S t})Tr[\rho_B] \tag{2.30}$$

In most cases, $Tr[\rho_B] = 1$. **Therefore, when coupling is not present in system but only the separate Hamiltonians, we observe an unitary dynamics in our system(subsystem) S governed by** $\boxed{\rho_S = e^{-\iota H_S t}\rho(0)e^{\iota H_S t}}$.

Interesting dynamics like in Open Quantum Systems, can be observed in the presence of coupling of the system with the environment. Entaglement-like phenomena arise where we can't write our ρ_{SB} into a factoring state like 2.27. Tracing out the environment is no longer trivial, and non-unitary dynamics are followed by System **S**.

- Initial density state is not entangled because coupling starts from $t > 0$. Postulates of Quantum Mechanics permit us to write any state of a combined system can be written as:

$$|\psi_i\rangle = \sum_{j,k} c_{i;jk} |j\rangle_S \otimes |k\rangle_B \tag{2.31}$$

$$\text{So, } \rho_{SB} = \sum_i p_i |\psi_i\rangle \langle\psi_i| \tag{2.32}$$

$$= \sum_i p_i (\sum_{j,k} c_{i;jk} |j\rangle_S \otimes |k\rangle_B)(\sum_{l,m} c^*_{i;lm} \langle l|_S \otimes \langle m|_B) \tag{2.33}$$

$$= \sum_{jlkm} \lambda_{jlkm} |j\rangle_S \langle l| \otimes |k\rangle_B \langle m| \tag{2.34}$$

where, $\lambda_{jlkm} = \sum_i p_i c_{i;jk} c^*_{i;lm}$. *2.34 can be considered as a representation of any density state of a combined subsystem, whether it is a pure, mixed, or entangled state. In an Open quantum system, where we can't write states such as 2.27 but even then 2.34 is permitted just because the basic postulates of quantum mechanics are utilized to derive it.*

If coupling is not present at $t \leq 0$, $\lambda_{jlkm} = \lambda_{jl}\lambda_{km}$. Then $\boxed{\rho_{SB}(0) = \rho(0) \otimes \rho_B}$, where $\rho(0)$ and ρ_B are mere linear combination of their respective eigenstates. Putting $t = 0$ in 2.27 gives the same result.

2.3 Two Level System- Spin 1/2 ensemble

We consider an ensemble of spin $\frac{1}{2}$ nuclei in a Zeeman field of magnitude B_0 in $z-$ direction and a transverse resonant drive oscillating with ω in the $x-$ as an experimentally realizable model of driven TLS connected to a heat bath. According to [1], The Hamiltonian is, therefore,

$$\mathcal{H}(t) = \mathcal{H}_S^0 + \mathcal{H}_{SL} + \mathcal{H}_L^0 + \mathcal{H}_S(t) + \mathcal{H}_L(t) \tag{2.35}$$
$$= \mathcal{H}_S^0 + \mathcal{H}_L^0 + \mathcal{H}_{\text{eff}}(t) + \mathcal{H}_L(t) \tag{2.36}$$

$\mathcal{H}_S^0 = \omega_0 I_z$ is bare Hamiltonian and $\mathcal{H}_S(t) = 2\omega_1 \cos(\omega t) I_x$ is the drive Hamiltonian. $(I_\alpha = \frac{1}{2}\sigma_\alpha)$ It's useful to remember that operators and Bath Hamiltonian $\mathcal{H}_L^0$ don't affect system operators, so they commute with the system operators.

Control over the system's state vector rotation in Bloch's sphere can be achieved by adjusting the magnitudes of ω_0 and ω_1. The parameter ω_0, associated with the Zeeman field, dictates the rate at which the state vector precesses around the z-axis on the Bloch sphere. This precession corresponds to the phase evolution between the two energy eigenstates. Meanwhile, the driving field ω_1 induces rotations around an axis within the xy-plane, with the direction of this rotation depending on the phase of the driving field. By modulating ω_1, the state vector can be rotated away from the z-axis, facilitating transitions between quantum states and enabling precise control over the system's dynamics.

We here assumed that the external drive $\omega = \omega_0 + \Delta\omega$ is nearly resonant with the ω_0, $\dfrac{\Delta\omega}{\omega_0} \to 0$. We will be concerned with the interaction representations of the relevant co-rotating spin-$\frac{1}{2}$ observables given by,

$$F_\alpha^R(t) = e^{\iota\omega_0 I_z t} I_\alpha e^{-\iota\omega_0 I_z t} \tag{2.37}$$

Like always, we will find the dynamics of the expectation value of $F_\alpha^R(t)$, denoted by $M_\alpha(t)$.

$$M_\alpha = Tr_S(F_\alpha^R(t)\rho_S(t) \tag{2.38}$$
$$\therefore \frac{d}{dt}M_\alpha(t) = Tr_S(\frac{d}{dt}F_\alpha^R(t)\rho_S(t) + F_\alpha^R(t)\frac{d}{dt}\rho_S(t)) \tag{2.39}$$

The relevant time scales in QME are, $\tau_c \ll \Delta t \ll \omega_1^{-1}, \omega_{SL}^{-1}$, and $\omega_0 \ll \Delta t$. Using the time-nonlocal QME, which has second-order contributions from external drive [1], we can sketch the dynamics of system. Now,

$$\frac{d}{dt}\rho_S(t) = -i \operatorname{Tr}_L \left[H_{\text{eff}}(t), \rho_S(t) \otimes \rho_L^{\text{eq}} \right]^{\text{sec}} - \int_0^\infty d\tau \operatorname{Tr}_L \left[H_{\text{eff}}(t), [H_{\text{eff}}(t-\tau), \rho_S(t) \otimes \rho_L^{\text{eq}}] \right]^{\text{sec}} e^{-|\tau|/\tau_c}. \tag{2.40}$$

Therefore,

$$\frac{d}{dt}M_\alpha(t) = \mathrm{Tr}_S\left\{\left\{\frac{d}{dt}F_\alpha^R(t)\right\}\rho_S(t)\right\} - i\,\mathrm{Tr}_S\left\{\mathrm{Tr}_L\left[H_{\mathrm{eff}}(t),\rho_S(t)\otimes\rho_L^{\mathrm{eq}}\right]^{\mathrm{sec}}F_\alpha^R(t)\right\}$$

$$-\int_0^\infty d\tau\,\mathrm{Tr}_S\left\{\mathrm{Tr}_L\left[H_{\mathrm{eff}}(t),[H_{\mathrm{eff}}(t-\tau),\rho_S(t)\otimes\rho_L^{\mathrm{eq}}]\right]^{\mathrm{sec}}e^{-|\tau|/\tau_c}F_\alpha^R(t)\right\}. \tag{2.41}$$

Driving Hamiltonian commutes with $\mathcal{H}_L^0$. So, in the interaction picture of $\mathcal{H}_S^0 + \mathcal{H}_L^0$, driving Hamiltonian becomes,

$$\mathcal{H}_S(t) = e^{\iota\omega_0 I_z t}(2\omega_1\cos(\omega t)I_x)e^{-\iota\omega_0 I_z t} \tag{2.42}$$

$$= 2\omega_1\cos(\omega t)e^{\iota\omega_0 I_z t}(\frac{I_+ + I_-}{2})e^{-\iota\omega_0 I_z t}$$

$$= 2\omega_1\cos(\omega t)(\frac{I_+ e^{\iota\omega_0 t} + I_- e^{-\iota\omega_0 t}}{2})$$

$$= 2\omega_1(\frac{e^{\iota\omega t} + e^{-\iota\omega t}}{2})(\frac{I_+ e^{\iota\omega_0 t} + I_- e^{-\iota\omega_0 t}}{2})$$

$$= \frac{\omega_1}{2}(I_+ e^{\iota\Omega t} + I_- e^{\iota\Delta\omega t} + I_+ e^{-\iota\Delta\omega t} + I_+ e^{-\iota\Omega t}) \tag{2.43}$$

$$= \omega_1(e^{\iota\Omega I_Z t}I_x e^{-\iota\Omega I_Z t} + e^{\iota\Delta\omega I_z t}I_x e^{-\iota\Delta\omega I_z t})$$

$$\therefore \mathcal{H}_S(t) = \omega_1(F_x^C(t) + F_x^R(t)) \tag{2.44}$$

Here, $F_x^C(t) = e^{\iota\Omega I_Z t}I_x e^{-\iota\Omega I_Z t}$ is counter rotating component of the drive-field. Note that in the interaction picture, transformed Hamiltonian (2.44 similar to $\mathcal{H}_I'$ of 2.14) obeys 2.15. So, it is now wise to use density matrices in Interaction representations.

In our system, we assume the most general form of $\mathcal{H}_{SL}$ for a Spin 1/2 ensemble,

$$H_{SL} = \omega_{SL}(I_+ R_- + I_- R_+ + I_z R_z) \tag{2.45}$$

It doesn't transform under rotations or any other transformations applied separately to the spin systems or its environment. In interaction representation of $H_S^0 + H_L^0$,

$$H_{SL}(t) = e^{\iota(H_S^0 + H_L^0)t}H_{SL}e^{-\iota(H_S^0 + H_L^0)t} \tag{2.46}$$

As system and bath operators commute with each other,

$$e^{\iota(H_S^0 + H_L^0)t}IRe^{-\iota(H_S^0 + H_L^0)t} = e^{\iota(H_S^0)t}Ie^{-\iota(H_S^0)t}e^{\iota(H_L^0)t}Re^{-\iota(H_L^0)t} \tag{2.47}$$

Therefore,

$$H_{SL}(t) = \omega_{SL}(I_+ e^{\iota\omega_o 0 t}R_-(t) + I_- e^{-\iota\omega_0 t}R_+ + I_z R_z(t)) \tag{2.48}$$

So, This coupled Hamiltonian $H_{SL}(t)$ and Drive Hamiltonian $H_s(t)$ operates the dynamics of equation 2.41. We will discuss some points about the calculations of different terms of 2.41 and then go to the Bloch Equations. Heat Bath is isotropic, and the expectation value of environment operators $B_i(t)$ in the equilibrium state ρ_L are zero due to the symmetry.

$$\langle B_i(t) \rangle = Tr_L(B_i(t)\rho_L) = 0 \tag{2.49}$$

$$\therefore Tr_L(H_{SL}(t)\rho_S(t)\rho_L) = \sum_i Tr_L((A_i \otimes B_i)(\rho_S(t) \otimes \rho_L))$$

$$= \sum_i A_i \rho_S(t) Tr_L(B_i \rho_L)$$

$$= 0$$

This ensures that first-order contributions in QME (second term in r.h.s. of equation (2.41)) from H_{SL} is zero. Only $H_S(t)$ contributes in first-order calculations of H_{eff}. In second-order calculations, H_{SL} leads to relaxation rates, T_1 and T_2 as well as the equilibrium value M_0.

Other than that, it also ensures that no cross terms between drive and coupling stay in second-order contributions (third term in r.h.s. of equation (2.41)). Because,

$$Tr_L(H_S H_{SL}(t)\rho_S(t)\rho_L) = H_S Tr_L(H_{SL}(t)\rho_S(t)\rho_L) = 0 \tag{2.50}$$

Bath operators have zero average, but they have correlations in time that make possible frequency-dependent terms ($\Gamma(\Omega)$) in bloch equations based on system coupling.

Another important point to evaluate 2.41 is keeping only secular terms. To have $|\omega|\Delta t \ll 1$, we ignore the terms with $\sigma = \omega + \omega_0$ and keep terms with $\Delta\omega = \omega - \omega_0$ in first-order calculations using $H_s(t)$. Whereas in second-order calculations, cross terms between $F_x^C(t)$ and $F_x^C(t)$ as well as the non-secular terms of $F_x^C(t)$ have negligible effects in secular integration.

2.4 Simulations

2.4.1 Differential Equations of Bloch Vectors

From equation 2.41,we find

$$\frac{d}{dt}M_x(t) = \Delta\omega_x M_y(t) - \Gamma_x M_x(t),$$

$$\frac{d}{dt}M_y(t) = -\Delta\omega_y M_x(t) - \omega_1 M_z(t) - \Gamma_y M_y(t) \tag{2.51}$$

$$\frac{d}{dt}M_z(t) = \omega_1 M_y(t) - \Gamma_z M_z(t) + \frac{1}{T_1}M_o.$$

where the decay rates are $\Gamma_x = \frac{1}{T_2} + \eta_x$, $\Gamma_y = \frac{1}{T_2} + \eta_y$, and $\Gamma_z = \frac{1}{T_1} + \eta_z$, with

$$
\begin{aligned}
\eta_x &= \omega_1^2 \left[\frac{1}{2} \left(\frac{\tau_c}{1 + \Omega^2 \tau_c^2} \right) \right], \\
\eta_y &= \omega_1^2 \left[\frac{1}{2} \left(\frac{\tau_c}{1 + \Omega^2 \tau_c^2} \right) + \frac{\tau_c}{1 + \Delta\omega^2 \tau_c^2} \right], \\
\eta_z &= \omega_1^2 \left[\frac{\tau_c}{1 + \Omega^2 \tau_c^2} + \frac{\tau_c}{1 + \Delta\omega^2 \tau_c^2} \right].
\end{aligned}
\tag{2.52}
$$

and,

$$
\begin{aligned}
\frac{1}{T_1} &= J(\omega_o) + K(\omega_o) \\
\frac{1}{T_2} &= \frac{1}{2}[J(\omega_o) + K(\omega_o)] + \frac{1}{2}J(0) \\
M_o &= \frac{1}{2} \left[\frac{J(\omega_o) - K(\omega_o)}{J(\omega_o) + K(\omega_o)} \right]
\end{aligned}
\tag{2.53}
$$

The frequency shifts are given by $\Delta\omega_x = \Delta\omega - \delta\omega_C$ and $\Delta\omega_y = \Delta\omega - \delta\omega_C + \delta\omega_R$, where

$$
\delta\omega_C = \frac{1}{2} \left(\frac{\omega_1^2 \Omega \tau_c^2}{1 + \Omega^2 \tau_c^2} \right)
\tag{2.54}
$$

is the frequency shift originating from the counter-rotating term $F_x^C(t)$, while

$$
\delta\omega_R = \frac{\omega_1^2 \Delta\omega \tau_c^2}{1 + \Delta\omega^2 \tau_c^2}
\tag{2.55}
$$

is the same from the resonant term $F_x^R(t)$.

Simulations of Bloch vectors using Equation 2.51

I want to see the time evolution of Bloch vectors in co-rotating frame (2.51) where the Initial density matrix is,

$$
\rho(0) = 0.5 \cdot \mathbb{I} + 0.4 \cdot \sigma_x
\tag{2.56}
$$

$Tr(\rho_0) = 1$, and the unity of trace is preserved throughout all its time dynamics.

Parameter Values: We will focus on the parameter regime presented in [1]. Although the choice of parameters may initially appear arbitrary, it is actually well-justified for practical purposes.

- $\omega_1 = 2\pi \cdot 10\text{kHz} = 20\pi \times 10^3 \text{ rad/s}$

- $\Delta\omega = 2\pi \cdot 5\text{kHz} = 10\pi \times 10^3 \text{ rad/s}$

- $\omega_0 = 2\pi \cdot 100\text{MHz} = 200\pi \times 10^6 \text{ rad/s}$

- $\omega = \omega_0 + \Delta\omega = 200\pi \times 10^6 \text{ rad/s} + 10\pi \times 10^3 \text{ rad/s}$

- $\Omega = \omega + \omega_0 = 200\pi \times 10^6 \text{ rad/s} + 200\pi \times 10^6 \text{ rad/s} + 10\pi \times 10^3 \text{ rad/s}$

- $\tau_c = 10^{-7} \text{ s}$

- $T_1 = 1 \text{ s}$

- $T_2 = 0.1 \text{ s}$

Here, $\frac{\Delta\omega}{\omega_0} = 0.5 \times 10^{-4}$, which is a good approximation as this ratio should be close to the zero value. Relevant quantities in equation 2.51 like $\Gamma_x, \Gamma_y, \Gamma_z, \delta\omega_x$, and $\delta\omega_y$ can be evaluated using this parameter values.

From the initial density matrix, $\rho(0)$, we can calculate the initial bloch vector values.

$$M_x(0) = Tr(I_x\rho(0))$$
$$= 0.4$$

Similarly, $M_y(0) = 0$, and $M_z(0) = 0$. Using RK4 method, from $t_{int} = 0$ to $t_{fin} = 15$ ms with timestep, $\Delta t = 0.1\mu s$, we evaluate $(M_x(t), M_y(t), M_z(t)$. It is important to notice that $\frac{\Delta t}{\tau_c} = 100$, a quite appropriate approximation respecting the arguments in [1].
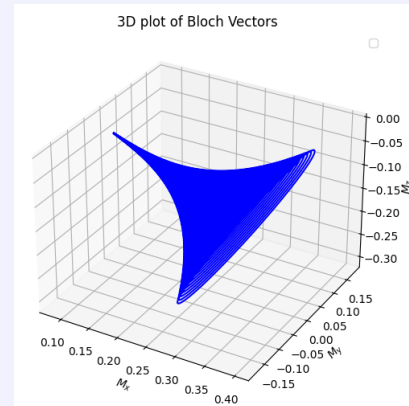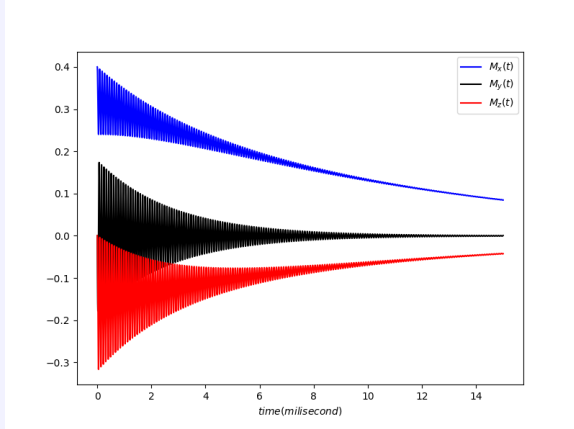
Note: At any point of time, you can check the trace of $\rho_S(t)$ and will find that trace is preserved at unity.

Results archived through numerical calculations are perfect as in the context of open quantum systems, the decay of the Bloch vectors is inevitable through different processes.

- *Relaxation (T_1 decay):* This is the process where the system loses energy to its environment, causing the component of the Bloch vector along the z-axis (the longitudinal component) to decay toward its equilibrium value.

- *Dephasing (T_2 decay):* This involves the loss of coherence between quantum states, leading to a decay in the transverse components (x and y) of the Bloch vector. This results in the vector's length shrinking over time, indicating the loss of information about the phase relationship between states.

If we are analyzing such a system, the presence of decay in the Bloch vector implies that the system's dynamics are not unitary (i.e., they do not conserve the length of the Bloch vector), and this non-unitarity is typically due to the coupling between the system and its environment. This coupling can lead to energy exchange and the randomization of phases, which contribute to the Bloch vector's overall decay.

2.4.2   Bloch Vectors Directly Using Quantum Master Equation

Now, our strategy is different to the previous one. Instead of figuring out the differential equations of Bloch Vectors, we will find the density matrix $\rho(t)$ for some time interval and then calculate $M_\alpha(t) = Tr[I_\alpha \rho(t)]$. In this case, we will use the Quantum Master Equation 2.40.

Putting $\mathcal{H}_{\mathit{eff}}(t) = \mathcal{H}_S(t) + \mathcal{H}_{SL}(t)$ from (2.44) and (2.48) in QME and performing secular integration , we have

$$\frac{d}{dt}\rho_S = -\frac{\iota\omega_1}{2}[I_+,\rho_S]e^{-\iota\Delta\omega t} - \frac{\iota\omega_1}{2}[I_-,\rho_S]e^{\iota\Delta\omega t} \tag{2.57}$$

$$-\frac{\omega_1^2}{4}\Gamma(\Omega)[I_+,[I_-,\rho_S]] - -\frac{\omega_1^2}{4}\Gamma^*(\Omega)[I_-,[I_+,\rho_S]] \tag{2.58}$$

$$-\omega_1^2\Gamma(\Delta\omega)[I_+,[I_-,\rho_S]]e^{-2\iota\Delta\omega t} - \omega_1^2\Gamma^*(\Delta\omega)[I_-,[I_+,\rho_S]]e^{2\iota\Delta\omega t} \tag{2.59}$$

$$-\omega_1^2\Gamma^*(\Delta\omega)[I_+,[I_-,\rho_S]] - \omega_1^2\Gamma(\Delta\omega)[I_-,[I_+,\rho_S]] \tag{2.60}$$

$$-p_+J(\omega)(\frac{1}{2}\{I_+I_-,\rho_S\} - I_-\rho_S I_+) - p_-J^*(\omega)(\frac{1}{2}\{I_-I_+,\rho_S\} - I_+\rho_S I_-) \tag{2.61}$$

Now, it's time to use Liouville formalism extensively. Instead of a matrix differential equation, using the Bra-Flipper Operator and superket property on the above equation, we have a vector differential equation that looks like-

$$\frac{d}{dt}|\rho_S(t)\rangle\rangle = \mathcal{L}(t)\,|\rho_S(t)\rangle\rangle \tag{2.62}$$

Here, $|\rho_S(t)\rangle\rangle$ is a 4-dimensional vector and $\mathcal{L}(t)$ is 4×4 super-operator.

Simulations of Bloch vectors using Quantum Master Equation 2.40

Taking initial density matrix and parameter as in the previous section, we can find $\rho_S(t)$. Instead of RK4 method, we can get to $\rho_S(t)$ in other way. Taking timestep Δt small enough,

$$\rho(t_{i+1}) = \exp\left(\Delta t \cdot \mathcal{L}(t_{i+1})\right) \cdot \rho(t_i) \tag{2.63}$$

From $t_{int} = 0$ to $t_{fin} = 15$ ms with $\Delta t = 0.1\mu$s, we evaluate $\rho_S(t)$ using 2.63. Now, $M_\alpha(t)$ can be evaluated according to the definition 2.38.
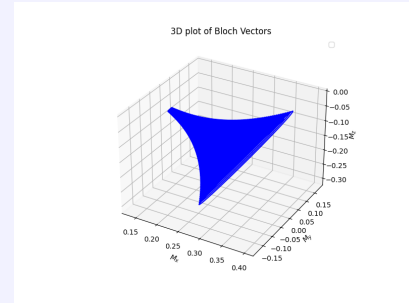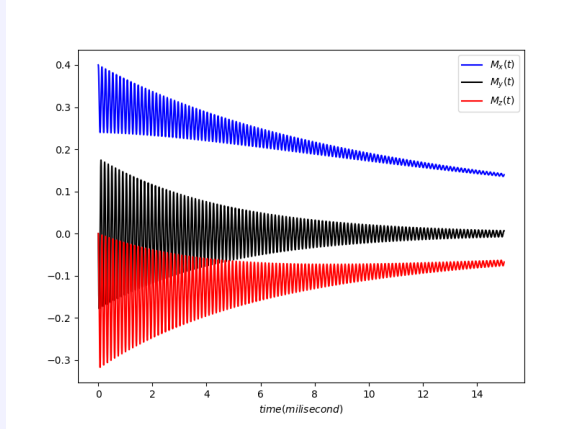
2.4.3 Fidelity between Initial And Final States

In Open Quantum Systems, our subsystem is subjected to decoherence due to environmental interactions. As shown in the previous two sections, Bloch matrices don't stay on the Bloch sphere surface but decay, which implies that the pure quantum state eventually becomes a mixed state.

Applying a z-direction Zeeman field induces a transition from the ground state to the excited state, an eigenstate of the system. However, the presence of a drive field causes the system to precess around an axis in the xy-plane, leading to a loss of coherence.

Furthermore, increasing ω_1 accelerates the decay of the system, while decreasing it exacerbates the effects of decoherence due to the system's interaction with the environment. As a result, the initially pure state of the system evolves into a mixed state, making it impossible to achieve an excited state in open quantum systems. *These conditions put our open quantum system into a speed limit while going from one state to another state contrary to the close quantum systems.*
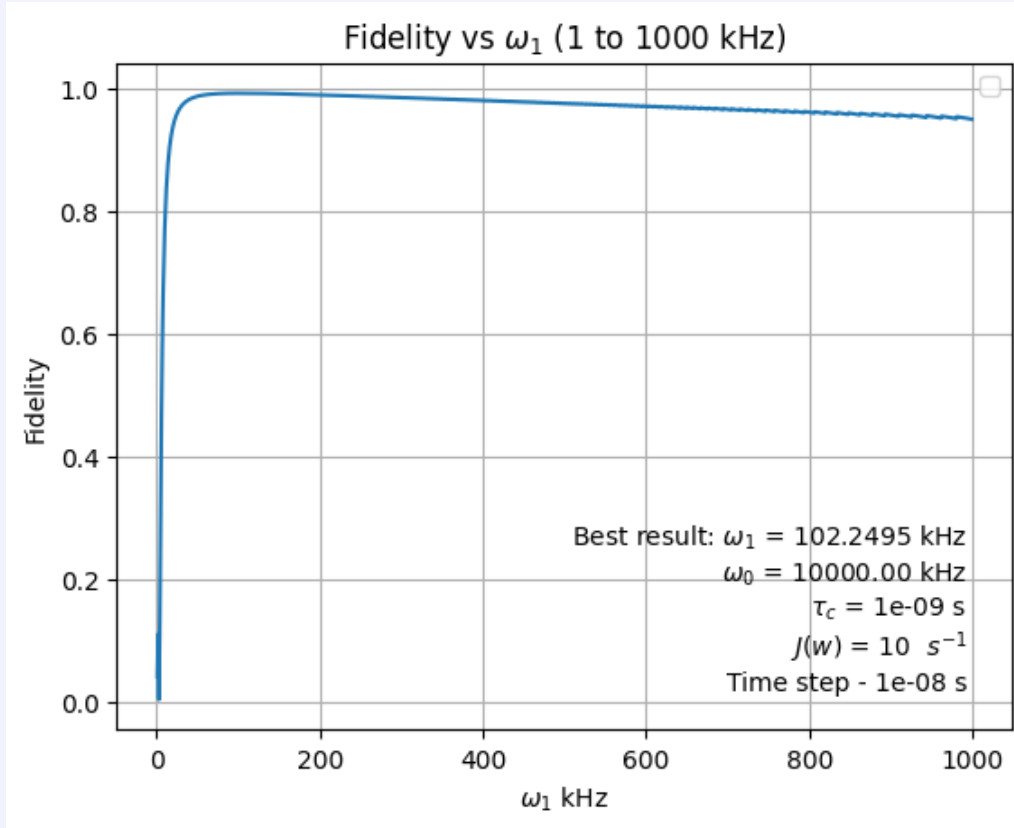

Finding ω_1 corresponded to the Maximum Fidelity

Let say, in discussed spin-1/2 ensemble, initially system is in the ground state, $|0\rangle$. so, initial density matrix(obviously a pure state) is,

$$\rho(0) = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{2.64}$$

There should be a particular ω_1 for which we can reach closest to our target state $|1\rangle$. Fidelity between initial ρ and final states σ, $F(\rho, \sigma) = \left(\mathrm{tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right)^2$ can be good measure how close the state is reaching to the final state. For any ρ and σ, $0 \leq F(\rho, \sigma) \leq 1$, and $F(\rho, \rho) = 1$.

For any ω_1, state would be the closest to the $|1\rangle$ at the first π rotation around the z-axis. Respecting the numerical purposes, we will evaluate the density matrices for every timestep $\Delta t = 10^{-8}s$ from $t_{int} = 0$ to $t_{fin} = 1.05 \cdot \dfrac{\pi}{\omega_1}s$ at some specific ω_1. Then, find where the state has the maximum fidelity $F_m(\omega_1)$. We then plot $F_m(\omega_1)$ vs ω_1.

Fidelity vs ω_1 (1 to 1000 kHz)

Best result: $\omega_1 = 102.2495$ kHz
$\omega_0 = 10000.00$ kHz
$\tau_c = 1e\text{-}09$ s
$J(w) = 10 \ s^{-1}$
Time step - 1e-08 s

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