Thermalization in Open Quantum Systems

A Thesis

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by

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Certificate

This is to certify that this dissertation entitled *Thermalization in Open Quantum Systems* towards the partial fulfillment of the BS-MS dual degree program at the Indian Institute of Science Education and Research, Pune, represents study/work carried out by Lokendra Singh Rathore at Indian Institute of Science Education and Research under the supervision of Sachin Jain, Department of Physics, Indian Institute of Science Education and Research, Pune, during the academic year 2023-2024.

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I dedicate this thesis to my parents for their endless love, support, and encouragement throughout my pursuit of education.

Declaration

I hereby declare that the matter embodied in the report entitled *Thermalization in Open Quantum Systems* are the results of the work carried out by me at the Department of Physics, Indian Institute of Science Education and Research, Pune, under the supervision of Sachin Jain and the same has not been submitted elsewhere for any other degree. Wherever others contribute, every effort is made to indicate this clearly, with due reference to the literature and acknowledgment of collaborative research and discussions.

L. Skethone

Lokendra Singh Rathore

List of Publications

This thesis is based on a pre-print that was written during the period of my MS research project.

1. Sakil Khan, Lokendra Singh Rathore, and Sachin Jain, "Steady state correlation function beyond the standard weak coupling limit and consistency with KMS relation", arxiv: 2401.16488 [quant-ph].

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Abstract

The thermalization of a system when interacting with a thermal bath poses an interesting problem. If a system eventually reaches a thermal state in the long-time limit, it is expected that its density matrix would resemble the mean-force Gibbs state. Moreover, the correlation function must satisfy the Kubo-Martin-Schwinger (KMS) condition or equivalently the Fluctuation-Dissipation Relation (FDR). In this work, we derive a formal expression for the non-Markovian two-point function within the context of the weak coupling limit. Using this expression, we explicitly compute the two-point function for specific models, demonstrating their adherence to the KMS condition. Additionally, we have formulated a non-perturbative approach in the form of a self-consistent approximation that includes partial resummation of perturbation theory. This approach can capture strong coupling phenomena while still relying on simple equations. Notably, we verify that the two-point function obtained through this method also satisfies the KMS condition. Another important idea discussed in this thesis is how perturbing around the thermal equilibrium helps us learn about dynamics far from equilibrium. Specifically, we demonstrate derived constraints on the master equation for open quantum systems from the positivity of the production of relative von Neumann entropy for small perturbations around the thermal equilibrium. We further show that these constraints are equivalent to the thermalization and stability constraints. Drawing motivation from recent work on hydrodynamics, we illustrate how the poles of the Green's function for the open system capture the spectrum of the Liouvillian governing open system dynamics.

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Part I

Introduction

Chapter 1

Introduction

In recent times, there has been a considerable amount of effort in developing quantum technologies, especially quantum computing. Understanding phenomena such as decoherence and entanglement is of fundamental importance for this purpose. Open quantum systems have served as a good realistic model for studying such phenomena. Therefore, understanding the process of thermalization in microscopic quantum systems in contact with a thermal quantum environment is an important problem. It has applications ranging from quantum technologies to the dynamics of black holes and that of the entire expanding universe.

We say that a certain quantity of the system has reached a steady state if its value has reached very close to an equilibrium value. At the same time, what one calls equilibrium is usually less than what's referred to as thermal equilibrium; in other words, not all systems in steady state have reached thermal equilibrium. The thermal state of a system is characterized by a few parameters such as temperature or chemical potential.

Consequently, in the process of going to thermal equilibrium, the system's local observables forget the information about the system's initial state. In recent times, there has been a growing interest in understanding the conditions and mechanisms governing thermalization in quantum many-body systems. In quantum many-body systems, the Eigenstate Thermalization Hypothesis (ETH) explains the conditions under which quantum many-body systems thermalize. Using the eigenstates of the many-body Hamiltonian as a tool to understand the dynamics, the Eigenstate thermalization Hypothesis states that if a quantum system at a given temperature indeed thermalizes for any initial state, then it should thermalize when any of the Hamiltonian eigenstates is its initial state, i.e. any eigenstates of many-body hamiltonian are thermal.

In recent times, there has been a growing interest in understanding the conditions and mechanisms governing the thermalization of a small (microscopic) open quantum system [1-9]. If the system's degrees of freedom are negligible compared to the bath degrees of freedom, one would naively expect that the system will go to a steady state at the long time limit. However, before addressing the question of whether the stationary state is thermal or not, it is necessary to identify criteria that allow a clear-cut detection of thermodynamic

equilibrium conditions in the stationary state. The precise density matrix state for an open quantum system is given by the Mean Force State. For correlation functions, the thermality constraint is known as the KMS condition.

In the first half of this thesis, we focus on the idea that perturbing the system around thermal equilibrium helps us learn about important features of the dynamics out of equilibrium. We first demonstrate how the Lindblad Master equation is constrained by the requirement of consistency with the Second Law of thermodynamics. That is, we demand the positivity of relative von Neumann entropy production for Open system dynamics. This gives us certain equality and inequality constraints on the coefficients of the Master equation. Then, we also look at thermalization and CPTP (Completely Positive Trace Preserving) constraints and show that the constraints from the positivity of entropy production reproduce the constraints from thermalization and stability.

Then, we demonstrate an abstract derivation of a general form for the retarded Green's function for a general model. Using this derivation, we systematically illustrate that the poles of the retarded Green's functions encapsulate the spectrum of the Liouvillian governing the density matrix dynamics. Moving forward, we extend this demonstration to any higher-order retarded correlation function, explaining how the poles of an n-point retarded Green's function capture the Liouvillian's spectrum. This result can be generalized to any out-of-time-ordered correlation function and its corresponding spectrum of the Liouvillian.

Moving forward, it is important to consider not only the static properties of the density matrix of the system, which describes its stationary state but also the dynamics of fluctuations. These fluctuations are encoded, for example, in the two-time correlation function (adhering to the KMS relation). More precisely, at the long time limit, (a) the density matrix of the system should be the mean-force density matrix [10, 11], and (b) the correlation function of the system at the long time must satisfy the KMS condition or equivalently the Fluctuation-Dissipation Relation (FDR) [1, 2, 12, 13].

A lot of work has already been done to address the first issue [10, 11]. However, till now, the discussion about the second issue is very limited in the literature. To fill this gap, in this paper, our central focus will be to answer this question as clearly as possible.

Except for exactly solvable models like Caldeira-Leggett [14], we generally resort to approximate techniques to explicitly compute the correlation function. In this context, it remains unclear whether the approximate correlation function adheres to the FDR, or, in other words, which approximation may violate it. Addressing this, L. Sieberer et al. [15, 16] recently discussed the constraints and symmetries imposed on the total Swinger-Keldysh (SK) action or, equivalently, on the total system-bath Hamiltonian. These constraints guide the system toward thermalization at the long time limit.

We employed an approximate technique called the image operator method [17–19]. We use this method to calculate the two-point correlation function, and then we explicitly demonstrate that the correlation function satisfies the KMS relation. However, it's important to note that the applicability of this method is limited to specific examples; it does not universally guarantee the satisfaction of the KMS relation for a generic system. Furthermore, the validity of this method is contingent upon the assumption of weak system-bath coupling.

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To go beyond the standard weak coupling limit, in the next part of our paper, we have developed a self-consistent non-perturbative technique[20–29], namely the self-consistent Born approximation [30, 31] or the NCA approach, following the Swinger-Keldysh path integral. Using this technique, we abstractly show that the correlation function must obey the FDR relation for a general class of systems. The FDR follows from the KMS relation [32, 33]. More precisely, the FDR is equivalent to a combination of quantum mechanical time reversal and the KMS condition [15].

Thermalization in Open Quantum Systems

Chapter 2

Preliminaries

Before delving into the work, I would like to present the basics of Open Quantum Systems and define thermalization in terms of the state and correlation functions of the system. This will allow us to concretely define thermalization and assess how accurately different techniques for calculating states and correlation functions describe the thermalization of open quantum systems.

2.1 Open Quantum Systems

An open quantum system is a quantum-mechanical system that interacts with an external quantum system, which is known as the environment or a bath. We can always write down the Hamiltonian of the total system as $H = H_S + H_R + \lambda H_{SR}$, where H_S is the Hamiltonian of the system of interest, H_R represents the Hamiltonian for the reservoir (bath), and H_{SR} is the coupling Hamiltonian between the system and the reservoir. Here, λ represents the coupling strength between the system and the bath. We can show that under the certain approximations the density operator of the system obeys the following Lindblad master equation

$$\frac{d}{dt}\rho_{\rm S}(t) = L[\rho_{\rm S}(t)],
L[\rho_{\rm S}(t)] = -i[H_S, \rho_{\rm S}(t)] + \sum_k \gamma_k \left(L_k \rho_S(t) L_k^{\dagger} - \frac{1}{2} \{ L_k^{\dagger} L_k, \rho_{\rm S}(t) \} \right),$$
(2.1.1)

where L_k 's are known as the jump operators of the system.

2.2 Mean Force Density Matrix

It is well known that the thermal state of a closed system with total Hamiltonian 'H' is given by the Gibbs state:

$$\rho_G = \frac{e^{-\beta H}}{Tr[\ e^{-\beta H}]} \tag{2.2.1}$$

So, for open quantum systems with the total Hamiltonian of the form $H_{tot} = H_S + \lambda H_{SR} + H_R$, where H_S is the Hamiltonian of the system of interest, H_R represents the Hamiltonian for the reservoir (bath), and H_{SR} is the coupling Hamiltonian between the system and the reservoir; the thermal density matrix for the total system is given by:

$$\rho_{tot} = \frac{e^{-\beta(H_S + \lambda H_{SR} + H_R)}}{Tr[\ e^{-\beta(H_S + \lambda H_{SR} + H_R)}]}$$
(2.2.2)

Tracing out the bath, we get the reduced density matrix for system, that is the true thermal state of the system. This state is called the Mean Force Density Matrix of the system.

$$\rho_{MF} = \frac{Tr_R[\ e^{-\beta(H_S + \lambda H_{SR})}]}{Tr[\ e^{-\beta(H_S + \lambda H_{SR})}]}$$
(2.2.3)

Obviously, at leading order in λ this is equal to the Gibbs state of the system.

2.3 KMS condition

The density matrix only captures the static properties of the system. The dynamical properties such as the spectral density and response of the system to external perturbations are captured by the correlation function. So, when a system reaches thermal equilibrium, the correlation functions satisfy a constarint independent of the density matrix. This constarint is called the KMS condition. For example, for a two-point function, the KMS condition is given by:

$$\langle A(t_A)B(t_B)\rangle = \langle B(t_B - i\beta/2)A(t_A + i\beta/2)\rangle$$
(2.3.1)

The genralization of KMS condition to multi-time correlation function is straightforward and givens

$$\langle A(t_{A,1}, t_{A,2}, \dots, t_{A,N}) B(t_{B,1}, t_{B,2}, \dots, t_{B,M}) \rangle = \langle B(t_{B,1} - i\beta/2, \dots, t_{B,M} - i\beta/2) A(t_{A,1} + i\beta/2, \dots, t_{A,N} + i\beta/2) \rangle$$

$$(2.3.2)$$

2.4 Image Operator Formalism

The Image Operator framework describes open quantum systems in the Heisenberg Picture. Describing the complete Heisenberg picture for an open quantum system this way involves multiple "image Heisenberg operators" for each system observable. For an operator O(t), an image operator $O_{\alpha\beta}(t)$ is defined as :

$$O_{\alpha\beta} = T^{\dagger}_{\alpha}O(t)T_{\beta}. \tag{2.4.1}$$

Where, $\{|i\rangle | i\epsilon I\}$ and $\{|\alpha\rangle | \alpha\epsilon A\}$ and thus, $\{|i\alpha\rangle | i\alpha\epsilon I, \alpha\epsilon A\}$ span the system, bath, and the total Hilbert space respectively. And, T_{α} is a projection operator defined as:

$$T_{\alpha} = |i\alpha\rangle \langle i| \,. \tag{2.4.2}$$

Clearly, the number of such image operators is equal to the environment Hilbert space. The key part of

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the formalism is a perturbative expansion of the image operators in terms of the single one-point operators, which is accurate up to arbitrary orders in the system bath coupling given as:

$$O_{\alpha\beta} = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \sum_{n_1,\dots,n_k=1}^{\infty} (-1)^k (\frac{\lambda}{\hbar})^{n+n_1+\dots+n_k} P_{\alpha\beta}^{(n)} P_S^{n_1} \dots P_S^{(n_k)} O_S(t).$$
(2.4.3)

Where, $O_S(t)$ is the reduced system operator, and

$$U_0(t) = e^{\frac{-iH_0t}{\hbar}},$$
(2.4.4)

$$\tilde{K}_{\alpha\beta}^{(n)}(t) = \int_0^t dt_1 \dots \int_0^{t_{n-1}} dt_n \tilde{H}_{I\alpha\gamma_1}(t_1) \dots \tilde{H}_{I\gamma_{n-1}\beta}(t_n), \qquad (2.4.5)$$

$$K_{\alpha\beta}^{(n)}(t) = e^{\frac{i(E_{\alpha} - E_{\beta})t}{\hbar}} \hbar U_0^{\dagger}(t) \tilde{K}_{\alpha\beta}^{(n)}(t) U_0(t), \qquad (2.4.6)$$

and finally,

$$P_{\alpha\beta}^{(n)}A(t) \equiv \sum_{r=0}^{n} i^{n-2r} K_{\gamma\alpha}^{(n-r)\dagger}(t) A(t) K_{\gamma\beta}^{(r)}(t), \qquad (2.4.7)$$

$$P_S^{(n)}A(t) \equiv P_{\alpha\beta}^{(n)}A(t)\rho_{\beta\alpha}.$$
(2.4.8)

One can observe that the image operators depend non-linearly on the state of the environment. This relationship is significant because it enables the construction of N-point-reduced system operators:

$$(O_1(t_1)...O_N(t_N))_S = (O_{1\alpha\gamma_1}(t_1)...O_{\gamma_{n-1}\beta}(t_N))\rho_{\beta\alpha}.$$
(2.4.9)

Thermalization in Open Quantum Systems

Part II

A close parallel between Open Quantum Systems and Hydrodynamics

Chapter 3

Entropy Production Constraints

3.1 Entropy Production Functional

The last decade has seen tremendous progress in understanding dissipative dynamics from the effective field theory approach. This has led to a better understanding of hydrodynamics. In the context of hydrodynamics, this approach has led to a new formulation based on symmetries [34], new constraints on the transport parameters [35], stability of hydrodynamic equations [36], and much more. In a beautiful paper by Bhattacharya et al. [35], it was shown that the coefficients in Navier-Stokes equations follow certain equality and inequality type relations in the higher derivative terms of the Navier-Stokes equation if one demands the positivity of the production of local entropy current for perturbations around the global equilibrium state. Taking inspiration from that work, in this chapter, I derive similar constraints on the coefficients of the Master Equation that describe the dynamics for Open Quantum systems.

3.1.1 Von Neumann Entropy

The von Neumann entropy is an important entropy functional. Given the state of an open quantum system, ensemble in terms of a density matrix is defined by

$$S[\rho_{\rm s}(t)] = -Tr[\rho_{\rm s}(t)\ln\rho_{\rm s}(t)]$$
(3.1.1)

3.1.2 Entropy Production Functional

Let's suppose that the canonical equilibrium distribution (Gibbs state)

$$\rho_{\rm s}^{th} = \frac{e^{-\beta H_{\rm s}}}{Tr_{\rm s}[e^{-\beta H_{\rm s}}]} \tag{3.1.2}$$

is a stationary solution of the master equation. This means that $L[\rho^{th}] = 0$.

For an Open Quantum System, the total entropy production at any time is

$$\sigma(t) = \frac{d}{dt}S(t) + J(t)$$
(3.1.3)

Where, S is the von Neumann entropy of the open system. The quantity J denotes the amount of entropy which is exchanged per unit of time between the open system and its environment. Let's consider an Open System obeying Lindblad dynamics. The time derivative of the von Neumann entropy is easily evaluated to be

$$\frac{d}{dt}S(t) = -k_B Tr[L(\rho_{\rm s}(t))\ln\rho_{\rm s}(t)]$$
(3.1.4)

And, entropy flux is evaluated to be

$$J(t) = k_B Tr[L(\rho_{\rm s}(t))\ln\rho_{\rm s}^{th}(t)]$$

$$(3.1.5)$$

So, the net entropy production is

$$\sigma(t) = k_B Tr[L(\rho_{\rm s}(t))(\ln \rho_{\rm s}^{th}(t) - \ln \rho_{\rm s}(t))]$$
(3.1.6)

3.1.3 Example: Harmonic Oscillator coupled with bath

Let's consider the same example where a simple harmonic oscillator is interacting with a bath. For simplicity, let's take these following two jump operators, $L_1 = a^{\dagger}$ and $L_2 = a$. Then the dynamics of $\rho_s(t)$ will govern by the following Lindblad master equation

$$\frac{d}{dt}\rho_{\rm s}(t) = -i\omega[a^{\dagger}a,\rho_{\rm s}(t)] + \gamma_1 \left(a^{\dagger}\rho_{\rm s}(t)a - \frac{1}{2} \{aa^{\dagger},\rho_{\rm s}(t)\}\right)
+ \gamma_2 \left(a\rho_{\rm s}(t)a^{\dagger} - \frac{1}{2} \{a^{\dagger}a,\rho_{\rm s}(t)\}\right)$$
(3.1.7)

Now if we do a small perturbation $\delta(t)$ in the entropy production around the thermal state then the first order term in $\delta(t)$ is

$$\sigma^{1}(\rho_{\rm s}^{th} + \delta(t)) = 2(-\gamma_{1}e^{-\beta E_{1}} + \gamma_{2}e^{-\beta E_{2}})\delta(t)$$
(3.1.8)

Since, $\sigma(\rho_s(t))$ is a convex function, so the first order term has to be zero which gives the following relation between γ_1 and γ_2

$$\gamma_1 = e^{-\beta\omega}\gamma_2 \,. \tag{3.1.9}$$

Similarly, the second order term in the perturbative parameter is

$$\sigma^2(\rho_{\rm s}^{th} + \delta(t)) = 2(1 + e^{-\beta\omega})\gamma_2 \ \delta^2(t) \ . \tag{3.1.10}$$

Since, $\sigma(\rho_s(t))$ is a convex function, so the second order term has to be non-negative which demands that γ_2 has to be non-negative i.e. $\gamma_2 \ge 0$ and using Eq.(3.1.9) we can say $\gamma_1 \ge 0$.

3.1.4 Multiple steady state and Entropy Production

If there exists multiple steady states then perturbation in different directions give different results. To understand this point we are going to take the example of a Dephasing Spin-Boson Model. The Hamiltonian of the dephasing spin-boson model is,

$$H = H_S + H_R + H_{SR}$$

= $\frac{\omega_0}{2}\sigma_z + \sum_k \omega_k b_k^{\dagger} b_k + \sum_k \alpha_k \sigma_z \otimes (b_k^{\dagger} + b_k)$ (3.1.11)

One can show that the reduced density operator obeys the following equation

$$\frac{d}{dt}\rho_{\rm s}(t) = -i\frac{\omega_0}{2}[\sigma_z, \rho_{\rm s}(t)] + \gamma_{11}(0)[\sigma_z\rho_{\rm s}(t)\sigma_z - \rho_{\rm s}(t)]$$
(3.1.12)

The solution of the above equation is

$$\rho_{\rm S}(t) = \begin{bmatrix} \rho_{\rm S}^{ee}(0) & e^{-(i\omega_0 + 2\gamma_{11}(0))t}\rho_{\rm S}^{eg}(0) \\ e^{(i\omega_0 - 2\gamma_{11}(0))t}\rho_{\rm S}^{ge}(0) & \rho_{\rm S}^{gg}(0) \end{bmatrix}$$
(3.1.13)

We can clearly see that this system has multiple steady states. Now if we do a diagonal perturbation $\delta(t)$

in the entropy production around the thermal state i.e. $\hat{\delta}(t) = \delta(t) \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$ then the change in entropy

production is zero. This result can be understood from the following fact that any diagonal perturbation in the thermal state is a steady state of this system, so there will be no entropic cost to go from one steady state to other. However, if we do an off-diagonal perturbation, the first order term is zero and the second order term will be positive only if $\gamma(0)$ is positive.

3.1.5 Convexity of Entropy Production Functional

The Lieb's theorem states that the functional

$$f_t(A,B) = -Tr[X^{\dagger}A^tXB^{1-t}]$$
(3.1.14)

is jointly convex in its arguments A and B. Here, A and B are positive operators, while X is an arbitrary fixed operator and t is a fixed number in the interval [0, 1]. By Lieb's theorem the functional

$$-Tr[(X\rho X^{\dagger} - X^{\dagger} X\rho)\ln\rho]$$
(3.1.15)

is convex.

Using this it can be shown that, the entropy production functional is non-negative and vanishes in a stationary state, if and only if all γ 's are non-negative. Moreover, in that case, $\sigma(\rho)$ is a convex functional on the state space of the open system.

3.1.6 Perturbative expansion for Entropy Production

We know,

$$\sigma(t) = -k_B Tr[L(\rho_{\rm s}(t))(\ln\rho_{\rm s}(t)) - \ln\rho_{\rm s}^{th}(t)]$$
(3.1.16)

Let's write, $\rho_S = \rho_S^{th} + \delta$ As, $L[\rho^{th}] = 0$, and $L[\rho_1 + \rho_2] = L[\rho_1] + L[\rho_2]$ We get,

$$\sigma(t) = -k_B Tr[L(\delta(t))(\ln(\rho_{\rm s}^{th}(t) + \delta(t)) - \ln\rho_{\rm s}^{th}(t)]$$

$$(3.1.17)$$

Using the Taylor Expansion for Matrix Logarithms, we get,

$$\sigma(t) = -k_B Tr[L(\delta(t))([\int_0^a (\rho_{\rm s}^{th}(t) + aI)^{-1}\delta(t)(\rho_{\rm s}^{th}(t) + aI)^{-1} + (\rho_{\rm s}^{th}(t) + aI)^{-1}\delta(t)(\rho_{\rm s}^{th}(t) + aI)^{-1}\delta(t)(\rho_{\rm s}^{th}(t) + aI)^{-1} + \dots])]$$

$$(3.1.18)$$

We know, $L[\delta(t)]$ is a linear functional in delta. So, clearly, the zeroth and first order terms in this perturbative expansion are zero. And, because of Lieb's theorem, imposing the non-negativity of the second order term (lowest order term in the expansion) is necessary and sufficient for imposing the non-negativity of entropy production.

3.2 Completely Positive Trace Preserving Map

Any Complete Positive Trace Preserving (CPTP) quantum map can be expressed in the following Kraus-operator representation

$$\rho_{\rm s}(t) = \sum_{\alpha} K_{\alpha}(t) \rho_{\rm s}(0) K_{\alpha}^{\dagger}(t) . \qquad (3.2.1)$$

Now the Lindblad equation (2.1.1) will have the Kraus operator representation if all the γ_k 's are non-negative. So, complete positivity (CP) demands $\gamma_k \ge 0$. Hence, the Eq.(3.1.12) preserve the positivity of probabilities only if γ_1 and γ_2 are both positive.

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3.3 Thermalization

If we demand that the thermal state should be a steady state solution of the Lindblad master equation (3.1.12) i.e. $L[\rho_s^{th}] = 0$, then it will give the following relation between γ_1 and γ_2

$$\gamma_1 = e^{-\beta\omega}\gamma_2. \tag{3.3.1}$$

3.4 Summary

In this section, we have demonstrated how the coefficients of the jump operators in the Lindblad Master equation adhere to specific equality and inequality-type relations by requiring the positivity of the production of the total von Neumann entropy during dissipative dynamics. Additionally, we have illustrated that the equality relations are equivalent to those obtained by requiring thermalization, while the inequality-type relations are equivalent to those obtained by demanding stability (or CPTP). Subsequently, we transition to the case of multiple steady states and elucidate how our results generalize in that context. Thermalization in Open Quantum Systems

Chapter 4

Spectrum of Lindbladian and Poles of Green's functions

The Liouvillian spectrum for open quantum systems contains crucial information about the system's dynamics. Specifically, it always resides on the left half of the complex plane due to the dissipative nature of the dynamics. Moreover, the lowest lying mode in the spectrum with a non-zero real part provides us with the timescale of the system's thermalization [37]. The distribution of the spectrum in a many-body system also offers hints about whether the underlying dynamics are chaotic or not [38].

In this section, we demonstrate how this spectrum, which governs the out-of-equilibrium dynamics, is neatly captured in the poles of the steady-state correlation functions of the system. This finding complements those of the previous section and illustrates how small perturbations around thermal equilibrium can assist us in understanding crucial aspects of truly out-of-equilibrium dynamics.

4.1 Spectrum of Lindbladian and poles of two-point function

The dynamics of an open system is governed by the following Lindblad equation in the Markovian regime

$$\frac{d}{dt}\rho_s = L\rho_s \tag{4.1.1}$$

The retarded two-point function is defined as

$$G^{R}(t,t') = -i\Theta(t-t')\langle [O_{1}(t), O_{2}(t')]\rangle$$
(4.1.2)

Let's assume t > t' and O_1 is one of the eigenvector of L i.e.

$$LO_1 = \lambda O_1 , \qquad (4.1.3)$$

where λ is one of the eigenvalue of the *L* operator. Using Quantum Regression Theorem(QRT) we can show that

$$G^{R}(t,t') = -i\Theta(t-t')e^{\lambda(t-t')} \langle [O_{1}(t'), O_{2}(t')] \rangle$$
(4.1.4)

Now at the steady state i.e. $t' \to \infty$ the retarded greens function becomes

$$G^R(\tau) = C\Theta(\tau)e^{\lambda\tau} , \qquad (4.1.5)$$

where $\tau = t - t'$ and C is a constant. The fourier transform of G^R is

$$G^R(\Omega) = \tilde{C} \frac{1}{i\Omega - \lambda} .$$
(4.1.6)

4.1.1 Exceptional point

The point in the spectrum where the eigenvectors coalesce is known as an exceptional point (EP). When two eigenvectors of the Lindbladian coalesce into one, a second-order non-Hermitian degeneracy is obtained. We refer to it as EP2. Let's assume k number of eigenvectors of L coalesce into one which we denoted by O_1^k . Then the retarded two-point function at the steady state will be

$$G^{R}(\tau) = -\lim_{t' \to \infty} i\Theta(t - t') \langle [O_{1}^{k}(t), O_{2}(t')] \rangle = C\Theta(\tau) \left(\sum_{j=0}^{k-1} d_{j}\tau^{j}\right) e^{\lambda\tau}$$
(4.1.7)

Fourier transform of G^R is

$$G^{R}(\Omega) = \sum_{j=0}^{k-1} \tilde{d}_{j} \frac{1}{(i\Omega - \lambda)^{j+1}} .$$
(4.1.8)

So if k numbers of eigenvectors coalesce then we will get poles of order k.

4.1.2 Examples

4.1.2.1 Caldeira-Legget model

For this model, we have calculated the spectrum of the L and they are given by (at T = 0)

$$\lambda_{nm} = -[(n+m)\gamma + i(n-m)\omega'_0], \qquad (4.1.9)$$

where n and m are non negative integers. Since, Lindbladian is infinite dimensional that's why we got infinite number of eigenvalues. For n = m = 0, $\lambda_{00} = 0$ which ensures the unique steady state.

Now let's calculate the following retarded two-point function at the steady state

$$G^{R}(t,t') = -i\Theta(t-t')\langle [a(t),a^{\dagger}(t')]\rangle$$

$$(4.1.10)$$

For the Caldeira-Legget model the above retarded correlation function is (using the QRT)

$$G^{R}(t,t') = -i\Theta(t-t') \ e^{-(i\omega'_{0}+\gamma)(t-t')}$$
(4.1.11)

In the frequency space it will be

$$G^R(\Omega) = \frac{1}{\Omega - \omega'_0 + i\gamma} \tag{4.1.12}$$

Hence, the retarded correlator has a pole at $\Omega = \omega'_0 - i\gamma$. The eigenvalue of Lindbladian for n = 1, m = 0 is $\lambda_{10} = -i\omega'_0 - \gamma$. So, the pole of retarded correlator and spectrum of the Lindbladian is related by

pole of
$$[G^R(\Omega)] = i$$
 [eigenvalue of \hat{L} for $n = 1, m = 0$]. (4.1.13)

Similarly, we have seen that other eigenvalues of \hat{L} are related to the retarded correlation function of different operators. For example, the pole of the following two-point function

$$G^{R}(t,t') = -i\Theta(t-t')\langle [a^{2}(t), a^{\dagger 2}(t')]\rangle$$
(4.1.14)

is related to the eigenvalue of \hat{L} for n = 2, m = 0.

General operator:

Let's consider the following operator

$$A_{nm}(t) = a^n a^{\dagger m}(t)$$
 (4.1.15)

For the CL model we can show that

$$\frac{d}{dt}\langle A_{nm}(t)\rangle = -[(n+m)\gamma + i(n-m)\omega_0']\langle A_{nm}(t)\rangle + 2nm\gamma\langle A_{n-1m-1}(t)\rangle$$
(4.1.16)

If we write the above equation in the matrix form we will get

$$\frac{d}{dt}\langle A_{nm}(t)\rangle = -[(n+m)\gamma + i(n-m)\omega_0']\langle A_{nm}(t)\rangle + 2nm\gamma\langle A_{n-1m-1}(t)\rangle$$
(4.1.17)

$$\frac{d}{dt} \begin{bmatrix} \langle A_{00} \rangle \\ \langle A_{01} \rangle \\ \vdots \\ \langle A_{0m} \rangle \\ \langle A_{10} \rangle \\ \vdots \\ \langle A_{10} \rangle \end{bmatrix} = \mathbf{M} \begin{bmatrix} \langle A_{00} \rangle \\ \langle A_{01} \rangle \\ \vdots \\ \langle A_{0m} \rangle \\ \langle A_{0m} \rangle \\ \langle A_{10} \rangle \\ \vdots \\ \langle A_{nm} \rangle \end{bmatrix} \quad (4.1.18)$$

This M_{ij} matrix is lower triangular with eigenvalues $\lambda_{nm}^M = -[(n+m)\gamma + i(n-m)\omega'_0]$. We can diagonlised this matrix by changing the operator, $A_{nm} \to \tilde{A}_{nm}$ i.e.

$$\frac{d}{dt}\langle \tilde{A}_{nm}\rangle = \lambda_{nm}^M \langle \tilde{A}_{nm}\rangle .$$
(4.1.19)

Now take the following retarded correlator

$$G^{R}(t,t') = -i\Theta(t-t')\langle [\tilde{A}_{nm}(t), f(a,a^{\dagger})(t')]\rangle$$
(4.1.20)

Using QRT, we can easily show that

$$G^{R}(\tau) = -i\Theta(\tau)e^{\lambda_{nm}^{M}\tau} \operatorname{Lt}_{t'\to\infty} \langle [\tilde{A}_{nm}(t'), f(a, a^{\dagger})(t')] \rangle , \qquad (4.1.21)$$

where we have set $t = t' + \tau$. Finally, we have

$$G^{R}(\tau) = -iC\Theta(\tau)e^{\lambda_{nm}^{M}\tau}, \qquad (4.1.22)$$

where $C = \text{Lt}_{t' \to \infty} \langle [\tilde{A}_{nm}(t'), f(a, a^{\dagger})(t')] \rangle$. In the frequency space it is given by

$$G^R(\Omega) = \frac{C}{\Omega - i\lambda_{nm}^M} \tag{4.1.23}$$

Hence, pole is at $\Omega = i\lambda_{nm}^M$. Now, $\lambda_{nm}^M = \lambda_{nm}$. Finally, we got the following relation

pole of
$$[G^R(\Omega)] = i$$
 [spectrum of \hat{L}]. (4.1.24)

4.1.2.2 Dissipative Spin-Boson model

For the dissipative spin-boson model, the Lindblad operator has the following form

$$L = \begin{bmatrix} -\gamma(\bar{n}+1) & 0 & 0 & \gamma\bar{n} \\ 0 & -[i\omega'_0 + \gamma(\bar{n}+1/2)] & 0 & 0 \\ 0 & 0 & -[-i\omega'_0 + \gamma(\bar{n}+1/2)] \\ \gamma(\bar{n}+1) & 0 & 0 & -\gamma\bar{n} \end{bmatrix}.$$
 (4.1.25)

Eigenvalues of this superoperator(L) are

$$\operatorname{Eig}(L) = \{0, 1\}.$$
 (4.1.26)

4.2 Spectrum of Lindbladian and poles of N-point function

N-point retarded greens function is defined as

$$G^{R}(t_{1}; t_{2}, ..., t_{N}) = (-i)^{N-1} \sum_{j} \theta(t_{1} - t_{j_{1}}) \theta(t_{j_{1}} - t_{j_{2}}) \theta(t_{j_{N-1}} - t_{j_{N}}) \\ \times [.....[[O_{1}(t_{1}), O_{j_{2}}(t_{j_{2}})], O_{j_{3}}(t_{j_{3}})], O_{j_{N}}(t_{j_{N}})]$$
(4.2.1)

On the right hand side of the above equation we sum over all permutations of the operators $\{O_2(t_2), ..., O_N(t_N)\}$, but leave $O_1(t_1)$ fixed. Now if we assume $t_1 > t_2..... > t_N$ then the above definition reduces to

$$G^{R}(t_{1}; t_{2},...,t_{N}) = (-i)^{N-1} \theta(t_{1} - t_{2}) \theta(t_{2} - t_{3}),...,\theta(t_{N-1} - t_{N})$$

$$\times [.....[[O_{1}(t_{1}), O_{2}(t_{2})], O_{3}(t_{3})],...,O_{N}(t_{N})]$$
(4.2.2)

Let's assume $\{\tilde{O}_n\}$ are the eigenvectors of L operator i.e.

$$L\tilde{O}_n = \lambda_n \tilde{O}_n \tag{4.2.3}$$

Now choose $\{O_n\}$ operators such that they satisfies the following relations

$$\tilde{O}_{1} = O_{1} ;$$

$$\tilde{O}_{2} = [O_{1}, O_{2}] ;$$

$$.$$

$$\tilde{O}_{n} = [\dots [[O_{1}, O_{2}], O_{3}] \dots , O_{n}]$$
(4.2.4)

Using Quantum Regression Theorem (QRT), we can easily calculate the following result

$$G^{R}(\tau_{1},\tau_{2},\ldots,\tau_{N-1},t_{N}) = (-i)^{N-1}\theta(\tau_{1})\theta(\tau_{2}),\ldots,\theta(\tau_{N-1})[\tilde{O}_{N-1}(t_{N}),O_{N}(t_{N})]\prod_{j}e^{\lambda_{j}\tau_{j}}$$
(4.2.5)

At the steady state i.e. $t_N \to \infty$ the retarded correlation becomes

$$G^{R}(\tau_{1}, \tau_{2}, ..., \tau_{N-1}) = C \ \theta(\tau_{1})\theta(\tau_{2}), ..., \theta(\tau_{N-1}) \prod_{j} e^{\lambda_{j}\tau_{j}} , \qquad (4.2.6)$$

where C is a constant. If we do the fourier transformation of G^R , we will get

$$G^{R}(\Omega_{1}, \Omega_{2}, ..., \Omega_{N-1}) = C \prod_{j=1}^{N-1} \left(\frac{1}{i\Omega_{j} - \lambda_{j}}\right).$$
(4.2.7)

So the poles of Ω_j 's are the eigenvalues of the Lindbladian. If we take the Fourier transform of G^R with respect to t_i rather τ_i , we will get

$$G^{R}(\omega_{1},\omega_{2},\ldots,\omega_{N-1}) = \tilde{C}\left(\frac{1}{\omega_{1}-i\lambda_{1}}\frac{1}{\omega_{1}+\omega_{2}-i\lambda_{2}},\ldots,\frac{1}{\omega_{1}+\omega_{2},\ldots+\omega_{N-1}-i\lambda_{N-1}}\right).$$
(4.2.8)

4.3 Summary

In this section, we first establish a direct correspondence between the poles of the retarded Green's function and the spectrum of the Liouvillian in an abstract manner. We utilize the quantum regression theorem to achieve this correspondence. Subsequently, we demonstrate this relationship using simple examples such as the Caldeira-Leggett model and the dissipative Spin-boson model.

Furthermore, we extend this correspondence by showing it abstractly for the poles of the N-point retarded Green's function and the Liouvillian. Although we focus on the retarded correlator in this discussion, we anticipate that such a correspondence holds for any of the out-of-time ordered correlators.

Part III

Steady State correlation function and consistency with KMS condition

Chapter 5

Steady State Correlation function under the standard weak coupling limit

In this section, we want to derive the two-point correlation function at the steady state up to the leading order in system-bath coupling strength. For our setup, we take the following general form of the total Hamiltonian

$$H = H_{S} + H_{R} + H_{SR} = H_{S} + \sum_{k} \Omega_{k} b_{k}^{\dagger} b_{k} + \sum_{k} \alpha_{k} (Sb_{k}^{\dagger} + S^{\dagger} b_{k}) , \qquad (5.0.1)$$

where b_k and b_k^{\dagger} represent the bosonic or fermionic annihilation and creation operator for the k-th mode, respectively. The third term in Eq.(5.0.1) represents the system-bath coupling with the generic system operator S coupled with the k-th bath mode with interaction strength α_k .

5.1 Two-point function and Image Operator Formalism

Our first aim is to calculate the two-point correlation function of the form

$$\langle O_1(t+\tau)O_2(t)\rangle = \text{Tr}_S \Big[[O_1(t+\tau)O_2(t)]_S \rho_S(0) \Big],$$
 (5.1.1)

where $[O_1(t+\tau)O_2(t)]_S$ denotes the two-point reduced operator [17, 18] defined as:

$$[O_1(t+\tau)O_2(t)]_S = \text{Tr}_B [O_1(t+\tau)O_2(t)\rho_B]$$
(5.1.2)

We follow the recipe of Ref. [18], to express the two-point reduced operator $[O_1(t + \tau)O_2(t)]_S$, up to the leading order in the system-bath coupling, in terms of one-point reduced operators $(O_{1S} \text{ and } O_{2S})$ (for details see Appendix-??). Note that, the dynamics of the reduced one-point operator is governed by the Born master equation [1].

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For the system defined in Eq.(5.0.1), we can explicitly show the two-point reduced operator is given by

$$[O_1(t+\tau)O_2(t)]_S = O_{1S}(t+\tau)O_{2S}(t) + D_1(t,\tau) + D_2(t,\tau) , \qquad (5.1.3)$$

In Appendix-??, we have given the details of this derivation. Note that, to derive the above expression we have only considered the weak coupling approximation i.e., we keep terms up to the leading order in the system-bath coupling. The two-point reduced operator is not just the product of one-point reduced operators, we also get two inhomogeneous terms $D_1(t, \tau)$ and $D_2(t, \tau)$ which are given by the following equations

$$D_{1}(t,\tau) = \sum_{j,l,m,n} \int \frac{d\Omega}{2\pi} F_{\eta}(\Omega) \ e^{i\Omega\tau} e^{-i(\omega_{j}+\omega_{m}')(t+\tau)} e^{-i(\tilde{\omega}_{l}-\omega_{n}')t} \int_{0}^{t+\tau} d\tau_{1}' \Big[O_{1jS}(\tau_{1}'), S_{m} \Big] e^{-i[\Omega-(\omega_{j}+\omega_{m}')]\tau_{1}'} \\ \int_{0}^{t} d\tau_{2}' \Big[S_{n}^{\dagger}, O_{2lS}(\tau_{2}') \Big] e^{i[\Omega+(\tilde{\omega}_{l}-\omega_{n}')]\tau_{2}'}, \quad (5.1.4)$$

$$D_{2}(t,\tau) = \sum_{j,l,m,n} \int \frac{d\Omega}{2\pi} \tilde{F}_{\eta}(\Omega) e^{-i\Omega\tau} e^{i(\omega_{m}^{\prime}-\omega_{j})(t+\tau)} e^{-i(\tilde{\omega}_{l}+\omega_{n}^{\prime})t} \int_{0}^{t+\tau} d\tau_{1}^{\prime} \Big[O_{1jS}(\tau_{1}^{\prime}), S_{m}^{\dagger} \Big] e^{i[\Omega+(\omega_{j}-\omega_{m}^{\prime})]\tau_{1}^{\prime}} \\ \int_{0}^{t} d\tau_{2}^{\prime} \Big[S_{n}, O_{2lS}(\tau_{2}^{\prime}) \Big] e^{i[(\tilde{\omega}_{l}+\omega_{n}^{\prime})-\Omega]\tau_{2}^{\prime}}$$
(5.1.5)

where $F_{\eta}(\Omega) = J(\Omega)n_{\eta}(\Omega)$ and $\tilde{F}_{\eta}(\Omega) = (J(\Omega) - \eta F_{\eta}(\Omega))$ with $J(\Omega)$ is the spectral density function of the bath which is defined as $J(\Omega) = 2\pi \sum_{k} |\alpha_{k}|^{2} \delta(\Omega - \Omega_{k})$. Note that, here $n_{\eta}(\Omega)$ represents the Bose or Fermi distribution function i.e. $F_{\eta}(\Omega) = [e^{\beta\Omega} + \eta]^{-1}$ with $\eta = +1$ and $\eta = -1$ are for fermions and bosons, respectively. ω_{j} corresponds to the possible energy differences between the bare system eigenenergies that appear by performing spectral decomposition for the operator O_{1S} . In other words, we use the fact that

$$O_{1S}(t) = \sum_{j} O_{1jS}(t - t')e^{-i\omega_j t'} + O(\alpha_k).$$
(5.1.6)

Similarly, $\tilde{\omega}_l$ and ω'_m correspond to the possible energy differences of the bare system for the operators O_{2S} and S respectively. Eq.(5.1.3)-Eq.(5.1.5) represents the two-point correlation function at any time.

For the rest of the paper, we focus on the steady-state correlation function. To obtain the steady state correlation function, we simply need to take the $t \to \infty$ limit in Eq.(5.1.3)-Eq.(5.1.5). Below, we will illustrate the calculation of the steady state correlation function using the image operator method for two paradigmatic models. Additionally, we will explicitly show that the obtained correlation function satisfies the KMS condition.

5.2 Two-point correlation function at the steady state and KMS for some specific models

Here, using the expression obtained in Eq.(5.1.3)-Eq.(5.1.5), we compute the correlation function for a dissipative non-interacting bosonic/fermion system and for the dissipative spin-boson model. For both these models, we show explicitly that the correlation function satisfies the KMS condition in the long-time limit.

5.2.1 Dissipative Bosonic/Fermionic Model

We treat a single bosonic or fermionic degree of freedom as a system that is coupled to a corresponding bosonic or fermionic thermal bath. The total Hamiltonian is given by

$$H = \omega_0 a^{\dagger} a + \sum_k \Omega_k b_k^{\dagger} b_k + \sum_k \alpha_k (a \, b_k^{\dagger} + a^{\dagger} \, b_k), \qquad (5.2.1)$$

where a and a^{\dagger} represent the bosonic or fermionic annihilation and creation operator for the system, respectively. For this model, we want to calculate $\langle a^{\dagger}(t+\tau)a(t)\rangle$ up to the leading order in system-bath coupling at the steady state using Eq.(5.1.3)-Eq.(5.1.5). Let us first note that, for this correlation function, $O_1 = a^{\dagger}$ and $O_2 = a$ in Eq. (5.1.3). With this identification, it is easy to show that the D_1 term (expressed in Eq.(5.1.4)) at the long time limit i.e. $t \to \infty$, takes this interesting form,

$$D_{1} = \int \frac{d\Omega}{2\pi} F_{\eta}(\Omega) \ e^{i\Omega\tau} \int_{0}^{\infty} d\tau_{1}' \Big[a_{S}^{\dagger}(\tau_{1}'), a \Big] e^{-i\Omega\tau_{1}'} \int_{0}^{\infty} d\tau_{2}' \Big[a^{\dagger}, a_{S}(\tau_{2}') \Big] e^{i\Omega\tau_{2}'} = \int \frac{d\Omega}{2\pi} F_{\eta}(\Omega) \ e^{i\Omega\tau} \Big[\tilde{a}_{S}^{\dagger}(i\Omega), a \Big] \Big[a^{\dagger}, \tilde{a}_{S}(-i\Omega) \Big] , \qquad (5.2.2)$$

where $\tilde{a}_S(-i\Omega)$ is the Laplace transformation of $a_S(t)$ i.e. $\tilde{a}_S(-i\Omega) = \int_0^\infty dt \ a_S(t)e^{i\Omega t}$. It is interesting to note that the Laplace transform is a feature specific to the steady state and appears naturally in the steady state limit. Similarly, we can show that D_2 (expressed in Eq. (5.1.5)) is zero for this model. Note that for this model, the first term of Eq.(5.1.3) is zero since $a_S(\infty) = a_S^{\dagger}(\infty) = 0$ and the Laplace transformation of $a_S(t)$ is (see Appendix-?? for details)

$$\tilde{a}_S(-i\Omega) = \frac{a}{\left[-i\left(\Omega - \omega_0 - \Sigma(\Omega)\right) + \frac{J(\Omega)}{2}\right]}.$$
(5.2.3)

Making these substitutions in Eq. (5.2.2), we get the following expression for the two-point correlation function at the steady state

$$\langle a^{\dagger}(t+\tau)a(t)\rangle_{\rm ss} = \int_0^\infty \frac{d\Omega}{2\pi} \frac{e^{i\Omega\tau} F_{\eta}(\Omega)}{\left[\left(\Omega - \omega_0 - \Sigma(\Omega)\right)^2 + \left(J(\Omega)/2\right)^2\right]} \,. \tag{5.2.4}$$

It is worth noting how the two-point correlator expressed by the seemingly complicated Eq.(5.1.3)-Eq.(5.1.5), takes on an elegant and simple form in the steady state limit. Another important feature of the above equation is that at $\tau = 0$, the right-hand side becomes the steady-state one-point expectation value $\langle a^{\dagger}a \rangle_{ss}$. We want to determine whether the correlation function obtained in Eq.(5.2.4) satisfies the KMS condition or not. The KMS condition states that:

$$\langle a^{\dagger}(t+\tau)a(t)\rangle_{\rm ss} = \langle a(t)a^{\dagger}(t+\tau-i\beta)\rangle_{\rm ss}$$
(5.2.5)

So, to check the KMS condition, we need to find the other correlator also, i.e., $\langle a(t)a^{\dagger}(t+\tau)\rangle$. Following the exact similar steps, one can easily compute the following correlator

$$\langle a(t)a^{\dagger}(t+\tau)\rangle_{\rm ss} = \int_0^\infty \frac{d\Omega}{2\pi} \frac{e^{i\Omega\tau} \left(1 - \eta \, n_\eta(\Omega)\right) J(\Omega)}{\left[\left(\Omega - \omega_0 - \Sigma(\Omega)\right)^2 + \left(J(\Omega)/2\right)^2\right]} \tag{5.2.6}$$

Looking at Eq.(5.2.4) and Eq.(5.2.6), it is clear that the above correlators satisfy the KMS condition at the steady state. Moreover, the obtained expression for the correlation functions in Eq.(5.2.4) and Eq.(5.2.6) turns out to be the exact correlation function at the steady state.

5.2.2 Dissipative Spin-Boson Model (Secular)

We want to apply the same method to calculate the correlation function for another paradigmatic model, namely the dissipative spin-boson model. The total Hamiltonian of the system is given by

$$H = \frac{\omega_0}{2}\sigma_z + \sum_k \Omega_k b_k^{\dagger} b_k + \sum_k \alpha_k (\sigma_- b_k^{\dagger} + \sigma_+ b_k) .$$
(5.2.7)

where $b_k(b_k^{\dagger})$ represents the bosonic annihilation (creation) operator and $\sigma_-(\sigma_+)$ is the lowering (raising) operator of the spin-half system. Our aim is to compute $\langle \sigma_+(t+\tau)\sigma_-(t)\rangle$ up to the leading order in the system-bath coupling. Let us first note that, $O_1 = \sigma_+$ and $O_2 = \sigma_-$ in Eq. (5.1.3). With this identification, it is easy to show that the D_1 term (expressed in Eq.(5.1.4)) at the long time limit i.e. $t \to \infty$, is given by

$$D_{1} = \int \frac{d\Omega}{2\pi} F_{-}(\Omega) e^{i\Omega\tau} \int_{0}^{\infty} d\tau_{1}' \Big[\sigma_{+S}(\tau_{1}'), \sigma_{-} \Big] e^{-i\Omega\tau_{1}'} \\ \int_{0}^{\infty} d\tau_{2}' \Big[\sigma_{+}, a_{-S}(\tau_{2}') \Big] e^{i\Omega\tau_{2}'} \\ = \int \frac{d\Omega}{2\pi} F_{-}(\Omega) e^{i\Omega\tau} \Big[\tilde{\sigma}_{+S}(i\Omega), \sigma_{-} \Big] \Big[\sigma_{+}, \tilde{\sigma}_{-S}(-i\Omega) \Big] , \qquad (5.2.8)$$

where $\tilde{\sigma}_{-S}(-i\Omega)$ is the Laplace transformation of $\sigma_{-S}(t)$ i.e. $\tilde{\sigma}_{-S}(-i\Omega) = \int_0^\infty dt \ \sigma_{-S}(t)e^{i\Omega t}$. Similarly, we can show that D_2 (expressed in Eq.(5.1.5)) is zero for this model. Finally, by substituting the Laplace transformation of the operators appearing in Eq. (5.2.8), we get the simple and explicit form of the two-point correlation function at the steady-state

$$\langle \sigma_{+}(t+\tau)\sigma_{-}(t)\rangle_{\rm ss} = \int_{0}^{\infty} \frac{d\Omega}{2\pi} \frac{e^{i\Omega\tau}F_{-}(\Omega)}{\left[\left(\Omega - \omega_{0} - \Sigma''(\Omega)\right)^{2} + \left(\left(n(\Omega) + 1/2\right)J(\Omega)\right)^{2}\right]}$$
(5.2.9)

By following the identical steps, we can find the following correlator

$$\langle \sigma_{-}(t+\tau)\sigma_{+}(t)\rangle_{\rm ss} = \int_{0}^{\infty} \frac{d\Omega}{2\pi} \frac{e^{-i\Omega\tau}(1+n_{-}(\Omega))J(\Omega)}{\left[\left(\Omega-\omega_{0}-\Sigma''(\Omega)\right)^{2}+\left((n(\Omega)+1/2)J(\Omega)\right)^{2}\right]} \,.$$
(5.2.10)

It is evident from Eq.(5.2.9) and Eq.(5.2.10) that the above correlators satisfy the KMS condition at the steady state. Note that, the above expressions of the correlation function are obtained under only the weak coupling limit.

5.3 Summary

Note that, by employing the image operator method developed in this section, we explicitly calculate the two-point correlation function at the steady state for specific examples and demonstrate that they satisfy the KMS relation. Our next aim is to develop a technique for calculating the correlation function that ensures consistency with the KMS condition for a generic model. To be more precise, our technique will provide insight into the KMS relation without explicit computation of the correlation function, Additionally, we aim to go beyond the standard weak coupling limit for calculating correlation functions.

To achieve our goal, in the next section, we have developed an approximate and self-consistent nonperturbative technique using the Swinger-Keldysh path integral. This technique not only enables us to comment on the KMS relation for a generic type of system but also allows us to go beyond the weak coupling limit. Thermalization in Open Quantum Systems

Chapter 6

Steady State Correlation function beyond the standard weak coupling limit

In this section, we initially develop a framework that will enable us to extend beyond the standard weak coupling limit for calculating the steady-state two-point function. We achieve this by applying the "self-consistent Born approximation" (or Non-Crossing Approximation, NCA). Then, we proceed to demonstrate that this approximation, while providing a simple method for calculating the two-point function, also ensures that the two-point correlators obey the Fluctuation-Dissipation Relation (FDR).

For this, we focus on a very general class of open quantum systems comprising a single bosonic mode coupled to a Gaussian bosonic bath, with the total Hamiltonian $H = H_S + H_B + H_{I,l} + H_{I,nl}$, where we take H_S to be an arbitrary system Hamiltonian, and

$$H_B = \sum_k \omega_k b_k^{\dagger} b_k, \quad H_{I,l} = \sum_k \alpha_k (a^{\dagger} b_k + a b_k^{\dagger}),$$

$$H_{I,nl} = \sum_k \alpha_k (a^{\dagger m} a^n b_k + a^{\dagger n} a^m b_k^{\dagger}). \tag{6.0.1}$$

Here, b_k and b_k^{\dagger} represent the bosonic annihilation and creation operators for the k-th bath mode, respectively. The third term, $H_{I,l}$ in Eq.(6.0.1), signifies the system-bath coupling through linear operators of the system, coupled to the k-th bath mode with an interaction strength of α_k . The fourth term, $H_{I,nl}$ represents the system-bath coupling employing a generic non-linear operator $(m, n \ge 0)$, coupled to the k-th bath mode with an interaction strength of α_k . Note that the non-linear system operator has been considered to be normally ordered in the second-quantization notation.

6.1 Steady State Green's function and Schwinger Keldysh path Integral

Our objective here is to study the steady-state green's function for the system. To accomplish this, we promote the total Hamiltonian to the Schwinger Keldysh Path Integral. The resulting Schwinger Keldysh Action is expressed in Eq. (C.0.1) of Appendix-C, in the classical-quantum (cl-q) basis for the field operators. The Schwinger-Keldysh functional integral, involving both system and bath degrees of freedom in the total action, is quadratic in the bath degrees field. Assuming that the bath is in a thermal state, we can integrate it out, resulting in an action expressed solely in system degrees of freedom. This action takes the form $S = S_S + S'_l + S'_{nl}$, as expressed in Eq.(C.0.2).

We employ the standard tool of Feynman diagrams to perturbatively calculate the self-energy ' $\tilde{\Sigma}(\omega)$ ' for the steady-state Green's function. The Dyson series

$$G(\omega) = G_{(0)}(\omega) + G_{(0)}(\omega)\bar{\Sigma}(\omega)G_{(0)}(\omega) + \dots$$

= $G_{(0)} + G_{(0)}\tilde{\Sigma}(\omega)G = (G_{(0)}^{-1}(\omega) - \tilde{\Sigma}(\omega))^{-1},$ (6.1.1)

relates the self-energy to the Green's function, where $G_{(0)}(\omega)$ represents the system's bare Green's function. For the class of models described by the Hamiltonian in Eq.(6.0.1), the self-energy always takes the form:

$$\tilde{\Sigma} = \tilde{\Sigma}_S + \tilde{\Sigma}_{I,l} + \tilde{\Sigma}_{I,nl}. \tag{6.1.2}$$

Here, $\tilde{\Sigma}_S$, $\tilde{\Sigma}_{I,l}$, and $\tilde{\Sigma}_{I,nl}$ represent contributions to the self-energy arising from S_S , S'_l , and S'_{nl} , and correspondingly from H_S , $H_{I,l}$, and $H_{I,nl}$, respectively.

6.2 Self Consistent Born Approximation for Steady State Green's fucntion

The 'standard Born approximation' involves expressing the Dyson series up to the leading order in the self-energy. In contrast, the self-consistent Born approximation constitutes a straightforward non-perturbative method that involves a partial resummation of perturbation theory. The self-consistent approximations are widely used in various contexts in many-body physics, such as quantum transport [20–23] problems and quantum impurity models, both in and out of equilibrium [24–28]. Moreover, it naturally appears in the physics of large-N systems [30, 31]. This approach is capable of capturing strong coupling phenomena while still relying on simple equations [29]. It is also referred to as the 'Non-Crossing Approximation' because, heuristically, it can also be implemented by considering all orders of Feynman diagrams, which can be drawn on the plane in such a way that the propagators don't cross each other and intersect only at the vertices. FIG. 6.1 depicts such diagrams for a simple example.

Implementing the self-consistent Born approximation involves two steps:

1. Write down the Dyson series with the Born approximation for the self-energy,

2. Replace the 'bare Green's function' inside self-energy with the total Green's function.

To demonstrate how to implement the self-consistent Born approximation, we consider the total Hamiltonian of the form given by Eq.(6.0.1), with the simplest non-linear interaction Hamiltonian $H_{I,nl}$:

$$H_{I,nl} = \sum_{k} \alpha_k a^{\dagger} a (b_k^{\dagger} + b_k) \tag{6.2.1}$$

Step 1: First, we calculate the self-energy at the leading order. Its form is expressed by Eq.(6.1.2). The contribution to the leading-order self-energy from the system Hamiltonian H_S , and interaction Hamiltonians $H_{I,l}$ and $H_{I,nl}$ respectively are:

$$\tilde{\Sigma}_{I,l}^{(2)}(\omega) = \begin{pmatrix} 0 & iJ(\omega) + \Sigma(\omega) \\ & \\ -iJ(\omega) + \Sigma(\omega) & -2iJ(\omega) \coth\left(\frac{\beta}{2}\omega\right) \end{pmatrix},$$
(6.2.3)

$$\tilde{\Sigma}_{I,nl}^{(2)}(\omega) = \int_{\tau} D_B(\tau) \circ G_{(0)}(\tau) e^{i\omega\tau}.$$
(6.2.4)

Here, $J(\omega)$ represents the bath spectral density function, and $\Sigma(\omega) = \mathcal{P} \int_{\omega'} \frac{1}{\pi} \frac{J(\omega')}{\omega - \omega'}$. Here, D_B' denotes the bath Green's function. The symbol 'o' is a concise representation of the Feynman diagrams arising from standard Wick contractions. Its definition is provided in Appendix E. The corresponding Dyson series gives the steady state Green's function under Born approximation:

$$G_B(\omega) = \left(G_{(0)}^{-1}(\omega) - \tilde{\Sigma}_S^{(2)}(\omega) - \tilde{\Sigma}_{I,l}^{(2)}(\omega) - \tilde{\Sigma}_{I,nl}^{(2)}(\omega)\right)^{-1}.$$
(6.2.5)

Step 2: Now, to implement the self-consistent Born approximation, we replace the bare Green's function in the above self-energy with the total Green's function. For our example, the self-energy $\tilde{\Sigma}_{S}^{(2)}(\omega)$ is independent of $G_{(0)}$. So, it remains unchanged under this approximation. Similarly, the self-energy $\tilde{\Sigma}_{I,l}$ and is always independent of $G_{(0)}$. So, it always remains unchanged under this approximation. However, the self-energy contribution $\tilde{\Sigma}_{I,nl}^{(2)}$, as expressed in Eq.(6.2.1), changes to:

$$\tilde{\Sigma}_{I,nl}^{SC}(\omega) = \int_{\tau} D_B(\tau) \circ G^{SC}(\tau) e^{i\omega\tau}, \qquad (6.2.6)$$

giving the self-consistent steady-state Green's function

$$G^{SC}(\omega) = \left(G^{-1}_{(0)}(\omega) - \tilde{\Sigma}_S(\omega) - \tilde{\Sigma}_{I,l}(\omega) - \tilde{\Sigma}^{SC}_{I,nl}(\omega)\right)^{-1}.$$
(6.2.7)

Let us note that $\tilde{\Sigma}_{S}(\omega)$, originating from the system Hamiltonian, is always a purely real function and does not contribute to the dissipative dynamics of the system. Consequently, it does not play a role in the Fluctuation Dissipation relation, which is our next focus. Additionally, $\tilde{\Sigma}_{I,l}$, being independent of the system Green's function, always remains unchanged under the self-consistent Born approximation. Therefore, in proving the consistency of the Non-Crossing Approximation with the Fluctuation Dissipation Relation, the self-energy contribution $\tilde{\Sigma}_{I,nl}$ plays a key role. Hence, it is useful to rewrite this Dyson series as follows:

$$G^{SC}(\omega) = \left(G_1^{-1}(\omega) - \tilde{\Sigma}_{I,nl}^{SC}(\omega)\right)^{-1},\tag{6.2.8}$$

defining,

$$G_1(\omega) = \left(G_{(0)}^{-1}(\omega) - \tilde{\Sigma}_S(\omega) - \tilde{\Sigma}_{I,l}(\omega)\right)^{-1}.$$
(6.2.9)

Doing this allows us to view G_1 as a redefined bare Green's function, and write a Dyson series with respect to the non-linear interaction. Henceforth, unless stated otherwise, we refer to G_1 as our bare Green's function.

6.3 Consistency of Non-Crossing Approximation with the Fluctuation Dissipation Relation

Here, focusing on the simple case for the non-linear interaction Hamiltonian as expressed by Eq.(6.2.1), we demonstrate that the self-consistent steady-state Green's function obeys the Fluctuation-Dissipation Relation (FDR), i.e.,

$$G_K^{SC}(\omega) = \left(G_R^{SC}(\omega) - G_A^{SC}(\omega)\right) \coth\left(\frac{\beta}{2}\omega\right).$$
(6.3.1)

The arguments used to do so are proven in Appendix D and Appendix E. We have proved them for the general class of models described by Hamiltonians in Eq.(6.0.1). So, analogous proof demonstrates FDR for each of these models.

To prove this, we focus on an iterative mechanism of implementing the self-consistent Born approximation. Upon substituting the Dyson equation for G^{SC} on the right-hand side in Eq.(6.2.8), the self-energy $\tilde{\Sigma}_{I,nl}^{SC}$ recursively appears on the right-hand side of the equation again. This is why, self-consistent Born approximation is termed "self-consistent" [30]. As a result, the self-consistent Born approximation can be implemented through the following iterative mechanism:

Initial Step: Write down the Dyson equation with the leading-order Green's function G_1 expressed by Eq.(6.2.9), appearing inside the leading order self-energy for the model under consideration, expressed by

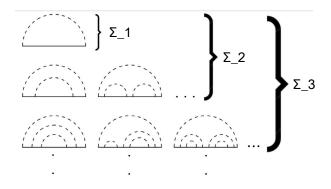


Figure 6.1: Non-crossing diagrams captured by the Self-Energy $\tilde{\Sigma}_{1,nl}$, $\tilde{\Sigma}_{2,nl}$ and $\tilde{\Sigma}_{3,nl}$, expressed by Eq.(6.3.2), Eq.(6.3.3) and Eq.(6.3.4) respectively. Here, the solid lines represent a system propagator, and the dashed lines represent a bath propagator.

Eq.(6.2.6), as follows:

$$\tilde{\Sigma}_{1,nl}(\omega) = \int_{\tau} D_B(\tau) \circ G_1(\tau) e^{i\omega\tau},$$

$$G_2(\omega) = \left(G_1^{-1}(\omega) - \tilde{\Sigma}_{1,nl}^{(2)}(\omega)\right)^{-1}.$$
(6.3.2)

Iteration 1: Define a new self-energy $\tilde{\Sigma}_{2,nl}$ and a corresponding Green's function G_3 with the Green's function G_2 appearing inside the self-energy:

$$\tilde{\Sigma}_{2,nl}(\omega) = \int_{\tau} D_B(\tau) \circ G_2(\tau) e^{i\omega\tau},$$

$$G_3(\omega) = \left(G_1^{-1}(\omega) - \tilde{\Sigma}_{2,nl}((\omega))\right)^{-1}.$$
(6.3.3)

Iteration 2: Further, define a new self-energy $\tilde{\Sigma}_{3,nl}$ and a corresponding Green's function G_4 with the Green's function G_3 appearing inside the self-energy:

$$\tilde{\Sigma}_{3,nl}(\omega) = \int_{\tau} D_B(\tau) \circ G_3(\tau) e^{i\omega\tau}$$

$$G_4(\omega) = \left(G_1^{-1}(\omega) - \tilde{\Sigma}_{3,nl}(\omega)\right)^{-1}$$
(6.3.4)

Performing this iteration infinitely generates all the NCA diagrams, and therefore, generates the selfconsistent Green's function G^{SC} . This is a method for implementing the self-consistent Born approximation. Now, to proceed further and use this to show that G^{SC} obeys the FDR, we have proved two key statements.

- 1. *Proved in Appendix D*: If the self-energy obeys the FDR, then the corresponding Green's function related to it by the Dyson series also obeys the same.
- 2. *Proved in Appendix E*: If the Green's functions appearing inside the self-energy obey the FDR, then the self-energy itself also obeys the same.

So, for the case of non-linear interaction Hamiltonian as expressed by Eq.(6.2.1), by alternately applying Statement 1 and Statement 2, one can observe that Green's function and self-energy generated at each step of the iterative process satisfy the FDR. Further, as depicted in FIG. 6.1, each subsequent iteration corresponds to a superclass of NCA diagrams with respect to the previous step. As mentioned earlier, performing this iteration infinitely generates all the NCA diagrams. Thus, this demonstrates that the self-consistent Green's function also satisfies the FDR. As previously stated, Statement 1 and Statement 2 have been proved abstractly for the class of models described by the Hamiltonian in Eq.(6.0.1), analogous proof demonstrates FDR for each of these models.

6.4 Comparison of greens function obtained using different techniques

In this section, we make a quantitative comparison between the self-consistent Green's function G^{SC} given by Eq.(6.2.8), Green's function G_2 given by Eq.(6.3.2), and Green's function G_B from the standard Born Approximation given by Eq.(6.2.5). The iterative mechanism for calculating the self-consistent Green's function discussed in the previous section highlights that Eq.(6.2.8) is not of the first order but rather of infinite order. Hence, we emphasize that the self-consistent Green's function might remain accurate even when the Green's function from the 'standard Born approximation' exhibits significant deviation. The self-consistent Green's function might also qualitatively capture the physics in the strong-coupling regime [39], while quantitative accuracy cannot be expected there.

The Green's function G^{SC} corresponds to the self-energy $\tilde{\Sigma}^{SC}$, which contains all the NCA diagrams. As depicted in FIG. 6.1, G_2 corresponds to the self-energy $\tilde{\Sigma}_1$, which represents the smallest class of NCA diagrams that satisfy the FDR. For the simple case of Hamiltonian given by Eq.(6.2.1), we explicitly demonstrate in Appendix F that G_2 satisfies the FDR. Conversely, in the same Appendix, we show that the steady-state Green's function G_B from the 'standard Born approximation' fails to satisfy the FDR.

Here, we perform a quantitative comparison of the steady-state Green's functions $G^{SC}(\tau)$, $G_2(\tau)$, and $G_B(\tau)$ for the Hamiltonian in Eq.(6.2.1). The explicit analytical derivation for $G_2(\tau)$ and $G_B(\tau)$ is provided in Appendix F. Meanwhile, we compute $G^{SC}(\tau)$ by numerically solving the integral-differential equation given by Eq.(6.2.8). Solving Eq.(6.2.8) requires $G^{SC}(0)$ and $\frac{dG^{SC}}{d\tau}(\tau)|_{\tau=0}$ as initial conditions, which are steady state one-point expectation values. Determining the precise initial condition amounts to computing a density matrix, denoted as $\rho(t)$ using a self-consistent dynamical map (as detailed in paper [39]), and then taking the $t \to \infty$ limit. This has a high computational cost. So, instead of doing this, we use steady-state

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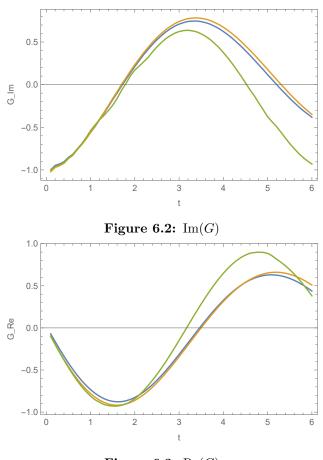


Figure 6.3: $\operatorname{Re}(G)$

Figure 6.4: This plot depicts a comparison between the steady state Green's functions G_2 , G_B , and G^{SC} for $\lambda^2 = 0.02$. The blue, orange and green lines represent G_B , G_2 , and G^{SC} , respectively.

one-point expectation values associated with the Gibbs state,

$$\rho_{Gibbs} = \frac{e^{-\beta H_S}}{\text{Tr}[e^{-\beta H_S}]},\tag{6.4.1}$$

to compute $G^{SC}(\tau)$. For weak coupling, we expect the initial condition ρ_{Gibbs} should be very close to the correct one. This is further supported by the observation that $G^{SC}(\tau)$ closely agrees with the other two Green's functions in FIG. 6.4. In contrast, for strong coupling, we expect the correct initial condition to deviate from the one obtained from ρ_{Gibbs} . Therefore, by $G^{SC}(\tau)$) plotted in FIG. 6.7 we aim to depict its qualitative behavior and quantitative precision isn't expected.

We consider here a thermal bath with the spectral density:

$$J(\omega) = \pi \frac{\omega}{1 + \omega^2}.$$
(6.4.2)

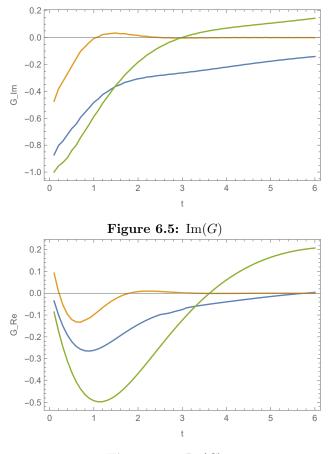


Figure 6.6: $\operatorname{Re}(G)$

Figure 6.7: This plot depicts comparison between G_B , G_2 , and G^{SC} for $\lambda^2 = 0.2$. The blue, orange, and green lines represent G_B , G_2 , and G^{SC} , respectively.

For comparison, we focus on the retarded Green's function of the system, given by:

$$G_R(\omega) = \left(G_{1R}^{-1}(\omega) - \tilde{\Sigma}_{nl,R}(\omega)\right)^{-1},\tag{6.4.3}$$

FIG. 6.4 demonstrates that for weaker coupling, with $\lambda^2 = 0.02$, $G^{SC}(\tau)$, $G_2(\tau)$ and $G_B(\tau)$ closely agree with each other. On the other hand, in FIG. 6.7 for stronger coupling, with $\lambda^2 = 0.2$, these functions exhibit significant differences. As discussed earlier, this deviation is expected because each of the steady-state Green's functions, G_B , G_2 , and G^{SC} , capture diagrams to different orders in perturbation theory. All these Green's functions display damped oscillatory behavior.

Part IV

Discussions and Outlook

Chapter 7

Conclusion

In the first half of this thesis, our focus is on the concept that perturbing the system around thermal equilibrium aids in understanding crucial aspects of dynamics beyond equilibrium. We begin by showcasing how the Lindblad Master equation is restricted by the need to comply with the Second Law of thermodynamics. Specifically, we insist on the positivity of relative von Neumann entropy production for Open system dynamics, leading to specific equality and inequality constraints on the coefficients within the Master equation. Additionally, we delve into thermalization and CPTP (Completely Positive Trace Preserving) constraints, demonstrating that the constraints stemming from entropy production positivity mirror those from thermalization and stability.

Furthermore, we present an abstract derivation outlining a general form for the retarded Green's function applicable to a broad model. Through this derivation, we methodically clarify that the poles of the retarded Green's functions encapsulate the spectrum of the Liouvillian that governs density matrix dynamics. Expanding on this concept, we extend our demonstration to encompass any higher-order retarded correlation function, elucidating how the poles of an n-point retarded Green's function capture the Liouvillian's spectrum. This outcome can be extended to encompass any out-of-time-ordered correlation function and its corresponding Liouvillian spectrum.

We anticipate that the advancements in understanding hydrodynamics over the past decade can offer more insights into open quantum systems. Specifically, the classification of coefficients in the higher derivative terms of the Navier-Stokes equation based on certain symmetries has provided valuable lessons on how these terms contribute to dissipative dynamics near equilibrium. Moreover, the Kubo formula in hydrodynamics offers an efficient method for computing out-of-time ordered correlators. It would be intriguing to explore whether analogous relations to the Kubo formula can be derived from an open quantum system governed by the Lindblad Master equation.

Additionally, significant work by Minwalla et al. [40] has demonstrated a precise mapping between the



Figure 7.1: Self Energy ' $\tilde{\Sigma}_{OCA}$ ' for One Crossing Approximation. Here, the solid line with a 'dot' represents the total system Green's function, and the dashed line represents a bath Green's function.

dynamical equations of black holes out of equilibrium and the nonlinear Navier-Stokes equation. Hence, we speculate that Black Hole Quasinormal Modes, which describe the behavior of black hole dynamics under small perturbations around equilibrium, can be modeled using Feynman-Vernon Influence functions or, equivalently, the Lindblad Master equation.

In open quantum systems, thermalization implies that multi-time correlation functions must conform to the KMS/FDR condition. In this paper, we specifically explore the KMS condition for the two-point correlation function. In instances of exactly solvable models like Caldeira-Leggett, we can explicitly verify the satisfaction of the KMS condition by the two-time correlation function at late times. However, for non-exactly solvable models, approximate techniques are required to compute the two-point function.

In the next part of the thesis, we employ the image operator method as an approximate technique, illustrating that the resultant correlation function adheres to the KMS relation. Nonetheless, this method establishes KMS only for specific examples and is reliant on the weak system-bath coupling approximation. To go beyond the standard weak coupling limit, the subsequent section of our paper introduces a self-consistent perturbative technique—the self-consistent Born approximation or NCA approach—based on the Schwinger-Keldysh path integral. Through this approach, we abstractly show that the steady-state correlation function must conform to the KMS relation for a generic system. This approach also allows us to go beyond the standard weak coupling limit. To demonstrate this, we perform a quantitative comparison of the steady-state Green's functions from the NCA approach with the Green's function from the standard weak coupling limit. These functions closely agree for weak coupling, whereas differ significantly in the stronger coupling, demonstrating that the NCA approach can help to go beyond the weak coupling limit.

It is worth mentioning that one can systematically go beyond the self-consistent Green's function approximation (NCA) by taking one crossing diagram (OCA). In other words, we can include a leading order diagram beyond the NCA to the self-energy and make a comparison similar to the one depicted in FIG. 6.4 and FIG. 6.7. The self-energy corresponding to the OCA is depicted diagrammatically in FIG. 7.1. It will again be interesting to see whether this bigger class of diagrams satisfies the KMS condition or not. Further, one can try to make a comparison between the accuracy of the steady state green's function derived using NCA, OCA, and higher-order self-consistent approximations [39]. The principle of Self-Consistency is not limited to expanding the two-point function. As an extension of our work, it will be interesting to check whether the self-consistent diagrams for four-point and higher-point functions satisfy the KMS condition. Along these lines, it would be interesting to investigate OTOC under the same set of ideas.

Another useful approximate way to calculate correlation function is the standard Quantum Regression Theorem (QRT). The QRT asserts that understanding the time evolution of a single-point function is adequate

Conclusion

for determining the time evolution of two-point or multi-point correlation functions. For calculating the one-point function and to go beyond the standard weak coupling limit, recently in [39], the NCA-Master equation or NCA Dynamical map was used. It is formally very similar and reduces to the standard master equations at sufficiently weak coupling. An intriguing avenue of exploration would involve incorporating the NCA Dynamical maps with the QRT to compute Green's function. This dynamic analysis could then be compared with the steady-state Green's function calculated using the NCA approach outlined in this paper.

We expect that this conceptual framework, the NCA approach, is extendable to out-of-equilibrium correlation functions [41]. Note that, to calculate the out-of-equilibrium correlation function we need information of the system's initial state. Additionally, it is known that out-of-equilibrium correlation functions break translational symmetry, rendering Fourier space analysis difficult. These two facts imply that, in general, calculating the out-of-equilibrium correlation function is technically challenging. However, we believe that this NCA technique is well-suited to go beyond the standard weak coupling limit in calculating the out-of-equilibrium correlation functions.

Appendix A

Image operator method

In this appendix, we present a detailed derivation of the two-point correlation function using the image operator method. It's important to note that our derivation applies to an arbitrary system Hamiltonian interacting with a bath through a generic system operator S. The total Hamiltonian for our configuration is given by the expression:

$$H = H_S + H_R + H_{SR}$$

= $H_S + \sum_k \Omega_k b_k^{\dagger} b_k + \sum_k \alpha_k (Sb_k^{\dagger} + S^{\dagger} b_k) ,$ (A.0.1)

here b_k and b_k^{\dagger} represent bosonic or fermionic annihilation and creation operators, respectively. We want to calculate the two-point function of the form, $\langle O_1(t+\tau)O_2(t)\rangle$, at the steady state i.e. at $t \to \infty$. To compute $\langle O_1(t+\tau)O_2(t)\rangle$, we are going to first express it in terms of one-point reduced operators. In Ref. [17, 18], it was shown that the two-point reduced operator can be written as

$$[O_1(t+\tau)O_2(t)]_S = O_{1S}(t+\tau)O_{2S}(t) + I[O_{1S}(t+\tau), O_{2S}(t)].$$
(A.0.2)

Here, O_{1S} and O_{2S} represent the reduced one-point operators whose evolution is governed by the Born master equation [1]. The term $I[O_{1S}(t + \tau), O_{2S}(t)]$ is referred to as the irreducible term, and it can be expressed in terms of the one-point reduced operator up to the leading order in system-bath coupling as

$$I[O_{1S}(t+\tau), O_{2S}(t)] = \int_{0}^{t+\tau} d\tau_{1} \int_{0}^{t} d\tau_{2} \ \beta(\tau_{2}-\tau_{1}) \Big[O_{1S}(t+\tau), \tilde{S}(-\tau_{1}) \Big] \Big[\tilde{S}^{\dagger}(-\tau_{2}), O_{2S}(t) \Big] \\ + \int_{0}^{t+\tau} d\tau_{1} \int_{0}^{t} d\tau_{2} \ \alpha(\tau_{2}-\tau_{1}) \Big[O_{1S}(t+\tau), \tilde{S}^{\dagger}(-\tau_{1}) \Big] \Big[\tilde{S}(-\tau_{2}), O_{2S}(t) \Big] , \qquad (A.0.3)$$

where $\tilde{S}(t)$ represents the interaction picture operator, defined as $\tilde{S}(t) = e^{-iH_S t} S e^{iH_S t}$. This operator can be decomposed as $\tilde{S}(t) = \sum_m S_m e^{i\omega'_m t}$, whereas $\alpha(\tau)$ and $\beta(\tau)$ are intricately connected to the bath correlation

function, or, to be more explicit,

$$\alpha(\tau) = \sum_{k} |\alpha_{k}|^{2} \operatorname{Tr}_{R} \left[b_{k} \tilde{b}_{k}^{\dagger}(-\tau) \rho_{R} \right] = \sum_{k} |\alpha_{k}|^{2} \left(1 - \eta \ n_{\eta}(\Omega_{k}) \right) e^{i\Omega_{k}\tau},$$

$$\beta(\tau) = \sum_{k} |\alpha_{k}|^{2} \operatorname{Tr}_{R} \left[b_{k}^{\dagger} \tilde{b}_{k}(-\tau) \rho_{R} \right] = \sum_{k} |\alpha_{k}|^{2} n_{\eta}(\Omega_{k}) e^{-i\Omega_{k}\tau}.$$
 (A.0.4)

In this context, $n_{\eta}(\Omega)$ denotes the Bose or Fermi distribution functions, expressed as $n_{\eta}(\Omega) = [e^{\beta\Omega} + \eta]^{-1}$, where $\eta = +1$ corresponds to fermions, and $\eta = -1$ corresponds to bosons. Now, let's focus on the first term of the irreducible part, $I[O_{1S}(t + \tau), O_{2S}(t)]$, in Eq.(A.0.3) i.e.

$$\int_{0}^{t+\tau} d\tau_{1} \int_{0}^{t} d\tau_{2} \ \beta(\tau_{2} - \tau_{1}) \Big[O_{1S}(t+\tau), \tilde{S}(-\tau_{1}) \Big] \Big[\tilde{S}^{\dagger}(-\tau_{2}), O_{2S}(t) \Big] \\
= \sum_{j,l,m,n} \int_{0}^{t+\tau} d\tau_{1} \int_{0}^{t} d\tau_{2} \ \beta(\tau_{2} - \tau_{1}) \Big[O_{1jS}(t+\tau-\tau_{1}), S_{m} \Big] \Big[S_{n}^{\dagger}, O_{2lS}(t-\tau_{2}) \Big] e^{-i(\omega_{j} + \omega_{m}')\tau_{1}} e^{-i(\tilde{\omega}_{l} - \omega_{n}')\tau_{2}} + O(|\alpha_{k}|^{4}) \\$$
(A.0.5)

In the last step of the above equation, we insert the following expressions

$$O_{1S}(t) = \sum_{j} O_{1jS}(t - t')e^{-i\omega_{j}t'} + O(|\alpha_{k}|^{2}),$$

$$O_{2S}(t) = \sum_{l} O_{2lS}(t - t')e^{-i\tilde{\omega}_{l}t'} + O(|\alpha_{k}|^{2}).$$
(A.0.6)

Let's define, $\tau'_1 = t + \tau - \tau_1$ and $\tau'_2 = t - \tau_2$, from the definition of τ'_1 it is clear that the limit of τ'_1 will be from $t + \tau$ to 0 and similarly the limit of τ'_2 will be from t to 0. In terms of these new variables, we get the following expression

$$\sum_{j,l,m,n} \int_{0}^{t+\tau} d\tau_{1} \int_{0}^{t} d\tau_{2} \ \beta(\tau_{2} - \tau_{1}) \Big[O_{1jS}(t+\tau-\tau_{1}), S_{m} \Big] \Big[S_{n}^{\dagger}, O_{2lS}(t-\tau_{2}) \Big] e^{-i(\omega_{j}+\omega_{m}')\tau_{1}} e^{-i(\tilde{\omega}_{l}-\omega_{n}')\tau_{2}} \\ = \sum_{j,l,m,n} \int_{0}^{t+\tau} d\tau_{1}' \int_{0}^{t} d\tau_{2}' \ \beta(\tau_{1}' - \tau_{2}' - \tau) \Big[O_{1jS}(\tau_{1}'), S_{m} \Big] \Big[S_{n}^{\dagger}, O_{2lS}(\tau_{2}') \Big] e^{-i(\omega_{j}+\omega_{m}')(t+\tau-\tau_{1}')} e^{-i(\tilde{\omega}_{l}-\omega_{n}')(t-\tau_{2}')} .$$
(A.0.7)

Similarly, we can simplify the other term of the irreducible part $I[O_{1S}(t+\tau), O_{2S}(t)]$, expressed in Eq.(A.0.3). Finally, by substituting α , β defined in Eq.(A.0.4), we get the two-point reduced operator formulated in Eq.(5.1.3).

Appendix B

Laplace transformation

In this appendix, we are going to find the Laplace transformation of $a_S(t)$. To do that we are going to first write down the equation of motion of $a_S(t)$

$$\frac{d}{dt}a_S(t) = -i\omega_0 a_S(t) - \int_0^t dt' K(t-t')a_S(t') , \qquad (B.0.1)$$

where $K(t-t') = \sum_k |\alpha_k|^2 e^{-i\omega_k(t-t')}$. Laplace transformation of the above equation gives

$$\tilde{a}_S(-i\Omega) = \frac{a}{i(\omega_0 - \Omega) + \tilde{K}(-i\Omega)} , \qquad (B.0.2)$$

where $\tilde{K}(-i\Omega) = J(\Omega)/2 + i\Sigma(\Omega)$.

Thermalization in Open Quantum Systems

Appendix C

Schwinger Keldysh Path Integral

The total Hamiltonian of Eq.(6.0.1) when promoted to the Schwinger-Keldysh Path Integral and expressed in the classical-quantum basis for field operators takes the form $S = S_S + S_B + S_{I,l} + S_{I,nl}$, where

$$S_{I,l} = \int_{\tau} \left(a_c^*(\tau) b_{k,q}(\tau) + a_q^*(\tau) b_{k,c}(\tau) + h.c. \right),$$

$$S_{I,nl} = \int_{\tau} \left((a^{*m} a^n)_c(\tau) b_{k,q}(\tau) + (a^{*m} a^n)_q(\tau) b_{k,c}(\tau) + h.c. \right).$$
(C.0.1)

Here, a and b are complex-valued fields associated with the coherent states of the system and bath, respectively. As the Schwinger-Keldysh functional integral, with a total action involving both system and bath degrees of freedom, is quadratic in the latter, the bath can be integrated out. After integrating out the bath, the reduced Schwinger-Keldysh action is, $S = S_s + S'_l + S'_{nl}$, where

$$\begin{split} S_l' &= \int_w \left(a_c^*(\omega) \quad a_q^*(\omega) \right) \left(\begin{array}{cc} -2iJ(\omega)(2n(\omega)+1) & -iJ(\omega)+\Sigma(\omega) \\ iJ(\omega)+\Sigma(\omega) & 0 \end{array} \right) \left(\begin{array}{c} a_c(\omega) \\ a_q(\omega) \end{array} \right), \\ S_{nl}' &= \int_w \left((a^{*m}a^n)_c(\omega)(a^{*m}a^n)_q(\omega) \right) \left(\begin{array}{c} -2iJ(\omega)(2n(\omega)+1) & -iJ(\omega)+\Sigma(\omega) \\ iJ(\omega)+\Sigma(\omega) & 0 \end{array} \right) \left(\begin{array}{c} (a^{*n}a^m)_c(\omega) \\ (a^{*n}a^m)_q(\omega) \end{array} \right). \quad (C.0.2) \end{split}$$

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Appendix D

$\mathbf{FDR}: \mathbf{Self\text{-}Energy} \leftrightarrow \mathbf{Green's} \ \mathbf{Function}$

In this section, we will demonstrate that if the self-energy $\tilde{\Sigma}_I$ due to system bath interaction satisfies the Fluctuation-Dissipation Relation (FDR), i.e.,

$$\tilde{\Sigma}_{K}(\omega) = \left(\tilde{\Sigma}_{R}(\omega) - \tilde{\Sigma}_{A}(\omega)\right) \coth\left(\frac{\beta}{2}\omega\right),\tag{D.0.1}$$

then the corresponding Green's function G, related to it by the Dyson series:

$$G(\omega) = \left(G_{(0)}^{-1}(\omega) - \tilde{\Sigma}_I(\omega)\right)^{-1},\tag{D.0.2}$$

must also obey the same relation. Here, $G_{(0)}$ is the bare Green's function with respect to the system-bathinteraction, i.e., calculated using H_S , and it is given by

$$G_{(0)}(\omega) = \begin{pmatrix} 0 & \frac{1}{\omega - \Sigma_S(\omega)} \\ \frac{1}{\omega - \Sigma_S(\omega)} & 0 \end{pmatrix},$$
 (D.0.3)

where ' Σ_S ' is the self-energy due to intra-system interactions, making it always a real-valued function. Using the Dyson equation, it is easy to show that

$$G(\omega) = \left(G_{(0)}^{-1}(\omega) - \tilde{\Sigma}_{I}(\omega)\right)^{-1}$$

$$= \left(\frac{\tilde{\Sigma}_{IK}(\omega)}{(\omega - \Sigma_{S}(\omega) - \tilde{\Sigma}_{IA}(\omega))(\omega - \Sigma_{S}(\omega) - \tilde{\Sigma}_{IR}(\omega))} \quad \frac{1}{\omega - \Sigma_{S}(\omega) - \tilde{\Sigma}_{IR}(\omega)}}{\frac{1}{\omega - \Sigma_{S}(\omega) - \tilde{\Sigma}_{IA}(\omega)} \quad 0}\right).$$
(D.0.4)

That implies,

$$\frac{G_K(\omega)}{G_R(\omega) - G_A(\omega)} = \frac{\tilde{\Sigma}_{IK}(\omega)}{\tilde{\Sigma}_{IR}(\omega) - \tilde{\Sigma}_{IA}(\omega)}.$$
 (D.0.5)

From here, it's transparent that Green's function G satisfies FDR if and only if $\tilde{\Sigma}_I$ satisfies the same.

Appendix E

Proof of FDR for the general form of leading order self-energy

In this section, working with the general class of models represented by the Action in Eq. (C.0.2), we demonstrate a condition under which the leading-order self-energy term satisfies the FDR. To do that, we first identify that the loops appearing in the leading-order self-energy diagrams can be classified into 'rainbow' and 'rings'. We can classify all the Feynman diagrams into diagrams with a ring, and diagrams without a ring. This classification is illustrated in FIG. E.3 for the total Hamiltonian of the form given by Eq. (6.0.1), with the simple non-linear interaction Hamiltonian $H_{I,nl} = a^{\dagger 2}ab_k + a^{\dagger}a^2b_k^{\dagger}$.

It will turn out, that only the rainbow part of these diagrams plays a non-trivial role in consistency with the FDR. The contribution from rings simply factors out from all the various time-ordered self-energies and, therefore, is inconsequential for the consistency with the FDR. Consequently, for simplicity, we first focus on the diagrams with no rings in the first subsection and prove the FDR. We then turn our attention to diagrams with rings in the next subsection.

E.1 Diagrams with no rings

Using the Schwinger-Keldysh path integral and employing the standard tool of Feynman diagrams that arise from the conventional Wick contraction, one can demonstrate that the leading-order self-energy diagrams with no rings (so only rainbow loops) are of the following general form:

$$\tilde{\Sigma}(\tau) = G_1(\tau_1) \circ G_2(\tau_2) \circ \dots \circ G_l(\tau_l), \tag{E.1.1}$$

where $\tau_j \in {\tau, -\tau}$ for all j, and $G_j(\tau_j)$ represents a system or bath Green's function. We establish the rule for the product ' \circ ' in accordance with the rules for Wick contraction. The product ' \circ ' is defined as follows:

for
$$L = \{1, 2, ..., l\}$$
,

$$\tilde{\Sigma}_{K}(\tau) = -i \sum_{\substack{S \subseteq L \\ n(S) \in 2\mathbb{Z}}} \left(\left(\prod_{\mu \in S} iG_{K\mu}(\tau_{\mu})\right) \left(\prod_{\substack{\nu \in \overline{S} \\ \tau_{\nu} = \tau}} iG_{R\nu}(\tau)\right) \left(\prod_{\substack{\nu \in \overline{S} \\ \tau_{\nu} = -\tau}} iG_{A\nu}(-\tau)\right) \right) - i \sum_{\substack{S \subseteq L \\ n(S) \in 2\mathbb{Z}}} \left(\left(\prod_{\mu \in S} iG_{K\mu}(\tau_{\mu})\right) \left(\prod_{\substack{\nu \in \overline{S} \\ \tau_{\nu} = -\tau}} iG_{R\nu}(-\tau)\right) \right) \right)$$

$$\tilde{\Sigma}_{R}(\tau) = -i \sum_{\substack{S \subseteq L \\ n(S) \in 2\mathbb{Z}+1}} \left(\left(\prod_{\mu \in S} iG_{K\mu}(\tau_{\mu})\right) \left(\prod_{\substack{\nu \in \overline{S} \\ \tau_{\nu} = \tau}} iG_{R\nu}(\tau)\right) \right) \left(\prod_{\substack{\nu \in \overline{S} \\ \tau_{\nu} = -\tau}} iG_{R\nu}(-\tau)\right) \right),$$

$$\tilde{\Sigma}_{A}(\tau) = -i \sum_{\substack{S \subseteq L \\ n(S) \in 2\mathbb{Z}+1}} \left(\left(\prod_{\mu \in S} iG_{K\mu}(\tau_{\mu})\right) \left(\prod_{\substack{\nu \in \overline{S} \\ \tau_{\nu} = \tau}} iG_{A\nu}(\tau)\right) \left(\prod_{\substack{\nu \in \overline{S} \\ \tau_{\nu} = -\tau}} iG_{R\nu}(-\tau)\right) \right),$$
(E.1.2)

where, n(S) denotes the number of elements in the set S, \overline{S} denotes the set complement to S, and $2\mathbb{Z}$ and

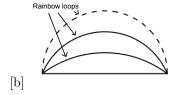


Figure E.1: Diagrams with no Rings

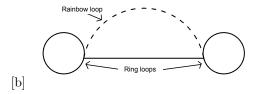


Figure E.2: Diagrams with Rings

Figure E.3: The two classes of Feynman diagrams for the simple case of the non-linear interaction Hamiltonian $H_{I,nl} = a^{\dagger 2}ab_k + a^{\dagger}a^2b_k^{\dagger}$. We define 'rainbow' as a loop that corresponds to two distinct vertices, whereas, we define 'ring' as a loop that has only one vertex associated with it. Here, the solid lines represent the system Green's functions, and the dashed lines represent the bath Green's functions.

 $2\mathbb{Z} + 1$ denote the sets of all even and odd integers, respectively. We represent the self-energy matrix in terms of the time-ordered self-energies as follows:

$$\tilde{\Sigma}(\tau) = \begin{pmatrix} 0 & \tilde{\Sigma}_A(\tau) \\ \\ \\ \tilde{\Sigma}_R(\tau) & \tilde{\Sigma}_K(\tau) \end{pmatrix}.$$
(E.1.3)

• •

As described in the paper [32], the contour-ordered thermal two-point correlators are related by the following structure:

$$\begin{pmatrix} G_K(\tau) & G_R(\tau) \\ G_A(\tau) & 0 \end{pmatrix} = \int_{\omega} \rho(\omega) \begin{pmatrix} \coth\left(\frac{\beta}{2}\omega\right) & \theta(\tau) \\ -\theta(-\tau) & 0 \end{pmatrix} e^{-i\omega\tau}.$$
 (E.1.4)

Where, ' $\rho(\omega)$ ' stands for 'spectral function' which is directly related to the Fourier Transform of commutators in the theory:

$$\int_{\omega} \rho(\omega) e^{-i\omega\tau} = \langle [\hat{a}^{\dagger}(\tau), \hat{a}(0)] \rangle.$$
(E.1.5)

So, for j such that $\tau_j = \tau$,

$$G_{j}(\tau) = \begin{pmatrix} G_{Kj}(\tau) & G_{Rj}(\tau) \\ G_{Aj}(\tau) & 0 \end{pmatrix}$$
$$= \int_{\omega_{j}} \rho_{j}(\omega_{j}) \begin{pmatrix} \coth\left(\frac{\beta}{2}\omega_{j}\right) & \theta(\tau) \\ -\theta(-\tau) & 0 \end{pmatrix} e^{-i\omega_{j}\tau}.$$
(E.1.6)

Next, for the convenience of denoting the product 'o', we perform the following transformation for $G_j(\tau_j)$ for which, $\tau_j = -\tau$:

$$G_{j}(-\tau) = \begin{pmatrix} G_{Kj}(-\tau) & G_{Aj}(-\tau) \\ G_{Rj}(-\tau) & 0 \end{pmatrix}$$
$$= \int_{\omega'_{j}} \rho'_{j}(\omega'_{j}) \begin{pmatrix} \coth\left(\frac{\beta}{2}\omega'_{j}\right) & \theta(\tau) \\ -\theta(-\tau) & 0 \end{pmatrix} e^{-i\omega'_{j}\tau}, \qquad (E.1.7)$$

where we define $\omega'_j = -\omega_j$ and $\rho'_j(\omega) = -\rho_j(-\omega)$. It is important to note that it assumes the same form as $G_j(\tau)$. This equivalence enables us to consistently express the self-energy term with no rings, as follows:

$$\tilde{\Sigma}(\tau) = G_1(\tau) \circ G_2(\tau) \circ \dots \circ G_l(\tau)$$
(E.1.8)

which gives, for $L=\{1,2,...,l\}$,

$$\tilde{\Sigma}_{K}(\tau) = -i \sum_{\substack{S \subseteq L\\n(S) \in 2\mathbb{Z}}} \left(\left(\prod_{\mu \in S} iG_{K\mu}(\tau)\right) \left(\prod_{\nu \in \overline{S}} iG_{R\nu}(\tau)\right) \right) - i \sum_{\substack{S \subseteq L\\n(S) \in 2\mathbb{Z}}} \left(\left(\prod_{\mu \in S} iG_{K\mu}(\tau)\right) \left(\prod_{\nu \in \overline{S}} iG_{A\nu}(\tau)\right) \right), \quad (E.1.9)$$

$$\tilde{\Sigma}_{R}(\tau) = -i \sum_{\substack{S \subseteq L\\n(S) \in 2\mathbb{Z}+1}} \left(\left(\prod_{\mu \in S} i G_{K\mu}(\tau) \right) \left(\prod_{\nu \in \overline{S}} i G_{R\nu}(\tau) \right) \right),$$
(E.1.10)

$$\tilde{\Sigma}_{A}(\tau) = -i \sum_{\substack{S \subseteq L\\n(S) \epsilon 2\mathbb{Z}+1}} \left(\left(\prod_{\mu \in S} iG_{K\mu}(\tau) \right) \left(\prod_{\nu \in \overline{S}} iG_{A\nu}(\tau) \right) \right)$$
(E.1.11)

Here, expressing the thermal Green's functions in the spectral function representation, one obtains,

$$\tilde{\Sigma}_{K}(\tau) = \int_{\omega_{1},\omega_{2},\dots,\omega_{l}} \left(\prod_{j \in L} \rho_{j}(\omega_{j})\right) \left(\sum_{\substack{S \subseteq L \\ n(\overline{S}) \in \mathbb{Z}}} \left(\prod_{j' \in \overline{S}} \coth\left(\frac{\beta}{2}\omega_{j'}\right)\right)\right) e^{-i(\sum_{j \in L} \omega_{j}\tau)}, \quad (E.1.12)$$

$$\tilde{\Sigma}_{R}(\tau) = \int_{\omega_{1},\omega_{2},\dots,\omega_{l}} \theta(\tau) \Big(\prod_{j \in L} \rho_{j}(\omega_{j})\Big) \Big(\sum_{\substack{S \subseteq L\\n(S) \in \mathbb{ZZ}+1}} \Big(\prod_{j' \in \overline{S}} \coth\left(\frac{\beta}{2}\omega_{j'}\right)\Big)\Big) e^{-i(\sum_{j \in L} \omega_{j}\tau)},$$
(E.1.13)

$$\tilde{\Sigma}_{A}(\tau) = \int_{\omega_{1},\omega_{2},\dots,\omega_{l}} -\theta(-\tau) \Big(\prod_{j \in L} \rho_{j}(\omega_{j})\Big) \Big(\sum_{\substack{S \subseteq L\\n(S) \in 2\mathbb{Z}+1}} \big(\prod_{j' \in \overline{S}} \coth\left(\frac{\beta}{2}\omega_{j'}\right)\big)\Big) e^{-i(\sum_{j \in L} \omega_{j}\tau)}.$$
(E.1.14)

The self-energy adheres to the spectral function representation, as can be observed by employing the identity

$$\operatorname{coth}\left(\sum_{i=1}^{l} x_{i}\right) = \frac{\sum_{\substack{n(S) \in 2\mathbb{Z} \\ n(S) \in 2\mathbb{Z}+1}} \left\{\prod_{i \in \overline{S}} \operatorname{coth}(x_{i})\right\}}{\sum_{\substack{n(S) \in 2\mathbb{Z}+1 \\ n(S) \in 2\mathbb{Z}+1}} \left\{\prod_{i' \in \overline{S}} \operatorname{coth}(x_{i'})\right\}},$$
(E.1.15)

and defining its spectral function as,

$$\varrho(\omega) = \int_{\omega_1, \omega_2, \dots, \omega_l} \left(\prod_{j \in L} \rho_j(\omega_j) \right) \delta\left(\omega - \sum_{j \in L} \omega_j \right),$$
(E.1.16)

giving,

$$\begin{pmatrix} 0 & \tilde{\Sigma}_A(\tau) \\ & \\ \tilde{\Sigma}_R(\tau) & \tilde{\Sigma}_K(\tau) \end{pmatrix} = \int_{\omega} \varrho(\omega) \begin{pmatrix} 0 & \theta(\tau) \\ & \\ -\theta(-\tau) & \coth\left(\frac{\beta}{2}\omega\right) \end{pmatrix} e^{-i\omega\tau}.$$
 (E.1.17)

This proves the FDR for leading-order self-energy rainbow diagrams when the Green's functions appearing in the self-energy obey the same.

E.2 Diagrams with Rings

Now, let's consider leading-order self-energy diagrams that also include rings. Firstly, due to the hermiticity of the interaction Hamiltonian, for any diagram with a ring involving the advanced Green's function, there exists a corresponding diagram with the ring involving the retarded Green's function. Therefore, the net contribution of these diagrams is proportional to $G_R(0) + G_A(0)$. Since $G_R(0) + G_A(0) = 0$ [42], these diagrams cancel out, leaving only the diagrams with all the rings involving Keldysh Green's function. Interestingly, these self-energy diagrams have the same general form as sunset diagrams with additional factors of the ring's Keldysh Green's functions, i.e., $G_{mK}(0)$. So, for a self-energy diagram with 'n' rings:

$$\tilde{\Sigma}(\tau) = \left(\prod_{m=1}^{n} G_{mK}(0)\right) G_1(\tau_1) \circ G_2(\tau_2) \circ \dots \circ G_l(\tau_l),$$
(E.2.1)

where $\tau_j \epsilon \{\tau, -\tau\}$ for all j. Because the ring Green's functions appear as common factors in all the time-ordered self-energies, the previous section's proof for FDR follows and we get:

$$\varrho(\omega) = \left(\prod_{m=1}^{n} G_{mK}(0)\right) \int_{\omega_1,\omega_2,\dots,\omega_l} \left(\prod_{j \in L} \rho_j(\omega_j)\right) \delta\left(\omega - \sum_{j \in L} \omega_j\right)$$
(E.2.2)

giving,

$$\begin{pmatrix} 0 & \tilde{\Sigma}_A(\tau) \\ & \\ \tilde{\Sigma}_R(\tau) & \tilde{\Sigma}_K(\tau) \end{pmatrix} = \int_{\omega} \varrho(\omega) \begin{pmatrix} 0 & \theta(\tau) \\ & \\ -\theta(-\tau) & \coth\left(\frac{\beta}{2}\omega\right) \end{pmatrix} e^{-i\omega\tau}.$$
 (E.2.3)

This completes the proof that if the Green's functions that appear inside the leading-order self-energy obey the FDR, then the self-energy obeys the same. Thermalization in Open Quantum Systems

Appendix F

Analytical calculation of steady state Green's functions G_B and G_2

In this section, we derive the explicit form of the steady-state Green's functions G_B and G_2 , expressed through the Dyson equations in Eq. (6.2.5) and (6.3.2), respectively. Additionally, we demonstrate that G_2 satisfies the Fluctuation-Dissipation Relation (FDR), whereas G_B fails to satisfy it.

Using the rules for product 'o' as stated in Appendix ??, the $\tilde{\Sigma}_B$ (Born) and $\tilde{\Sigma}_{1,nl}^{(2)}$ self energies defined in Section IV are:

$$\begin{split} \tilde{\Sigma}_{BK}(\tau) &= i(D_{BK}(\tau)G_{(0)K}(\tau) + D_{BR}(\tau)G_{(0)R}(\tau) + D_{BA}(\tau)G_{(0)A}(\tau)) \\ &= -i\sum_{k} |\alpha_{k}|^{2}e^{-i(\omega_{0}+\omega_{k})\tau} \mathbf{F}.\mathbf{T}. - 2iJ(\omega - \omega_{0}) \\ \tilde{\Sigma}_{BR}(\tau) &= i(D_{BK}(\tau)G_{(0)R}(\tau) + D_{BR}(\tau)G_{(0)K}(\tau)) \\ &= -i\theta(\tau)\sum_{k} |\alpha_{k}|^{2} \coth\left(\frac{\beta}{2}\omega_{k}\right)e^{-i(\omega_{0}+\omega_{k})\tau} \mathbf{F}.\mathbf{T}. - iJ(\omega - \omega_{0}) \coth\left(\frac{\beta}{2}(\omega - \omega_{0})\right) + \mathcal{P}\int_{\omega'} \frac{J(\omega - \omega_{0}) \coth\left(\frac{\beta}{2}(\omega' - \omega_{0})\right)}{\pi(\omega - \omega')} \\ \tilde{\Sigma}_{BA}(\tau) &= i(D_{BK}(\tau)G_{(0)A}(\tau) + D_{BA}(\tau)G_{(0)K}(\tau)) \\ &= i\theta(-\tau)\sum_{k} |\alpha_{k}|^{2} \coth\left(\frac{\beta}{2}\omega_{k}\right)e^{-i(\omega_{0}+\omega_{k})\tau} \mathbf{F}.\mathbf{T}.iJ(\omega - \omega_{0}) \coth\left(\frac{\beta}{2}(\omega - \omega_{0})\right) + \mathcal{P}\int_{\omega'} \frac{J(\omega - \omega_{0}) \coth\left(\frac{\beta}{2}(\omega' - \omega_{0})\right)}{\pi(\omega - \omega')} \\ (\mathbf{F}.0.1) \end{split}$$

Clearly,

$$\tilde{\Sigma}_{BK}(\omega) = (\tilde{\Sigma}_{BR}(\omega) - \tilde{\Sigma}_{BA}(\omega)) \frac{1}{\coth\left(\frac{\beta}{2}(\omega - \omega_0)\right)}$$
(F.0.2)

Note that, it does not satisfy the FDR. As a result, as proved in Appendix ??, the corresponding Green's function G_B also doesn't satisfy the FDR. Similarly, if

$$G_{1K}(\tau) = \int_{\omega} \rho(\omega) \begin{pmatrix} \coth\left(\frac{\beta}{2}\omega\right) & \theta(\tau) \\ -\theta(-\tau) & 0 \end{pmatrix} e^{-i\omega\tau}$$
(F.0.3)

Then,

$$\begin{split} \tilde{\Sigma}_{1K}^{(2)}(\tau) &= i(D_{BK}(\tau)G_{1K}(\tau) + D_{BR}(\tau)G_{1R}(\tau) + D_{BA}(\tau)G_{1A}(\tau)) \\ &= \int_{\omega} \rho(\omega) \sum_{k} |\alpha_{k}|^{2} (\coth\left(\frac{\beta}{2}\omega_{k}\right) \coth\left(\frac{\beta}{2}\omega\right) + 1)e^{-i(\omega+\omega_{k})\tau} \\ \text{F.T.} &- 2i\sum_{i} J(\omega-\omega_{i}) (\coth\left(\frac{\beta}{2}(\omega-\omega_{i})\right) \coth\left(\frac{\beta}{2}\omega_{i}\right) + 1) \\ \tilde{\Sigma}_{1R}^{(2)}(\tau) &= i(D_{BK}(\tau)G_{1R}(\tau) + D_{BR}(\tau)G_{1K}(\tau)) \\ &= -i\theta(\tau)\sum_{i} r_{i}\sum_{k} |\alpha_{k}|^{2} (\coth\left(\frac{\beta}{2}\omega_{k}\right) + \coth\left(\frac{\beta}{2}\omega_{i}\right))e^{-i(\omega_{i}+\omega_{k})\tau} \\ \text{F.T.} \sum_{i} (-iJ(\omega-\omega_{i}) (\coth\left(\frac{\beta}{2}(\omega-\omega_{i})\right) + \coth\left(\frac{\beta}{2}\omega_{i}\right)) + \mathcal{P}\int_{\omega'} \frac{J(\omega'-\omega_{i}) (\coth\left(\frac{\beta}{2}(\omega'-\omega_{i})\right) + \coth\left(\frac{\beta}{2}\omega_{i}\right))}{\pi(\omega-\omega')}) \\ \tilde{\Sigma}_{1A}^{(2)}(\tau) &= i(D_{BK}(\tau)G_{1A}(\tau) + D_{BA}(\tau)G_{1K}(\tau)) \\ &= i\theta(-\tau)\sum_{i} r_{i}^{*}\sum_{k} |\alpha_{k}|^{2} (\coth\left(\frac{\beta}{2}\omega_{k}\right) + \coth\left(\frac{\beta}{2}\omega_{i}^{*}\right))e^{-i(\omega_{i}^{*}+\omega_{k})\tau} \\ \text{F.T.} \sum_{i} (-iJ(\omega-\omega_{i}) (\coth\left(\frac{\beta}{2}(\omega-\omega_{i})\right) + \coth\left(\frac{\beta}{2}\omega_{i}^{*}\right)) + \mathcal{P}\int_{\omega'} \frac{J(\omega'-\omega_{i}) (\coth\left(\frac{\beta}{2}(\omega'-\omega_{i})\right) + \coth\left(\frac{\beta}{2}\omega_{i}\right))}{\pi(\omega-\omega')} \\ \text{F.T.} \sum_{i} (-iJ(\omega-\omega_{i}) (\coth\left(\frac{\beta}{2}(\omega-\omega_{i})\right) + \coth\left(\frac{\beta}{2}\omega_{i}^{*}\right)) + \mathcal{P}\int_{\omega'} \frac{J(\omega'-\omega_{i}) (\coth\left(\frac{\beta}{2}(\omega'-\omega_{i})\right) + \coth\left(\frac{\beta}{2}\omega_{i}\right))}{\pi(\omega-\omega')} \\ \end{array}$$

Using,

$$\coth(x_1 + x_2) = \frac{\coth(x_1)\coth(x_2) + 1}{\coth(x_1) + \coth(x_2)}$$
(F.0.4)

$$\implies \tilde{\Sigma}_{1K}^{(2)}(\omega) = \left(\tilde{\Sigma}_{1R}^{(2)}(\omega) - \tilde{\Sigma}_{1A}^{(2)}(\omega)\right) \coth\left(\frac{\beta}{2}\omega\right)$$
(F.0.5)

So, the self-energy satisfies FDR. As a result, as proved in Appendix ??, the corresponding Green's function G_B also satisfies the FDR.

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