On Quantum Master Equation and its application to driven dissipative two-level systems.

A report submitted in fulfilment of the Summer Internship

by

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Declaration

I, Pritish Karmakar, hereby declare that the summer internship report titled *"On Quantum Master Equation and its application to driven dissipative two-level systems"* is undertaken by me as a part of the Summer Internship under Prof. Rangeet Bhattacharyya at Indian Institute of Science Education & Research, Kolkata from 20.05.24 to 25.07.24. I affirm that the content of this report is based on my reading, research, and comprehension of the materials provided or recommended by my internship supervisor and all the information, quotations, or ideas taken from external sources have been duly acknowledged and cited.

I hereby submit this report in fulfilment of this summer internship and for further evaluation and assessment.

Sincerely,
Pritish Karmakar

भारतीय विज्ञान शिक्षा एव अनुसंधान संस्थान कोलकाता
(भारत सरकार के शिक्षा मंत्रालय के अधीन एक स्वायत्त संस्थान)
INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH KOLKATA
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TO WHOMSOEVER IT MAY CONCERN

This is to certify that

Pritish Karmakar

a student of

Indian Institute of Science Education and Research Kolkata

has satisfactorily completed a Summer Project
on

“Simulations of open quantum systems”

Under the supervision of

Rangeet Bhattacharyya

of

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Despite my best efforts, if any errors or inaccuracies are found in this report, I kindly request readers to inform me at pritishkarmakar7@gmail.com so that necessary corrections can be made.

Pritish Karmakar

On Quantum Master Equation and its application to driven dissipative two-level systems.

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Abstract

This report begins with discussing the evolution of open quantum systems and corresponding Quantum Master Equation (QME). The main emphasis is given to the Fluctuation Regulated Quantum Master Equation (FRQME) and its applications on the dynamics of driven dissipative two-level systems (TLS) and quantum optimal control of that TLS. I have also presented the results of numerical simulations for the solutions of the FRQME in the report.

Contents

1 Introduction

Open quantum system deals with the system which interacts with the environment or thermal reservoir, unlike the closed system which is completely isolated from the environmental interactions. A typical open

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quantum system is modeled by the Hamiltonian

$$H = H_S^\circ \otimes \mathbb{1} + \mathbb{1} \otimes H_R^\circ + H_{SR}$$

where H_S°, H_R° are the static Hamiltonian of system and reservoir respectively and H_{SR} is Hamiltonian corresponding to the interaction between system and reservoir (see figure 1). From the quantum mechanics we know

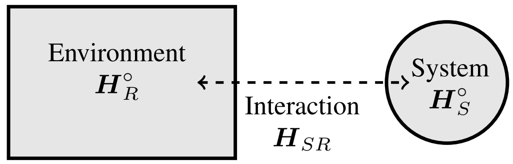


Figure 1: Schematic diagram of typical open quantum system.

that a closed system is evolved under unitary transformation, but in case of open system, if we look particularly the evolution of the subsystem of the total open system, it in general, is not dictated by unitary evolution. In the later section we will discuss the Quantum Master Equation, which describe the evolution of the system.

2 Theory on Quantum Master Equation (QME).

We will start with the microscopic derivation of Quantum master equation and briefly discuss about the Fluctuation regulated quantum master equation. We will not discuss the operator sum representation of quantum master equation here. Readers are requested to refer [3] or for a brief and concise discussion refer the previous term project report here.

2.1 Microscopic derivation of QME

Let our open quantum system can be described by the Hamiltonian,

$$H = H_S^\circ \otimes \mathbb{1} + \mathbb{1} \otimes H_R^\circ + H_{SR} \equiv H_S^\circ + H_R^\circ + H_{SR} \tag{2.1}$$

where H_S°, H_R° denote the static Hamiltonian of system and bath, respectively and H_{SR} denotes system-bath coupling Hamiltonian. And the corresponding Von-Neumann equation is

$$\dot{\rho}_T(t) = -i[H_T(t), \rho_T(t)] \tag{2.2}$$

We denote density operator of total system as

$$\rho_T = \rho_S \otimes \rho_R \tag{2.3}$$

where ρ_S and ρ_R denote the density operator of system and bath, respectively. We mostly work on interaction picture, so for a operator O in Hiesenberg picture, in interaction picture it is

$$\tilde{O}(t) = e^{i(H_S^\circ + H_R^\circ)t} O e^{-i(H_S^\circ + H_R^\circ)t}, \tag{2.4}$$

and

$$\tilde{\rho}_T(t) = e^{i(H_S^\circ + H_R^\circ)t} \rho_T(t) e^{-i(H_S^\circ + H_R^\circ)t}. \tag{2.5}$$

With this, the equation of motion is

$$\dot{\tilde{\rho}}_T(t) = -i[\tilde{H}_{SR}(t), \tilde{\rho}_T(t)] \tag{2.6}$$

$$\tilde{\rho}_T(t') = \tilde{\rho}_T(t) - i\int_t^{t'} dt_1 [\tilde{H}_{SR}(t_1), \tilde{\rho}_T(t_1)] \tag{2.7}$$

Iterating repeatedly, we get

$$\tilde{\rho}_T(t+\delta t) = \tilde{\rho}_T(t) - i\int_t^{t+\delta t} dt_1 [\tilde{H}_{SR}(t_1), \tilde{\rho}_T(t_1)] \tag{2.8}$$

$$\begin{aligned}\tilde{\rho}_T(t+\delta t) = \tilde{\rho}_T(t) &- i\int_t^{t+\delta t} dt_1 [\tilde{H}_{SR}(t_1), \tilde{\rho}_T(t)] \\ &- \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2 [\tilde{H}_{SR}(t_1), [\tilde{H}_{SR}(t_2), \tilde{\rho}_T(t_2)]]\end{aligned} \tag{2.9}$$

$$\begin{aligned}\tilde{\rho}_T(t+\delta t) = \tilde{\rho}_T(t) &- i\int_t^{t+\delta t} dt_1 [\tilde{H}_{SR}(t_1), \tilde{\rho}_T(t)] \\ &- \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2 [\tilde{H}_{SR}(t_1), [\tilde{H}_{SR}(t_2), \tilde{\rho}_T(t)]] + \mathcal{O}(H_{SR}^3)\end{aligned} \tag{2.10}$$

Following [1],[2] and [3] we will take couple of approximations and steps, as follows:

a. Weak coupling approximation

In this approximation we neglect the term of $\mathcal{O}(H_{SR}^3)$ due to weak coupling strength, i.e.,

$$\begin{aligned}\tilde{\rho}_T(t+\delta t) = \tilde{\rho}_T(t) &- i\int_t^{t+\delta t} dt_1 [\tilde{H}_{SR}(t_1), \tilde{\rho}_T(t)] \\ &- \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2 [\tilde{H}_{SR}(t_1), [\tilde{H}_{SR}(t_2), \tilde{\rho}_T(t)]]\end{aligned} \tag{2.11}$$

$$\begin{aligned}\tilde{\rho}_S(t+\delta t) = \tilde{\rho}_S(t) &- i\int_t^{t+\delta t} dt_1 \,\mathrm{Tr}_R[\tilde{H}_{SR}(t_1), \tilde{\rho}_T(t)] \\ &- \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2 \,\mathrm{Tr}_R[\tilde{H}_{SR}(t_1), [\tilde{H}_{SR}(t_2), \tilde{\rho}_T(t)]]\end{aligned} \tag{2.12}$$

b. Born-Markov approximation

Assuming the weak coupling strength, the system-bath correlation time τ_c is sufficiently small. We consider $\tilde{\rho}_R(t) = \mathrm{Tr}_S(\tilde{\rho}_T(t))$ does not evolve over the δt interval coarse-grained time scale, i.e.,

$$\tilde{\rho}_R(t+\delta t) = \tilde{\rho}_R(t) \quad \text{for} \quad \delta t \gg \tau_c. \tag{2.13}$$

We also consider the fact that $\delta t \ll \tau_s$ where τ_s is the timescale of the system. Finally the coarse-grain time interval is as follows:

$$\tau_c \ll \delta t \ll \tau_s \tag{2.14}$$

Let us define correlation density operator $\tilde{\rho}_{correl}$ as,

$$\tilde{\rho}_{corre}(t) = \tilde{\rho}_T(t) - \mathrm{Tr}_R(\tilde{\rho}_T(t)) \otimes \mathrm{Tr}_S(\tilde{\rho}_T(t)) = \tilde{\rho}_T(t) - \tilde{\rho}_S(t) \otimes \tilde{\rho}_R(t) \tag{2.15}$$

Let us assume that at $t = 0$, H_{SR} is just turned on. So just before $t = 0$, let

$$\tilde{\rho}_T(0) = \tilde{\rho}_S(0) \otimes \tilde{\rho}_R(0) \tag{2.16}$$

$$\tilde{\rho}_{correl}(0) = 0 \tag{2.17}$$

Now after δt time, keeping (2.14) and (2.13) in mind,

$$\tilde{\rho}_T(\delta t) \approx \tilde{\rho}_S(\delta t) \otimes \tilde{\rho}_R(\delta t) \approx \tilde{\rho}_S(0) \otimes \tilde{\rho}_R(\delta t) \tag{2.18}$$

$$\tilde{\rho}_{corre}(\delta t) \approx \tilde{\rho}_S(0) \otimes (\tilde{\rho}_R(\delta t) - \tilde{\rho}_R(0)) \approx 0 \tag{2.19}$$

Taking slightly stronger approximation, for a finite time $t = n\delta t$,

$$\tilde{\rho}_{corre}(t) = \tilde{\rho}_{corre}(n\delta t) = \tilde{\rho}_{corre}((n-1)\delta t) = \cdots = \tilde{\rho}_{corre}(\delta t) = 0 \tag{2.20}$$

$$\tilde{\rho}_R(t) = \tilde{\rho}_R(n\delta t) = \tilde{\rho}_R(0) = \tilde{\rho}_R^{eq} \tag{2.21}$$

which allow us to write the total density operator as

$$\tilde{\rho}_T(t) = \tilde{\rho}_S(t) \otimes \tilde{\rho}_R^{eq}. \tag{2.22}$$

The $\tilde{\rho}_R^{eq}$ can be taken as canonical thermal equilibrium density operator, i.e,

$$\rho_R^{eq} = \frac{1}{Z} \exp\left(-\frac{H_R^\circ}{k_b T}\right) \tag{2.23}$$

$$\tilde{\rho}_R^{eq} = \rho_R^{eq} \quad \text{as} \quad [H_R^\circ, \rho_R^{eq}] = 0. \tag{2.24}$$

c. Expression of coupling Hamiltonian.

We take the coupling Hamiltonian to be

$$H_{SB} = \sum_j A_j \otimes B_j \tag{2.25}$$

$$\tilde{H}_{SB}(t) = \sum_j \tilde{A}_j(t) \otimes \tilde{B}_j(t) \tag{2.26}$$

Then

$$\begin{aligned} \tilde{\rho}_S(t+\delta t) = \tilde{\rho}_S(t) - i \int_t^{t+\delta t} dt_1 [\tilde{A}_j(t_1), \tilde{\rho}_S(t)] \operatorname{Tr}\Big(\tilde{B}_j(t)\tilde{\rho}_R^{eq}\Big) \\ - \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2 \operatorname{Tr}_R[\tilde{H}_{SR}(t_1), [\tilde{H}_{SR}(t_2), \tilde{\rho}_T(t)]] \end{aligned} \tag{2.27}$$

We can always choose $\tilde{H}_{SR}$ such that $\langle B_j \rangle = \operatorname{Tr}(B_j \rho_R^{eq}) = \operatorname{Tr}\Big(\tilde{B}_j(t)\tilde{\rho}_R^{eq}\Big) = 0$, then

$$\tilde{\rho}_S(t+\delta t) = \tilde{\rho}_S(t) - \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2 \operatorname{Tr}_R[\tilde{H}_{SR}(t_1), [\tilde{H}_{SR}(t_2), \tilde{\rho}_T(t)]] \tag{2.28}$$

$$\begin{aligned} \frac{\delta \tilde{\rho}_S}{\delta t}(t) &= \frac{\tilde{\rho}_S(t+\delta t) - \tilde{\rho}_S(t)}{\delta t} \\ &= -\frac{1}{\delta t} \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2 \operatorname{Tr}_R[\tilde{H}_{SR}(t_1), [\tilde{H}_{SR}(t_2), \tilde{\rho}_T(t)]] \end{aligned} \tag{2.29}$$

d. Change of integrand variables

Change the variables as

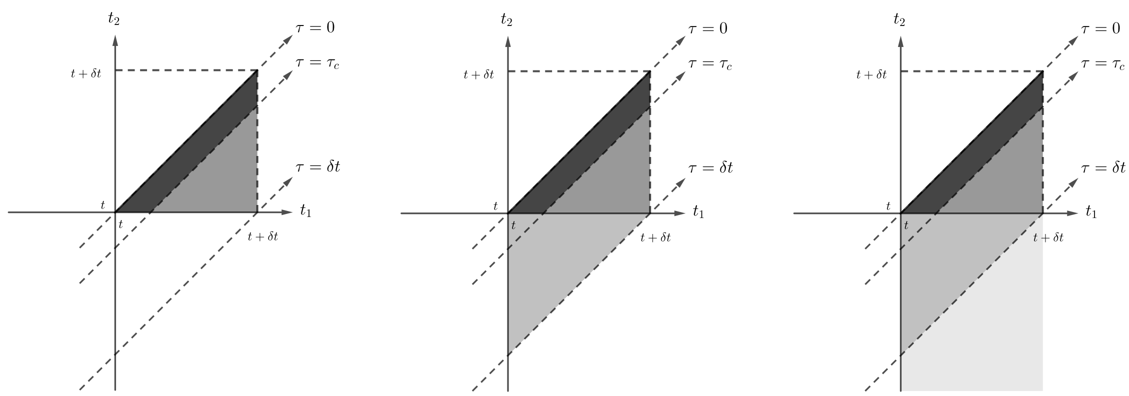
$$(t_1, t_2) \longrightarrow (t_1, \tau) \;\; \text{where} \;\; \tau = t_1 - t_2 \tag{2.30}$$

$$\int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2 \longrightarrow \int_0^{\delta t} d\tau \int_{t+\tau}^{t+\delta t} dt_1 \tag{2.31}$$

Considering $\tau > \tau_c$ has negligible contribution we can approximate the integral limit as (see Figure 2)

$$\int_0^{\delta t} d\tau \int_{t+\tau}^{t+\delta t} dt_1 \approx \int_0^{\delta t} d\tau \int_t^{t+\delta t} dt_1 \approx \int_0^{\infty} d\tau \int_t^{t+\delta t} dt_1 \tag{2.32}$$

Following that



(a) $\int_0^{\delta t} d\tau \int_{t+\tau}^{t+\delta t} dt_1$ (b) $\int_0^{\delta t} d\tau \int_t^{t+\delta t} dt_1$ (c) $\int_0^{\infty} d\tau \int_t^{t+\delta t} dt_1$

Figure 2: Figure shows the corresponding domain of the integration. Darkest shade in between $\tau = 0$ and $\tau = \tau_c$ has most significant contribution. With increase of τ, the contribution decrease rapidly.

$$\frac{\delta \tilde{\rho}_S}{\delta t}(t) = -\int_0^{\infty} d\tau \frac{1}{\delta t} \int_t^{t+\delta t} dt_1 \, \mathrm{Tr}_R[\tilde{H}_{SR}(t_1), [\tilde{H}_{SR}(t_1 - \tau), \tilde{\rho}_T(t)]] \tag{2.33}$$

$$= -\int_0^{\infty} d\tau \frac{1}{\delta t} \int_t^{t+\delta t} dt_1 \Big\{ [\tilde{A}_j(t_1), \tilde{A}_k(t_1 - \tau)\tilde{\rho}_S(t)] \, \mathrm{Tr}\Big(\tilde{B}_j(t_1)\tilde{B}_k(t_1 - \tau)\tilde{\rho}_R^{eq}\Big) - [\tilde{A}_j(t_1), \tilde{\rho}_S(t)\tilde{A}_k(t_1 - \tau)] \, \mathrm{Tr}\Big(\tilde{B}_k(t_1 - \tau)\tilde{B}_j(t_1)\tilde{\rho}_R^{eq}\Big) \Big\} \tag{2.34}$$

By cyclic property of Trace and $[H_R^{\circ}, \rho_R^{eq}] = 0$, one can show that

$$g_{jk}(\tau) = \mathrm{Tr}\Big(\tilde{B}_j(t_1)\tilde{B}_k(t_1 - \tau)\tilde{\rho}_R^{eq}\Big) = \mathrm{Tr}\Big(\tilde{B}_j(\tau)\tilde{B}_k(0)\tilde{\rho}_R^{eq}\Big) \tag{2.35}$$

$$g_{kj}(-\tau) = \mathrm{Tr}\Big(\tilde{B}_k(t_1 - \tau)\tilde{B}_j(t_1)\tilde{\rho}_R^{eq}\Big) = \mathrm{Tr}\Big(\tilde{B}_k(-\tau)\tilde{B}_j(0)\tilde{\rho}_R^{eq}\Big) = \mathrm{Tr}\Big(\tilde{B}_k(0)\tilde{B}_j(\tau)\tilde{\rho}_R^{eq}\Big) = g_{jk}^*(\tau) \tag{2.36}$$

which leads

$$\frac{\delta\tilde{\rho}_S}{\delta t}(t) = -\int_0^\infty d\tau \frac{1}{\delta t}\int_t^{t+\delta t} dt_1 \Big(g_{jk}(\tau)[\tilde{A}_j(t_1), \tilde{A}_k(t_1-\tau)\tilde{\rho}_S(t)] + g^*_{jk}(\tau)[\tilde{A}_j(t_1), \tilde{\rho}_S(t)\tilde{A}_k(t_1-\tau)]\Big). \tag{2.37}$$

This is a form of *quantum master equation*.

e. Spectral decomposition & Secular time approximation

We proceed by spectral decomposition of $\tilde{A}_j(t_1)$ in the energy eigenbasis of the system i.e., $\{|n\rangle\}$ with energy eigenvalue of $|n\rangle$ be $E_n = \omega_n$ and we get

$$\begin{aligned}
\tilde{A}_j(t_1) &= \sum_{m,n} \langle m|\tilde{A}_j(t_1)|n\rangle\, |m\rangle\langle n| \\
&= \sum_{m,n} e^{-i\omega_{nm}t} \langle m|A_j|n\rangle\, |m\rangle\langle n|\,, \quad \text{where } \omega_{nm} = \omega_n - \omega_m \\
&= \sum_{m,n} e^{-i\omega_{nm}t} A_j^{(m,n)}\, |m\rangle\langle n|\,, \quad \text{where } A_j^{(m,n)} = \langle m|A_j|n\rangle \\
&= \sum_{\omega} e^{-i\omega t}\Big(\sum_{\substack{m,n \\ \text{s.t., } \omega_{nm}=\omega}} A_j^{(m,n)}\, |m\rangle\langle n|\Big) \\
&= \sum_{\omega} e^{-i\omega t} A_j(\omega), \quad \text{where } A_j(\omega) \sum_{\substack{m,n \\ \text{s.t., } \omega_{nm}=\omega}} A_j^{(m,n)}\, |m\rangle\langle n|\,.
\end{aligned} \tag{2.38}$$

As A_j is Hermitian, we can write

$$\tilde{A}_j(t_1) = \sum_{\omega} e^{-i\omega t} A_j(\omega) = \sum_{\omega} e^{i\omega t} A_j^\dagger(\omega) \tag{2.39}$$

Now putting these expressions in the expression (2.37)

$$\begin{aligned}
\frac{\delta\tilde{\rho}_S}{\delta t}(t) &= -\int_0^\infty d\tau \frac{1}{\delta t}\int_t^{t+\delta t} dt_1 \Big(g_{jk}(\tau)[\tilde{A}_j(t_1), \tilde{A}_k(t_1-\tau)\tilde{\rho}_S(t)] - h.c.\Big) \\
&= -\sum_{\omega,\omega'} \int_0^\infty d\tau \frac{1}{\delta t}\int_t^{t+\delta t} dt_1 \Big(g_{jk}(\tau)[e^{i\omega t_1} A_j^\dagger(\omega), e^{-i\omega'(t_1-\tau)} A_k(\omega')\tilde{\rho}_S(t)]\Big) + h.c. \\
&= -\sum_{\omega,\omega'} \underbrace{\int_0^\infty d\tau\, g_{jk}(\tau) e^{i\omega'\tau}}_{\Gamma_{jk}(\omega')} \frac{1}{\delta t}\int_t^{t+\delta t} dt_1\, e^{-i(\omega'-\omega)t_1} [A_j^\dagger(\omega), A_k(\omega')\tilde{\rho}_S(t)] + h.c. \\
&= -\sum_{\omega,\omega'} \Gamma_{jk}(\omega')\, [A_j^\dagger(\omega), A_k(\omega')\tilde{\rho}_S(t)] \left(\frac{1}{\delta t}\int_t^{t+\delta t} dt_1\, e^{-i(\omega'-\omega)t_1}\right) + h.c.
\end{aligned} \tag{2.40}$$

From the above, we see t_1-dependant terms of the integrand in eq (2.37) are of the form $e^{-i(\omega'-\omega)t_1}$. The local time-average of terms like $e^{-i(\omega'-\omega)t_1}$ is

$$\frac{1}{\delta t}\int_t^{t+\delta t} dt_1 e^{i(\omega-\omega')t_1} = e^{i(\omega-\omega')t}\, e^{i(\omega-\omega')\delta t/2}\, \frac{\sin((\omega-\omega')\delta t/2)}{(\omega-\omega')\delta t/2} \tag{2.41}$$

$$\approx \begin{cases} e^{i(\omega-\omega')t}, & \text{if} \quad |\omega-\omega'|\,\delta t \ll 1 \\ 0, \quad \text{if} & |\omega-\omega'|\,\delta t \gg 1. \end{cases} \tag{2.42}$$

This is *secular time approximation*. We denote it as

$$\left(e^{i(\omega-\omega')t}\right)_{\text{sec}} = \begin{cases} e^{i(\omega-\omega')t}, & \text{if} \quad |\omega-\omega'|\,\delta t \ll 1 \\ 0, & \text{if} \quad |\omega-\omega'|\,\delta t \gg 1. \end{cases} \tag{2.43}$$

When considering of the secular approximation, we can get rid of time variable t_1 and the the QME is represented as

$$\frac{\delta\tilde{\rho}_S}{\delta t}(t) = -\int_0^\infty d\tau\,\Big(g_{jk}(\tau)[\tilde{A}_j(t),\tilde{A}_k(t-\tau)\tilde{\rho}_S(t)]_{\text{sec}} - h.c.\Big) \tag{2.44}$$

$$= -\sum_{\omega,\omega'}\Gamma_{jk}(\omega')\,[A_j^\dagger(\omega),A_k(\omega')\tilde{\rho}_S(t)]\,\left(e^{i(\omega-\omega')t}\right)_{\text{sec}} + h.c. \tag{2.45}$$

If we work with single frequency ω and $\omega=\omega'$, then the above QME is nicely written as

$$\frac{\delta\tilde{\rho}_S}{\delta t}(t) = -\Gamma_{jk}(\omega)\,[A_j^\dagger(\omega),A_k(\omega)\tilde{\rho}_S(t)] + \Gamma_{jk}^*(\omega)\,[A_j(\omega),\tilde{\rho}_S(t)A_k^\dagger(\omega)]. \tag{2.46}$$

- **QME in Schrodinger picture:**

The expression of QME discussed before is in interaction picture. In Schrodinger picture,

$$\rho_S(t) = e^{-iH_S^\circ t}\rho_T(t)e^{iH_S^\circ t} \tag{2.47}$$

Then [1]

$$\frac{\delta\rho_S(t)}{\delta t} = -i[H_S^\circ t,\rho_S(t)] + e^{-iH_S^\circ t}\frac{\delta\tilde{\rho}_S(t)}{\delta t}e^{iH_S^\circ t}$$
$$= -i[H_S^\circ t,\rho_S(t)] - \int_0^\infty d\tau\,\Big(g_{jk}(\tau)[A_j,e^{-iH_S^\circ t}A_k e^{iH_S^\circ t}\rho_S(t)]_{\text{sec}} - h.c.\Big) \tag{2.48}$$

- **QME in Liouville Space:**

Let the density operator $\tilde{\rho}_S$ represented as column vector form in Liouville space be $||\tilde{\rho}_S\rangle\rangle$ (For more about this, see Appendix A). Using the identity A.4 the QME (2.45) is written as

$$\frac{\delta}{\delta t}\,||\tilde{\rho}_S\rangle\rangle\,(t) = -\sum_{\omega,\omega'}\Gamma_{jk}(\omega')\,\left(e^{i(\omega-\omega')t}\right)_{\text{sec}}\,||[A_j^\dagger(\omega),A_k(\omega')\tilde{\rho}_S(t)]\rangle\rangle\; + h.c.$$
$$= \mathfrak{L}(t)\,||\tilde{\rho}_S(t)\rangle\rangle \tag{2.49}$$

where $\mathfrak{L}$ is called the *Lindbladian*, and the expression of the Lindbladian is

$$\mathfrak{L}(t) = -\sum_{\omega,\omega'}\Big\{\Gamma_{jk}(\omega')\,\left(e^{i(\omega-\omega')t}\right)_{\text{sec}}\Big(A_j^\dagger(\omega)A_k(\omega')\otimes\mathbb{1} - A_j^\dagger(\omega)\otimes A_k^T(\omega')\Big)$$
$$-\Gamma_{jk}^*(\omega')\,\left(e^{-i(\omega-\omega')t}\right)_{\text{sec}}\Big(A_j^\dagger(\omega)\otimes A_k^*(\omega') - \mathbb{1}\otimes A_j^T(\omega)A_k^*(\omega')\Big)\Big\} \tag{2.50}$$

For further extension and modification of the QME in the later sections, we will primarily follow the microscopic derivation as it give more physical understanding about the system.

[1] Considering $\frac{\delta\rho_S(t)}{\delta t}$ behaves same as $\frac{d\rho_S(t)}{dt}$.

2.2 QME with external drive

In a type of problems where there is external drive on the system, the Hamiltonian is

$$H = H_S^\circ \otimes \mathbb{1} + \mathbb{1} \otimes H_R^\circ + H_{SR} + H_D(t) \otimes \mathbb{1} \equiv H_S^\circ + H_R^\circ + H_{SR} + H_D(t) \tag{2.51}$$

where $H_D(t)$ denotes Hamiltonian corresponding external drive. Let $H_{\text{eff}}(t) = H_{SR} + H_D(t)$, then

$$H = H_S^\circ + H_R^\circ + H_{\text{eff}}(t) \tag{2.52}$$

Then analogous to the eq (2.12), we have

$$\begin{aligned} \tilde{\rho}_S(t+\delta t) &= \tilde{\rho}_S(t) - i\int_t^{t+\delta t} dt_1 \, \mathrm{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \tilde{\rho}_T(t)] \\ &\quad - \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2 \, \mathrm{Tr}_R[\tilde{H}_{\text{eff}}(t_1), [\tilde{H}_{eff}(t_2), \tilde{\rho}_T(t)]] \end{aligned} \tag{2.53}$$

$$\begin{aligned} \frac{\delta\tilde{\rho}_S}{\delta t}(t) &= -\frac{i}{\delta t}\int_t^{t+\delta t} dt_1 \, \mathrm{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \tilde{\rho}_T(t)] \\ &\quad - \frac{1}{\delta t}\int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2 \, \mathrm{Tr}_R[\tilde{H}_{\text{eff}}(t_1), [\tilde{H}_{\text{eff}}(t_2), \tilde{\rho}_T(t)]] \end{aligned} \tag{2.54}$$

Using the fact that $\langle B_j \rangle = \mathrm{Tr}\Big(\tilde{B}_j(t)\tilde{\rho}_R^{eq}\Big) = 0$ and following the similar prescription shown before, one can show that

$$\begin{aligned} \frac{\delta\tilde{\rho}_S}{\delta t}(t) &= -\frac{i}{\delta t}\int_t^{t+\delta t} dt_1 [\tilde{H}_D(t_1), \tilde{\rho}_S(t)] \\ &\quad - \int_0^\infty d\tau \frac{1}{\delta t}\int_t^{t+\delta t} dt_1 [\tilde{H}_D(t_1), [\tilde{H}_D(t_1-\tau), \tilde{\rho}_s(t)]] \\ &\quad - \int_0^\infty d\tau \frac{1}{\delta t}\int_t^{t+\delta t} dt_1 \, \mathrm{Tr}_R[\tilde{H}_{SR}(t_1), [\tilde{H}_{SR}(t_2), \tilde{\rho}_T(t)]] \end{aligned} \tag{2.55}$$

$$\begin{aligned} \frac{\delta\tilde{\rho}_S}{\delta t}(t) &= -i[\tilde{H}_D(t), \tilde{\rho}_S(t)]_{\text{sec}} - \int_0^\infty d\tau [\tilde{H}_D(t), [\tilde{H}_D(t-\tau), \tilde{\rho}_s(t)]]_{\text{sec}} \\ &\quad - \int_0^\infty d\tau \Big(g_{jk}(\tau)[\tilde{A}_j(t_1), \tilde{A}_k(t_1-\tau)\tilde{\rho}_S(t)]_{\text{sec}} - h.c.\Big) \end{aligned} \tag{2.56}$$

Now using the prescription given before, one can easily write the equation in Lindbladian form.

- **A second approach:**

Analogous to the (2.8),

$$\tilde{\rho}_S(t+\delta t) = \tilde{\rho}_S(t) - i\int_t^{t+\delta t} dt_1 \, \mathrm{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \tilde{\rho}_T(t_1)] \tag{2.57}$$

$$= \tilde{\rho}_S(t) - i\int_t^{t+\delta t} dt_1 \, \mathrm{Tr}_R[\tilde{H}_{\text{eff}}(t_1), U(t_1,t)\tilde{\rho}_T(t)U^\dagger(t_1,t)] \tag{2.58}$$

where

$$U(t_1,t) = T\exp\Big(-i\int_t^{t_1} dt_2 \tilde{H}_{\text{eff}}(t_2)\Big) \tag{2.59}$$

In interaction picture, we know

$$\frac{d}{dt_1}U(t_1,t) = -i\tilde{H}_{\text{eff}}(t_1)U(t_1,t) \tag{2.60}$$

$$U(t_1,t) = \mathbb{1} - i\int_t^{t_1} dt_2\, \tilde{H}_{\text{eff}}(t_2)\, U(t_2,t) \tag{2.61}$$

$$= \mathbb{1} - i\int_t^{t_1} dt_2\, \tilde{H}_{\text{eff}}(t_2) \, + \mathcal{O}(\tilde{H}_{\text{eff}}^2) \tag{2.62}$$

and putting this expression in (2.58) we get

$$\begin{aligned}\tilde{\rho}_S(t+\delta t) = \tilde{\rho}_S(t) - i\int_t^{t+\delta t} dt_1\, \text{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \tilde{\rho}_T(t)] \\ - \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2\, \text{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \tilde{H}_{\text{eff}}(t_2)\tilde{\rho}_T(t)] \\ - \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2\, \text{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \tilde{\rho}_T(t_2)\tilde{H}_{\text{eff}}(t)] + \mathcal{O}(\tilde{H}_{\text{eff}}^3)\end{aligned} \tag{2.63}$$

which leads to the same expression as (2.54).

2.3 Fluctuation Regulated Quantum Master Equation (FRQME)

In most practical cases environmental fluctuations present in open quantum system. Here, we will follow the prescription given in [4]. In this problem, the total Hamiltonian is

$$H = H_S^\circ \otimes \mathbb{1} + \mathbb{1} \otimes H_R^\circ + H_{SR} + H_D \otimes \mathbb{1} + \mathbb{1} \otimes H_R \equiv H_S^\circ + H_R^\circ + H_{SR} + H_D + H_{st} \tag{2.64}$$

where H_{st} denotes stochastic Hamiltonian corresponding to local environmental fluctuations. We define H_{st} as

$$H_{st}(t) = \sum_j f_j(t)\, |\phi_j\rangle\langle\phi_j| \tag{2.65}$$

where $\{|\phi_j\rangle\}$ is the eigenbasis of H_R° with eigen values $\{\epsilon_j\}$, and $f_j(t)$'s are independent, Gaussian, δ-correlated white noises with

$$\overline{f_j(t)} = 0 \tag{2.66}$$

$$\overline{f_j(s)f_k(t)} = \kappa^2\, \delta(s-t)\, \delta_{j,k} \tag{2.67}$$

To get the QME for this case, we follow the second approach in the previous section so that we can incorporate the effect of the environmental fluctuation and look from the perspective of ensemble average of the dynamical evolution. The concerned time-scale of the problem is that of (2.14). Let

$$V(t) = H_{\text{eff}}(t) + H_{st}(t) = H_{SR} + H_D(t) + H_{st}(t) \tag{2.68}$$

Analogous to the (2.58),

$$\tilde{\rho}_S(t+\delta t) = \tilde{\rho}_S(t) - i\int_t^{t+\delta t} dt_1\, \text{Tr}_R[\tilde{V}(t_1), \tilde{\rho}_T(t_1)] \tag{2.69}$$

$$= \tilde{\rho}_S(t) - i\int_t^{t+\delta t} dt_1\, \text{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \tilde{\rho}_T(t_1)], \quad \text{as } [\tilde{H}_{st}, \tilde{\rho}_R^{eq}] = 0 \tag{2.70}$$

$$= \tilde{\rho}_S(t) - i\int_t^{t+\delta t} dt_1\, \text{Tr}_R[\tilde{H}_{\text{eff}}(t_1), U(t_1,t)\tilde{\rho}_T(t)U^\dagger(t_1,t)] \tag{2.71}$$

where

$$U(t_1,t) = T\exp\left(-i\int_t^{t_1} dt_2 \tilde{V}(t_2)\right) \tag{2.72}$$

$$\Rightarrow \quad \frac{d}{dt_1}U(t_1,t) = -i\tilde{V}(t_1)U(t_1,t) \tag{2.73}$$

$$\Rightarrow \quad U(t_1,t) = \mathbb{1} - i\int_t^{t_1} dt_2\, \tilde{V}(t_2)\, U(t_2,t) \tag{2.74}$$

$$= \mathbb{1} - i\int_t^{t_1} dt_2\, \tilde{H}_{st}(t_2)\, U(t_2,t) - i\int_t^{t_1} dt_2\, \tilde{H}_{\text{eff}}(t_2)\, U(t_2,t) \tag{2.75}$$

$$= U_{st}(t_1,t) - i\int_t^{t_1} dt_2\, \tilde{H}_{\text{eff}}(t_2)\, U(t_2,t) \tag{2.76}$$

where

$$U_{st}(t_1,t) = T\exp\left(-i\int_t^{t_1} dt_2 \tilde{H}_{st}(t_2)\right) \Rightarrow U_{st}(t_1,t) = \mathbb{1} - i\int_t^{t_1} dt_2\, \tilde{H}_{st}(t_2)\, U_{st}(t_2,t) \tag{2.77}$$

Moreover, we know timescale of the noises is far less than that of $\tilde{H}_{\text{eff}}$ and $(t_2 - t) \leq \delta t \ll \tau_s$, which follows

$$U(t_2,t) = T\exp\left(-i\int_t^{t_2} dt_3 \tilde{V}(t_3)\right) \approx T\exp\left(-i\int_t^{t_2} dt_3 \tilde{H}_{st}(t_3)\right) = U_{st}(t_2,t). \tag{2.78}$$

Incorporating all the trickery steps we finally get

$$U(t_1,t) = U_{st}(t_1,t) - i\int_t^{t_1} dt_2\, \tilde{H}_{\text{eff}}(t_2)\, U_{st}(t_2,t). \tag{2.79}$$

and putting it in (2.71) we get

$$\begin{aligned}\tilde{\rho}_S(t+\delta t) = \tilde{\rho}_S(t) &- i\int_t^{t+\delta t} dt_1\, \text{Tr}_R[\tilde{H}_{\text{eff}}(t_1), U_{st}(t_1,t)\tilde{\rho}_T(t)U_{st}^\dagger(t_1,t)] \\ &- \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2\, \text{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \tilde{H}_{\text{eff}}(t_2)U_{st}(t_2,t)\tilde{\rho}_T(t)U_{st}^\dagger(t_1,t)] \\ &+ \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2\, \text{Tr}_R[\tilde{H}_{\text{eff}}(t_1), U_{st}(t_1,t)\tilde{\rho}_T(t)U_{st}^\dagger(t_2,t)\tilde{H}_{\text{eff}}(t_2)] + \mathcal{O}(\tilde{H}_{\text{eff}}^3)\end{aligned} \tag{2.80}$$

But we are interested in ensemble average of the evolution of the density operator, which means

$$\tilde{\rho}_S(t+\delta t) = \tilde{\rho}_S(t) - i\int_t^{t+\delta t} dt_1\, \text{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \overline{U_{st}(t_1,t)\tilde{\rho}_T(t)U_{st}^\dagger(t_1,t)}] \tag{2.81}$$

$$\begin{aligned}&- \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2\, \text{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \tilde{H}_{\text{eff}}(t_2)\overline{U_{st}(t_2,t)\tilde{\rho}_T(t)U_{st}^\dagger(t_1,t)}] \\ &+ \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2\, \text{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \overline{U_{st}(t_1,t)\tilde{\rho}_T(t)U_{st}^\dagger(t_2,t)}\tilde{H}_{\text{eff}}(t_2)]\end{aligned} \tag{2.82}$$

Now we need to find the ensemble average of those quantities.

$$\begin{aligned}\overline{U_{st}(t_2,t)\tilde{\rho}_T(t)U_{st}^\dagger(t_1,t)} &= \tilde{\rho}_S(t) \otimes \sum_j \frac{e^{-\beta\epsilon_j}}{Z}\, |\phi_j\rangle\langle\phi_j|\, \overline{\exp\left(i\int_{t_2}^{t_1} dt_3 f_j(t_3)\right)} \\ &= \exp\left(-\frac{\kappa^2}{2}(t_1 - t_2)\right)\tilde{\rho}_T(t) \quad \text{using (C.13)}\end{aligned} \tag{2.83}$$

Similarly,

$$\overline{U_{st}(t_1,t)\tilde{\rho}_T(t)U_{st}^{\dagger}(t_2,t)} = \exp\left(-\frac{\kappa^2}{2}(t_1-t_2)\right)\tilde{\rho}_T(t),\ \overline{U_{st}(t_1,t)\tilde{\rho}_T(t)U_{st}^{\dagger}(t_1,t)} = \tilde{\rho}_T(t) \tag{2.84}$$

Finally putting this in (2.82) and identifying $2/\kappa^2$ as τ_c (correlation time), we obtain

$$\begin{aligned}\tilde{\rho}_S(t+\delta t) = \tilde{\rho}_S(t) - i\int_t^{t+\delta t} dt_1\, \mathrm{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \tilde{\rho}_T(t)] \\ - \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2\, \mathrm{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \tilde{H}_{\text{eff}}(t_2)\tilde{\rho}_T(t)] \\ - \int_t^{t+\delta t} dt_1 \int_t^{t_1} dt_2\, \mathrm{Tr}_R[\tilde{H}_{\text{eff}}(t_1), \tilde{\rho}_T(t_2)\tilde{H}_{\text{eff}}(t)]\ \exp\left(-\frac{t_1-t_2}{\tau_c}\right)\end{aligned} \tag{2.85}$$

Doing the procedure shown multiple times before

$$\frac{\delta\tilde{\rho}_S}{\delta t}(t) = -i[\tilde{H}_D(t), \tilde{\rho}_S(t)]_{\text{sec}} - \int_0^{\infty} d\tau\, \mathrm{Tr}_R[\tilde{H}_{\text{eff}}(t), [\tilde{H}_{\text{eff}}(t-\tau), \tilde{\rho}_T(t)]]_{\text{sec}}\, e^{-\tau/\tau_c} \tag{2.86}$$

$$\begin{aligned}= -i[\tilde{H}_D(t), \tilde{\rho}_S(t)]_{\text{sec}} - \int_0^{\infty} d\tau [\tilde{H}_D(t), [\tilde{H}_D(t-\tau), \tilde{\rho}_S(t)]]_{\text{sec}}\, e^{-\tau/\tau_c} \\ - \int_0^{\infty} d\tau\, \mathrm{Tr}_R[\tilde{H}_{SR}(t), [\tilde{H}_{SR}(t-\tau), \tilde{\rho}_S(t)\otimes\tilde{\rho}_R^{eq}]]_{\text{sec}}\, e^{-\tau/\tau_c}\end{aligned} \tag{2.87}$$

we obtain *Fluctuation regulated Quantum Master Equation*.

3 Applications using FRQME

Application of the QME is diverse. This report is particularly focused on two level system (TLS).

3.1 Driven dissipative TLS

We consider a scenario of a TLS (take spin-1/2 system) in a constant z-magnetic field with a nearly resonating oscillatory perturbative drive (x-magnetic field). Here we will reproduce the results in [4] and visualize the dynamics of the system and concerned observable. The different quantities of the Hamiltonian are as follows

$$H_S^{\circ} = \omega_0 I_z, \tag{3.1}$$

$$H_D = 2\omega_1\cos(\omega t)I_x \quad \text{with } \omega \approx \omega_0, \tag{3.2}$$

$$H_{SR} = \omega_{SR}(I_+R_- + I_-R_+ + I_zR_z) \tag{3.3}$$

Let $\omega - \omega_0 = \delta\omega$ and $\omega + \omega_0 = \Omega$, then in interaction picture,

$$\begin{aligned}\tilde{H}_D &= e^{i\omega_0 tI_z}\ H_D\ e^{-i\omega_0 tI_z} \\ &= \frac{\omega_1}{2}e^{i\omega_0 tI_z}\left(e^{i\omega t} + e^{-i\omega t}\right)\left(I_+ + I_-\right)e^{-i\omega_0 tI_z} \\ &= \omega_1(F_x^C(t) + F_x^R(t))\end{aligned} \tag{3.4}$$

where

$$F_x^C = e^{i\Omega tI_z}I_x e^{-i\Omega tI_z} = \frac{\omega_1}{2}(I_+e^{i\Omega t} + I_-e^{-i\Omega t}) \tag{3.5}$$

$$F_x^R = e^{i\delta\omega tI_z}I_x e^{-i\delta\omega tI_z} = \frac{\omega_1}{2}(I_+e^{-i\delta\omega t} + I_-e^{i\delta\omega t}) \tag{3.6}$$

Our task is to find the evolution of a state with time. The time scale of our problem is

$$\tau_c \ll \delta t \ll \omega_1^{-1}, \omega_{SR}^{-1} \tag{3.7}$$

$$\omega_0^{-1} \ll \delta t \ll \delta\omega^{-1} \tag{3.8}$$

which leads

$$\left(e^{\pm i\omega t}\right)_{\text{sec}} = 0, \left(e^{\pm i\omega_1 t}\right)_{\text{sec}} = 0, \left(e^{\pm i\Omega t}\right)_{\text{sec}} = 0, \tag{3.9}$$

$$\left(e^{\pm i\delta\omega t}\right)_{\text{sec}} = e^{\pm i\delta\omega t} \tag{3.10}$$

Calculating first order drive term in the FRQME 2.87 using the secular approximation stated before,

$$\begin{aligned}\mathbf{I}_D &= -i[\tilde{H}_D(t), \tilde{\rho}_S(t)]_{\text{sec}} \\ &= -i\frac{\omega_1}{2}\Big(e^{-i\delta\omega t}\,[I_+, \tilde{\rho}_S(t)] + e^{i\delta\omega t}\,[I_-, \tilde{\rho}_S(t)]\Big)\end{aligned} \tag{3.11}$$

$$\mathfrak{L}_D^{(1)}(t)\,||\tilde{\rho}_S(t)\rangle\rangle \equiv -i\frac{\omega_1}{2}\Big(e^{-i\delta\omega t}\,\hat{I}_+ + e^{i\delta\omega t}\,\hat{I}_-\Big)\,||\tilde{\rho}_S(t)\rangle\rangle \tag{3.12}$$

The equivalent Lindbladian form is also given where $\hat{I}_\pm = I_\pm \otimes \mathbb{1} - \mathbb{1} \otimes I_\mp$ (see Appendix A). The second order drive term is

$$\begin{aligned}\mathbf{II}_D &= -\int_0^\infty d\tau[\tilde{H}_D(t), [\tilde{H}_D(t-\tau), \tilde{\rho}_S(t)]]_{\text{sec}}\, e^{-\tau/\tau_c} \\ &= -\frac{\omega_1^2}{4}\Big((\Gamma(\Omega) + \Gamma^*(\delta\omega))\,[I_+, [I_-, \tilde{\rho}_S(t)]] + (\Gamma^*(\Omega) + \Gamma(\delta\omega))\,[I_-, [I_+, \tilde{\rho}_S(t)]] \\ &\qquad + \Gamma(\delta\omega)\,e^{-i2\delta\omega t}\,[I_+, [I_+, \tilde{\rho}_S(t)]] + \Gamma^*(\delta\omega)\,e^{i2\delta\omega t}\,[I_-, [I_-, \tilde{\rho}_S(t)]]\Big) \\ \mathfrak{L}_D^{(2)}(t)\,||\tilde{\rho}_S(t)\rangle\rangle &\equiv -\frac{\omega_1^2}{4}\Big((\Gamma(\Omega) + \Gamma^*(\delta\omega))\,\hat{I}_+\hat{I}_- + (\Gamma^*(\Omega) + \Gamma(\delta\omega))\,\hat{I}_-\hat{I}_+ \\ &\qquad + \Gamma(\delta\omega)\,e^{-i2\delta\omega t}\,\hat{I}_+\hat{I}_+ + \Gamma^*(\delta\omega)\,e^{i2\delta\omega t}\,\hat{I}_-\hat{I}_-\Big)\,||\tilde{\rho}_S(t)\rangle\rangle\end{aligned} \tag{3.13}$$

where

$$\Gamma(\nu) = \int_0^\infty d\tau e^{i\nu t} e^{-\tau/\tau_c} = \frac{\tau_c}{1 - i\nu\tau_c} = \Gamma^*(-\nu) \tag{3.14}$$

Now we have to calculate the second order coupling term. The Hamiltonian in interaction picture is

$$\tilde{H}_{SR} = \omega_{SR}(e^{i\omega_0 t} I_+ \tilde{R}_- + e^{-i\omega_0 t} I_- \tilde{R}_+ + I_z R_z) \tag{3.15}$$

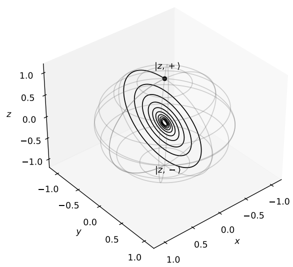
Following the prescription given in [6], and neglecting the Lamb-shift Hamiltonian we get

$$\begin{aligned}\mathbf{II}_{SR} &= -\int_0^\infty d\tau\,\mathrm{Tr}_R[\tilde{H}_{SR}(t), [\tilde{H}_{SR}(t-\tau), \tilde{\rho}_S(t) \otimes \tilde{\rho}_R^{eq}]]_{\text{sec}}\, e^{-\tau/\tau_c} \\ &= -J(\omega_0)\left(\frac{1}{2}\{I_- I_+, \tilde{\rho}_R^{eq}\} - I_+ \tilde{\rho}_R^{eq} I_-\right) - K(\omega_0)\left(\frac{1}{2}\{I_- I_+, \tilde{\rho}_R^{eq}\} - I_+ \tilde{\rho}_R^{eq} I_-\right) \\ &\quad - j(0)\left(\frac{1}{4}\tilde{\rho}_R^{eq} - I_z \tilde{\rho}_R^{eq} I_z\right) \\ \mathfrak{L}_{SR}\,||\tilde{\rho}_S(t)\rangle\rangle &\equiv -\Big(\frac{J(\omega_0)}{2}\,(I_+ I_- \otimes \mathbb{1} + \mathbb{1} \otimes I_+ I_- - 2I_- \otimes I_-) \\ &\quad + \frac{K(\omega_0)}{2}\,(I_- I_+ \otimes \mathbb{1} + \mathbb{1} \otimes I_+ I_+ - 2I_+ \otimes I_+) \\ &\quad + \frac{j(0)}{4}(\mathbb{1} \otimes \mathbb{1} - 4I_z \otimes I_z)\Big)\,||\tilde{\rho}_S(t)\rangle\rangle\end{aligned} \tag{3.16}$$

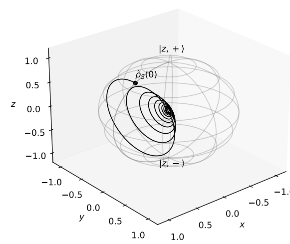
where $J(\omega_0), K(\omega_0)$ and $j(0)$ are some constants. Combining all the quantities, our FRQME for the problem is

$$\frac{\delta}{\delta t}\,||\tilde{\rho}_S(t)\rangle\rangle = (\mathfrak{L}_D^{(1)}(t) + \mathfrak{L}_D^{(2)}(t) + \mathfrak{L}_{SR})\,||\tilde{\rho}_S(t)\rangle\rangle \tag{3.17}$$

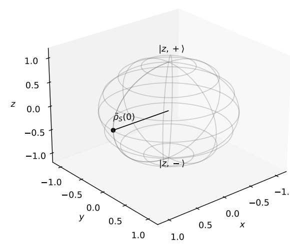
Taking different initial states and solving FRQME numerically by 4th order Runge-Kutta (RK4) we visualize the trajectory of the state in Bloch sphere in figure 3.



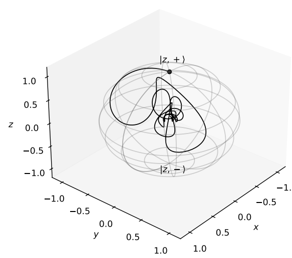
(a) $|\psi(0)\rangle = |z,+\rangle$



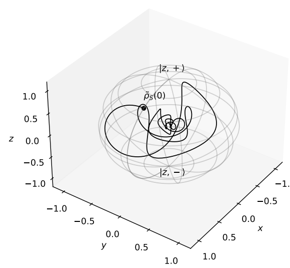
(b) $|\psi(0)\rangle = \frac{3}{5}\,|x,+\rangle + \frac{4}{5}\,|z,+\rangle$



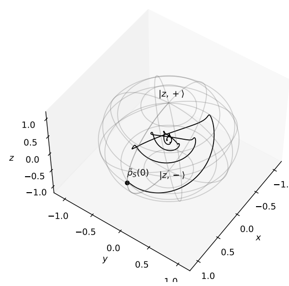
(c) $|\psi(0)\rangle = |x,+\rangle$



(d) $|\psi(0)\rangle = |z,+\rangle$



(e) $|\psi(0)\rangle = \frac{3}{5}\,|x,+\rangle + \frac{4}{5}\,|z,+\rangle$



(f) $|\psi(0)\rangle = |x,+\rangle$

Figure 3: Figure shows the trajectory for different initial states $\tilde{\rho}_S(0) = |\psi(0)\rangle\langle\psi(0)|$. The values of different parameters are $\omega_0 = 200\pi$ MHz, $\omega_1 = 20\pi$ KHz, $T_1 = 10$ ms, $T_2 = 0.2$ ms, $\tau_c = 0.1$ μs. For figure 3a, 3b and 3c the $\delta\omega = 0$, but for figure 3d, 3e and 3f the $\delta\omega = 10\pi$ KHz.

Now we are interested in looking the observable I_x, I_y and I_z (magnetic moments). As mentioned in [4], heterodyne detection followed by low-pass filter is equivalent to measuring in co-rotating frame with ω frequency. So the observables I_α we want to measure in co-rotating frame are as follows,

$$M_\alpha(t) = \langle e^{-i\omega t I_z} I_\alpha e^{i\omega t I_z}\rangle = \mathrm{Tr}\big(e^{-i\omega t I_z} I_\alpha e^{i\omega t I_z}\tilde{\rho}_S(t)\big) = \mathrm{Tr}\big(F_\alpha^R(t)\tilde{\rho}_S(t)\big) \tag{3.18}$$

Now

$$\frac{d}{dt}M_\alpha(t) = \mathrm{Tr}\left(\tilde{\rho}_S(t)\,\frac{d}{dt}F_\alpha^R(t)\right) + \mathrm{Tr}\left(F_\alpha^R(t)\,\frac{\delta}{\delta t}\tilde{\rho}_S(t)\right) \tag{3.19}$$

Following [6] we get the differential equations,

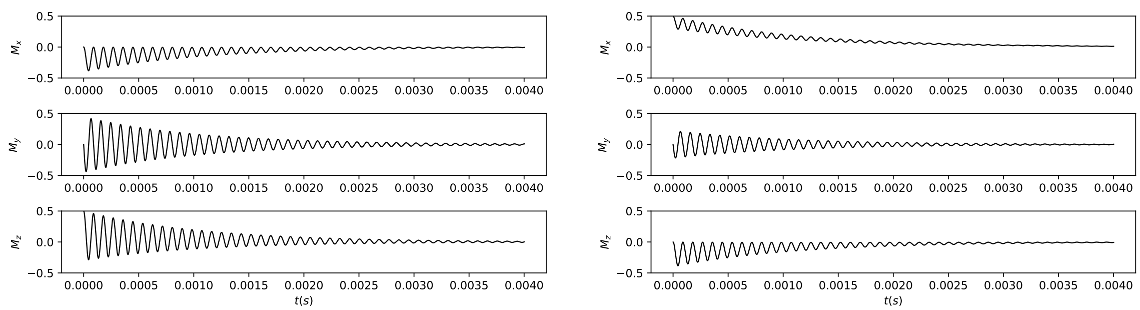
$$\frac{d}{dt}\begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix} = \begin{pmatrix} -\eta_x - 1/T_2 & \delta\omega - \delta\omega_C & 0 \\ \delta\omega_C - \delta\omega_R - \delta\omega & -\eta_y - 1/T_2 & -\omega_1 \\ 0 & \omega_1 & -\eta_z - 1/T_1 \end{pmatrix}\begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix} + \frac{1}{T_1}\begin{pmatrix} 0 \\ 0 \\ M_0 \end{pmatrix} \tag{3.20}$$

where

$$\delta\omega_C = \frac{1}{2}\Big(\frac{\omega_1^2\Omega\tau_c^2}{1+\Omega^2\tau_c^2}\Big),\ \delta\omega_R = \frac{\omega_1^2\delta\omega\tau_c^2}{1+\delta\omega^2\tau_c^2},\ \eta_x = \frac{1}{2}\Big(\frac{\omega_1^2\tau_c}{1+\Omega^2\tau_c^2}\Big),$$
$$\eta_y = \frac{1}{2}\Big(\frac{\omega_1^2\tau_c}{1+\Omega^2\tau_c^2}\Big) + \frac{\omega_1^2\tau_c}{1+\delta\omega^2\tau_c^2},\ \eta_Z = \frac{\omega_1^2\tau_c}{1+\Omega^2\tau_c^2} + \frac{\omega_1^2\tau_c}{1+\delta\omega^2\tau_c^2},$$
$$\frac{1}{T_1} = J(\omega_0) + K(\omega_0),\ \frac{1}{T_1} = \frac{1}{2}(J(\omega_0) + K(\omega_0) + j(0)), \tag{3.21}$$

the constants T_1, T_2 are the relaxation times and M_0 is equilibrium magnetic moment.

Taking different initial magnetic moments and solving the above coupled differential equation by RK4, we plot the variation of observables in the figure 4. Note that the value of M_0 is taken as zero as after very long time, our final state will approach to maximally mixed state i.e., $\tilde{\rho}_S(t\to\infty) = \frac{1}{2}\mathbb{1}$ due to decoherence.



(a) $\vec{M}(0) = (0, 0, 0.5)$ (b) $\vec{M}(0) = (0.5, 0, 0)$

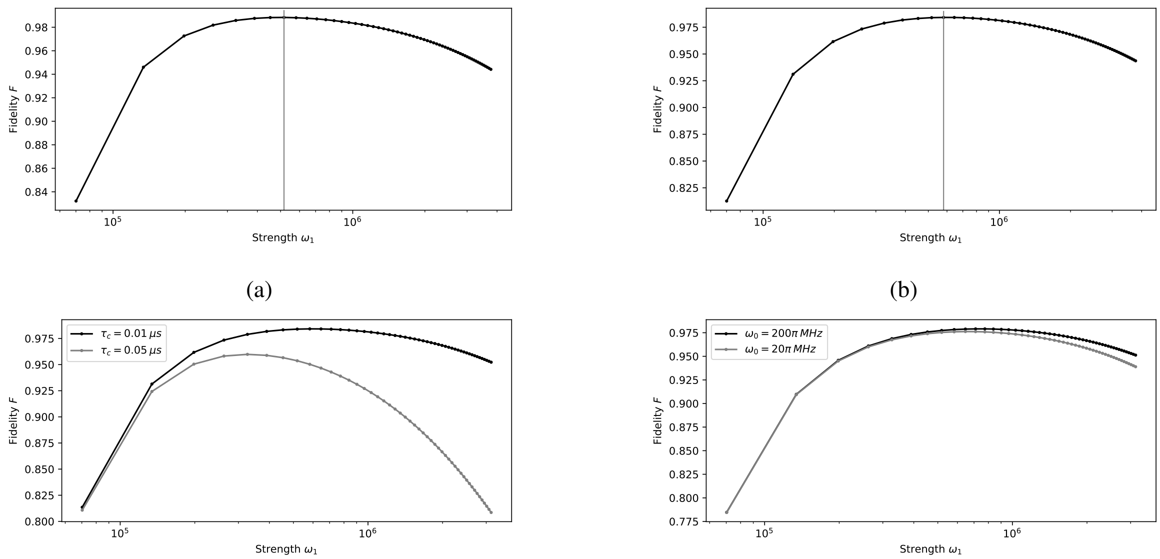
Figure 4: Variation of observable M_x, M_y and M_z with time for different initial magnetic moments $\vec{M}(0) = (M_x(0), M_y(0), M_z(0))$. The values of different parameters are $\omega_0 = 200\pi$ MHz, $\omega_1 = 20\pi$ KHz, $\delta\omega = 10\pi$ KHz, $T_1 = 50$ ms, $T_2 = 1$ ms, $\tau_c = 0.1\ \mu$s, $M_0 = 0$.

3.2 Maximum fidelity drive strength

Fidelity is a measure of the 'distance' between two operator in a Liouville space. Let σ and ρ be two operator in Liouville space then the fidelity in between them is defined as

$$F(\sigma,\rho) = \Big(\mathrm{Tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\Big)^2 \tag{3.22}$$

In this section we want to find the optimum drive strength ω_1 for which we can achieve the maximum fidelity between the the final state and desired target state. We start from the state $|z,+\rangle$ and drive the system by $\sim\pi/2$ pulse (not exactly $\pi/2$, but slightly more than that) of varying strength ω_1 and find the maximum fidelity between the final state evolved by the FRQME and target state $|z,-\rangle$ for each strength ω_1 and plot it in the figure 5.We see that initially in lower frequency the fidelity is rising as the first order drive term is dominant over the other two but, in higher frequency the second order drive term and the coupling term dominate which leads to the net decrease in fidelity. In between this, we achieve the optimal strength. We also see that with increase the correlation time τ_c the plot decays faster as the extent of environment fluctuation effect increases. Another observation is that the plot is not significantly changing with the change of ω_0. These are the notable observations.



(a) (b)

(c) (d)

Figure 5: Figures show the variation of fidelity with strength ω_1. For the figure 5a, we do not consider coupling Hamiltonian of FRQME during calculation but in 5b we have the full FRQME. Optimal strength ω_1 is shown by the vertical line in both plot. Figure 5c and 5d show the variation of plot for two different τ_c and two different ω_0, respectively. Primary values of the parameters are $\omega_0 = 200\pi\,\text{MHz}$, $\omega_1 = 20\pi\,\text{KHz}$, $\delta\omega = 10\pi\,\text{KHz}$, $T_1 = 10\,\text{ms},\ T_2 = 0.2\,\text{ms},\ \tau_c = 0.01\,\mu\text{s}$.

3.3 Quantum optimal control of spin-1/2 system

In the previous section, we discussed how controlling the drive strength can achieve high fidelity. However, in that scenario, the number of control parameters is very limited, as we can only adjust the drive strength and not its direction. In this section we desire to get maximum fidelity within a fixed time window. To attain higher fidelity, we will vary the direction of the drive throughout its evolution in the given time window in a optimal way. Here, we will discuss how we can achieve this by following the Gradient Ascent Pulse Engineering (or GRAPE) algorithm. For the GRAPE algorithm, we follow the method outlined in [7] and [8], and apply that to our driven dissipative system of spin-1/2. In this case our drive Hamiltonian is parameterized by two control parameter ω_x and ω_y, as follows

$$H_D(t|\omega_x, \omega_y) = 2\omega_x \cos(\omega t) I_x + 2\omega_y \cos(\omega t) I_y \tag{3.23}$$

which allow us to change the direction of the drive. In interaction picture,

$$\begin{aligned}\tilde{H}_D(t) &= \omega_x (F_x^C(t) + F_x^R(t)) + \omega_y (F_y^C(t) + F_y^R(t)) \\ &= \frac{1}{2}\Big(\omega_d^*\, e^{i\Omega t}\, I_+ + \omega_d\, e^{-i\Omega t}\, I_- + \omega_d^*\, e^{i\delta\omega t}\, I_+ + \omega_d\, e^{i\delta\omega t}\, I_-\Big)\end{aligned} \tag{3.24}$$

where $\omega_d = \omega_x + i\,\omega_y$. Using this, the first and second order drive term of the FRQME in Lindbladian form are,

$$\mathfrak{L}_D^{(1)}(t) = -\frac{i}{2}\Big(\omega_d^*\, e^{-i\delta\omega t}\, \hat{I}_+ + \omega_d\, e^{i\delta\omega t}\, \hat{I}_-\Big) \tag{3.25}$$

$$\mathfrak{L}_D^{(2)}(t) = -\frac{1}{4}\Big(|\omega_d|^2\, (\Gamma(\Omega) + \Gamma^*(\delta\omega))\, \hat{I}_+\hat{I}_- + |\omega_d|^2\, (\Gamma^*(\Omega) + \Gamma(\delta\omega))\, \hat{I}_-\hat{I}_+ + \omega_d^{*2}\, \Gamma(\delta\omega)\, e^{-i2\delta\omega t}\, \hat{I}_+\hat{I}_+ + \omega_d^2\, \Gamma^*(\delta\omega)\, e^{i2\delta\omega t}\, \hat{I}_-\hat{I}_-\Big) \tag{3.26}$$

and the coupled term $\mathfrak{L}_{SR}$ is same as before. Let us define $\mathfrak{L}_D(t) = \mathfrak{L}_D^{(1)}(t) + \mathfrak{L}_D^{(2)}(t)$ which is controled by the control parameter ω_x and ω_y. To get the maximum fidelity we will vary the ω_x and ω_y throughout its evolution as stated before. Then the FRQME and its solution is given by

$$\frac{\delta}{\delta t}\, ||\tilde{\rho}_S(t)\rangle\rangle = (\mathfrak{L}_D(t|\omega_d(t)) + \mathfrak{L}_{SR})\, ||\tilde{\rho}_S(t)\rangle\rangle \tag{3.27}$$

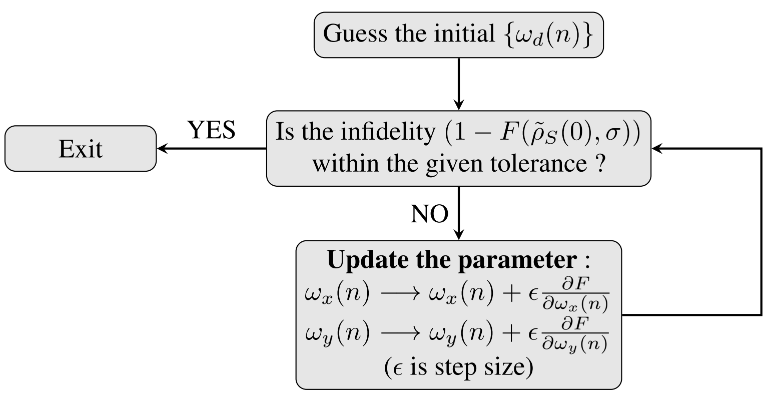
$$||\tilde{\rho}_S(t)\rangle\rangle = T\ \exp\bigg(\int_0^t dt_1\, (\mathfrak{L}_D(t_1|\omega_d(t_1)) + \mathfrak{L}_{SR})\bigg)\, ||\tilde{\rho}_S(0)\rangle\rangle \tag{3.28}$$

Although we will not vary $\omega_d(t)$ continuously as it is not feasible for numerical calculation or experimental purpose. We divide the time window (say from 0 to T) in N equal sub-window of length T/N, and will keep the value of $\omega_d(t)$ constant in each sub-window. Let $\omega_d(n)$ be the complex drive frequency which is constant in the nth subwindow, i.e. from $(n-1)T/N$ to nT/N. Then the solution of the FRQME is modified to

$$||\tilde{\rho}_S(t)\rangle\rangle = T\ \exp\left(\sum_{n=1}^{N}\int_{(n-1)T/N}^{nT/N} dt_1\, (\mathfrak{L}_D(t_1|\omega_d(n)) + \mathfrak{L}_{SR})\right) ||\tilde{\rho}_S(0)\rangle\rangle \tag{3.29}$$

Our task is to optimize the set of parameters $\{\omega_d(n)\}$, such that fidelity $F(\tilde{\rho}_S(0), \sigma)$ is maximum, where σ is the target state.

The optimization of $\{\omega_d(n)\}$ by GRAPE algorithm is in a loop as follows:



The key step of the GRAPE algorithm is the updating the parameter and calculating the gradient of fidelity $\{\frac{\partial F}{\partial \omega_x(n)}, \frac{\partial F}{\partial \omega_y(n)}\}$. *The numerical implementation of this algorithm for our problem has not been completed due to time constraint.*

4 Conclusions

I have presented a brief overview of dynamics of open quantum systems, the Quantum Master Equation, the Fluctuation Regulated Quantum Master Equation and showed the dynamics of the driven dissipative TLS through numerical simulation of FRQME and infer from the simulation plots. We gave a brief introduction to the quantum optimal control over the specified system. I hope this report serves as a foundation for further studies in understanding the complex dynamics of open quantum systems.

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Appendices

A Liouvillean formalism

Here we will very briefly discuss about Liouville space, density matrix in Liouville space and some properties required for the report. For detailed explanation, readers are requested to refer to [5]. As we know that a pure state can be represented as a element ('ket' state) of a Hilbert space ($\mathcal{H}$). But a mixed state being 'weighted average' of multiple ket states, cannot be represented as an single element of Hilbert space. Here comes the Liouville space. A Liouville space ($\mathcal{L}$) is a inner product space in which all the operators of a Hilbert space ($\mathcal{H}$) reside. So for any $|\psi\rangle, |\phi\rangle \in \mathcal{H}$, the operator

$$O = \sum_{\phi,\psi} |\phi\rangle\langle\psi| \in \mathcal{L}. \tag{A.1}$$

Sometimes the elements of Liouville space be represented in a column vector form

$$||O\rangle\rangle = \sum_{\phi,\psi} |\phi\rangle \otimes |\psi\rangle^* \tag{A.2}$$

For a 1-qubit state, it is

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} \longleftrightarrow ||\rho\rangle\rangle = \begin{pmatrix} \rho_{11} \\ \rho_{12} \\ \rho_{21} \\ \rho_{22} \end{pmatrix} \tag{A.3}$$

Now the following identity we will discuss, is very important and frequently utilized. For operators $A, B, C \in \mathcal{L}$, the column vector form of $ABC \in \mathcal{L}$ i.e., $||ABC\rangle\rangle$ is written as

$$||ABC\rangle\rangle = (A \otimes C^T)\,||B\rangle\rangle\,. \tag{A.4}$$

Using this identity, we can write the Von-Neumann equation for $||\rho\rangle\rangle$,

$$\dot{\rho}(t) = -i[H(t), \rho(t)] \tag{A.5}$$

$$\begin{aligned} ||\dot{\rho}\rangle\rangle(t) &= -i\,||[H(t), \rho(t)]\rangle\rangle \\ &= -i\,||\Big(H(t)\rho(t) - \rho(t)H(t)\Big)\rangle\rangle \\ &= -i\Big(||H(t)\rho(t)\mathbb{1}\rangle\rangle - ||\mathbb{1}\rho(t)H(t)\rangle\rangle\Big) \\ &= -i\Big(H(t)\otimes\mathbb{1} - \mathbb{1}\otimes H^T(t)\Big)\,||\rho(t)\rangle\rangle\,. \end{aligned} \tag{A.6}$$

So we can write any commutator of the form

$$||[H(t), \rho(t)]\rangle\rangle = \hat{H}(t)\,||\rho(t)\rangle\rangle \tag{A.7}$$

where $\hat{H}(t)$ is called the *superoperator* (in this context its *Lindbladian*) with

$$\hat{H}(t) = H(t)\otimes\mathbb{1} - \mathbb{1}\otimes H^T(t). \tag{A.8}$$

Now we look for the solution of the following equation

$$||\dot{\rho}\rangle\rangle(t) = \hat{H}(t)\,||\rho(t)\rangle\rangle \tag{A.9}$$

which is

$$||\rho(t)\rangle\rangle = T\ \exp\left(\int_0^t ds\,\hat{H}(s)\right)||\rho(0)\rangle\rangle \tag{A.10}$$

B Time ordering operator

Often we encounter the unitary propagator of a system with Hamiltonian H, in the form of

$$U(T, T_0) = T\ \exp\left(-i\int_{T_i}^{T_f} dt_1 H(t_1)\right) \tag{B.1}$$

where T is a time ordering operator. A time ordering operator operates on Hamiltonian as follows:

$$T(H(t_{\pi_1})H(t_{\pi_2})\dots H(t_{\pi_n})) = H(t_1)H(t_2)\dots H(t_n) \tag{B.2}$$

where π is any permutation of $\{1, 2, \dots, n\}$ and $t_1 > t_2 > \cdots > t_n$. For example, if $t_1 > t_2$,

$$T(H(t_1)H(t_2)) = T(H(t_2)H(t_1)) = H(t_1)H(t_2) \tag{B.3}$$

As $\{1, 2, \dots, n\}$ can be permuted in $n!$ different ways, there are $n!$ ways one can get the same result. We do not consider the cases when any two times become equal i.e., $t_i = t_j$, as they form measure-zero set. Now to justify the expression of unitary propagator, take two cases:

Case 1: H(t) does not commutes each other for different t.
Then

$$\begin{aligned} U(T_f, T_i) &= T\ \exp\left(-i\int_{T_i}^{T_f} dt_1 H(t_1)\right) \\ &= \mathbb{1} + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} T\left(\int_{T_f}^{T_i} dt_1 \cdots \int_{T_f}^{T_i} dt_n H(t_1)\dots H(t_n)\right) \end{aligned} \tag{B.4}$$

And by the fact that there are $n!$ different set of values of $\{t_1, \dots, t_n\}$ for which we get the same result of $T(H(t_1)\dots H(t_n))$, one can show that

$$T\left(\int_{T_f}^{T_i} dt_1 \cdots \int_{T_f}^{T_i} dt_n H(t_1)\dots H(t_n)\right) = n! \int_{T_f}^{T_i} dt_1 \int_{T_f}^{t_1} dt_2 \cdots \int_{T_f}^{t_{n-1}} dt_n H(t_1)\dots H(t_n) \tag{B.5}$$

using the result,

$$U(T_f, T_i) = \mathbb{1} + \sum_{n=1}^{\infty} (-i)^n \int_{T_f}^{T_i} dt_1 \int_{T_f}^{t_1} dt_2 \cdots \int_{T_f}^{t_{n-1}} dt_n H(t_1)\dots H(t_n) \tag{B.6}$$

we recover the *Dyson series*.

Case 2: H(t) commutes each other for different t.
This means $H(t_{\pi_1})H(t_{\pi_2})\dots H(t_{\pi_n}) = H(t_1)H(t_2)\dots H(t_n)$. For any $\{t_1, \dots, t_n\}$, we have

$$T(H(t_1)H(t_2)\dots H(t_n)) = H(t_1)H(t_2)\dots H(t_n) \tag{B.7}$$

this follows

$$\begin{aligned} U(T_f, T_i) &= T\ \exp\left(-i\int_{T_i}^{T_f} dt_1 H(t_1)\right) \\ &= \mathbb{1} + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{T_f}^{T_i} dt_1 H(t_1) \cdots \int_{T_f}^{T_i} dt_n H(t_n) \\ &= \mathbb{1} + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \left(\int_{T_f}^{T_i} dt_1 H(t_1)\right)^n = \exp\left(-i\int_{T_i}^{T_f} dt_1 H(t_1)\right) \end{aligned} \tag{B.8}$$

C Kubo cumulant expansion

Kubo cumulant expansion is a very useful mathematical tool when we work with Hamiltonian having a stochastic part. Consider as an example our Hamiltonian described in the hilbert space $\mathcal{H}$ be

$$H = H^{\circ}(t) + H_{st}(t) \tag{C.1}$$

where H°, H_{st} be the non-stochastic and stochastic part of the Hamiltonian. The propagator in this case is

$$U(t) = T\ \exp\left(-i\int_0^t dt_1 H(t_1)\right). \tag{C.2}$$

Starting with a state $|\psi(0)\rangle \in \mathcal{H}$, in a later time the state will be

$$|\psi(t)\rangle = U(t)\,|\psi(0)\rangle \tag{C.3}$$

Due to the presence of stochastic term in Hamiltonian, the final state will have a probability distribution in Hilbert space (there is no certainty that the initial state will reach to a particular final state with unit probability). But we are interested in the 'statistical ensemble average' of the final states. To get the ensemble average of final state i.e., $\overline{|\psi(t)\rangle}$, we have to take the ensemble average of the propagator such that,

$$\overline{|\psi(t)\rangle} = \overline{U(t)}\,|\psi(0)\rangle \tag{C.4}$$

Let,

$$\overline{U(t)} = \overline{T\ \exp\left(-i\int_0^t dt_1 H(t_1)\right)} = e^{k(t)} \tag{C.5}$$

Now look at the RHS of the above expression. We first do Taylor series expansion of the function $k(t)$ around $t = 0$, then we put that into the expression in RHS.

$$k(t) = \sum_{n=1} \frac{(-i)^n}{n!} k_n t^n, \quad k_0 = 0 \text{ as } \overline{U(0)} = \mathbb{1} \tag{C.6}$$

$$\begin{aligned} e^{k(t)} &= \mathbb{1} + \sum_{m=1} \frac{k^m(t)}{m!} \\ &= \mathbb{1} + \sum_{m=1} \frac{1}{m!}\Big(\sum_{n=1} \frac{(-i)^n}{n!} k_n t^n\Big)^n \\ &= \mathbb{1} - ik_1 t - \frac{1}{2}(k_2 - k_1^2)t^2 + \mathcal{O}(t^3) \end{aligned} \tag{C.7}$$

Now from the expression (B.4), we get

$$\overline{U(t)} = \mathbb{1} + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} T\left(\int_0^t dt_1 \cdots \int_0^t dt_n \overline{H(t_1)\dots H(t_n)}\right) \tag{C.8}$$

and comparing above two expressions, we get,

$$k_1 = \frac{1}{t}\int_0^t dt_1\ \overline{H(t_1)} \tag{C.9}$$

$$k_2 = \frac{1}{t^2}\ T\left(\int_0^t \int_0^t dt_1 dt_2\ \overline{H(t_1)H(t_2)}\right) - k_1^2. \tag{C.10}$$

and so on. Now writing the ensemble-averaged propagator

$$
\begin{aligned}
\overline{U(t)} &= \overline{T\ \exp\left(-i\int_0^t dt_1 H(t_1)\right)} = e^{k(t)} \\
&\approx \exp\left\{-i\int_0^t dt_1 \overline{H(t_1)} - \frac{1}{2}\ T\left(\int_0^t\int_0^t dt_1 dt_2 \overline{H(t_1)H(t_2)}\right) + \left(\int_0^t dt_1\ \overline{H(t_1)}\right)^2\right\}
\end{aligned} \tag{C.11}
$$

This is *Kubo cumulant expansion*. The advantage of this expansion is that we need to know the average value and the autocorrelation function of the Hamiltonian.

The integration we will encounter in this report is of the form

$$
\overline{\exp\left(\pm i\int_{t_2}^{t_1} dt_3 f_j(t_3)\right)} \quad \text{with } t_1 \geq t_2 \text{ and } \begin{cases} \overline{f_j(t)} = 0 \\ \overline{f_j(s) f_j(t)} = \kappa^2\ \delta(s-t) \end{cases} \tag{C.12}
$$

then using (C.11),

$$
\begin{aligned}
\overline{\exp\left(\pm i\int_{t_2}^{t_1} dt_3\ f_j(t_3)\right)} &\approx \exp\left\{-\frac{1}{2}\int_{t_2}^{t_1}\int_{t_2}^{t_1} dt_3 dt_4\ \overline{f_j(t_3) f_j(t_4)}\right\} \\
&= \exp\left\{-\frac{\kappa^2}{2}\int_{t_2}^{t_1}\int_{t_2}^{t_1} dt_3 dt_4\ \delta(t_3 - t_4)\right\} \\
&= \exp\left\{-\frac{\kappa^2}{2}(t_1 - t_2)\right\}
\end{aligned} \tag{C.13}
$$