

# Re-deriving a General Kubo Formulation for Open Finite Quantum Systems

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## Supervision

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## Abstract

This research project aims to generalize the Kubo Formulation for Open Finite Quantum Systems by studying the Master Equation approach and applying its findings to build a general model considering the initial correlation conditions of the system environment bath. The following report is a collection of all the literature reviews that have been carried out in an effort to understand Open Quantum Systems and the various methods involved in their theoretical and computational analysis in the hopes of deriving a generalized Kubo Formula applicable to particular Markovian Dynamics.

## 1 Introduction

The Kubo formula is a widely used equation in Linear Response Theory. It is able to express the linear response of an observable quantity placed under a time dependent perturbation. This allows us to calculate system responses due to external mechanical force or vibrations or the susceptibilities of systems under magnetic and/or electric fields. However, the formulation is often times limited in its functionality in Open Quantum Systems with certain conditions[1]. For example, in thermal conductivity, the Green-Kubo Formula can not be used for small systems pertaining to single particles or for systems with anomalous transport (often seen in low dimensional systems)[2]. This report will introduce the reader to Linear Response Theory, Fundamentals of the Kubo Formulation, and the Master Equation Approach used to solve Open Quantum Systems.

## 2 Linear Response Theory

Linear response theory is a powerful calculation tool used in classical and quantum systems, describing a system's evolution towards or away from equilibrium

under certain perturbative conditions. Using its formalism, we aim to decipher how systems react to external (driving) forces. Usually, these forces include pressure, magnetic fields, and electric fields. Real quantities that can be observed under this theory are called response functions. We will study the theory by examining a weakly perturbed non-equilibrium system and show that for small changes in the state, the equilibrium fluctuations serve as a good indicator for non-equilibrium responses [3].

## 2.1 Weakly Perturbed System

We will examine a state given by the Hamiltonian  $H_0$  and see how it interacts with an external time-dependent stimulus  $V(t)$ . In this case, the system is moving away from equilibrium via the external stimuli by absorbing energy. Obviously, there is a weak coupling between the system and the external agent, and we assume that the external agent interacts with our equilibrium system through an internal variable  $A$ . This makes our Hamiltonian take the following form:

$$H = H_0 - f(t)A. \quad (1)$$

In the above equation, we symbolize the time dependence of the external agent using  $f(t)$ . An illustration of the complete system is given below.

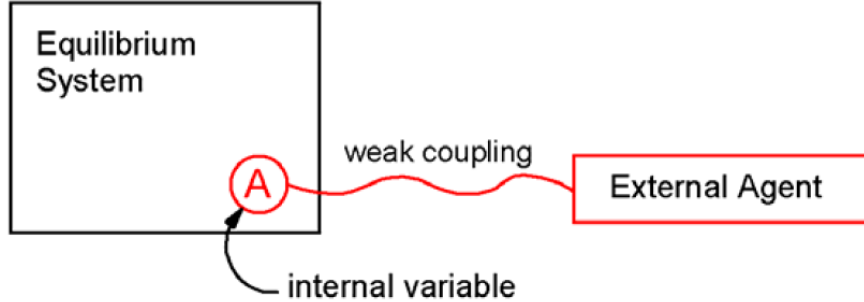


Figure 1: Equilibrium system coupled with external agent

We describe the system's behavior through an ensemble setup where the ensemble is initially at thermal equilibrium by assuming that each item in the ensemble interacts equally with the external agent and ensemble averaging. In this state, the internal variable  $A$  can be characterized by an equilibrium ensemble average  $\langle A \rangle$ . The external agent is then applied; we note this time as  $t_0$ , moving the system away from equilibrium. The new ensemble is called the non-

equilibrium ensemble average  $\overline{A(t)}$  where  $\langle A \rangle \neq \overline{A(t)}$  as shown in the diagram below:

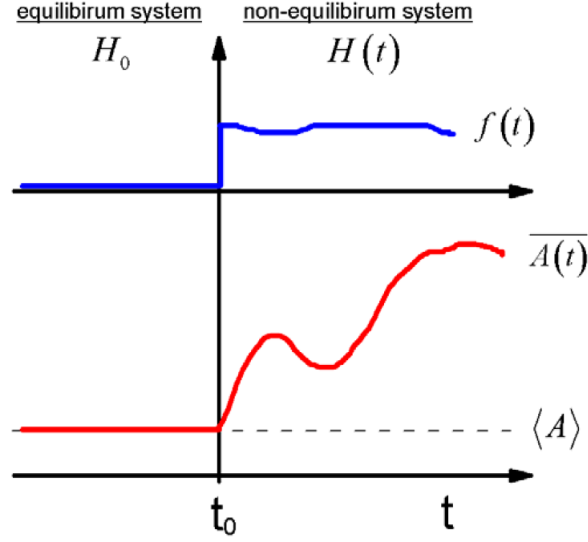


Figure 2: Disequilibrium due to interaction with external agent

We can now perform a power expansion of  $f(t)$  in order to illustrate  $\overline{A(t)}$  since it is a weak interaction.

$$\overline{A(t)} = (\text{terms } f^{(0)}) + (\text{terms } f^{(1)}) + \dots \quad (2)$$

$$\overline{A(t)} = \langle A \rangle + \int dt_0 R(t, t_0) f(t_0) + \dots \quad (3)$$

In this expression, the external agent begins acting on the system at  $t_0$ , and we begin our observations of the system at  $t$ . The leading term in the expansion is independent of  $f$ , meaning it must be  $\langle A \rangle$ . The next term in equation 3 represents the deviation from the equilibrium position through the linear dependence on the external agent. The linear response function  $R(t, t_0)$  is the quantity that contains the microscopic information describing how the system responds to the applied stimulus. We integrate the response function to depict that the non-equilibrium behavior corresponds to the whole history of the application of the external agent and not just the exact time we are measuring. We now analyze the various properties of the response function to express it quantitatively.

## 2.2 Properties of the Response Function

### 2.2.1 Causality

This idea states that a system can not respond to the stimulus before it has been applied. Hence,  $R(t, t_0) = 0$  for  $t < t_0$  and the time-dependent change in  $A$  is:

$$\delta \overline{A(t)} = \overline{A(t)} - \langle A \rangle = \int_{-\infty}^t dt_0 R(t, t_0) f(t_0) \quad (4)$$

The negative infinity in the integration's lower limit represents that the system is initially at equilibrium, and the upper limit is that we observe the system. We can also reflect the causality principle by introducing a step function in the integral such that:

$$\Theta(t - t_0) = \begin{cases} 0 & \text{if } (t < t_0) \\ 1 & \text{if } (t \geq t_0) \end{cases} \quad (5)$$

### 2.2.2 Stationarity

Just like our discussion of the correlation function, the time dependence of the system only depends on the time interval between the application of the stimulus as the observation. Hence we can write  $R(t, t_0) = R(t - t_0)$  and

$$\delta \overline{A(t)} = \int_{-\infty}^t dt_0 R(t - t_0) f(t_0). \quad (6)$$

The above expression confirms that the observed response of the system to the agent is a convolution of the physical response with the time development of the applied force. Rather than measuring in absolute time intervals, we define a time interval  $\tau$  which is equal to  $t - t_0$  so we can rewrite our equation as:

$$\delta \overline{A(t)} = \int_0^\infty d\tau R(\tau) f(t - \tau). \quad (7)$$

### 2.2.3 Impulse Response

Since we have a perturbation in terms of the delta function:

$$f(t) = \lambda \delta(t - t_0), \quad (8)$$

we can obtain:

$$\delta \overline{A(t)} = \lambda R(t - t_0). \quad (9)$$

Hence,  $R$  describes how the system evolves when a sudden perturbation is applied, this is usually called the impulse response function, and an illustration is shown below.

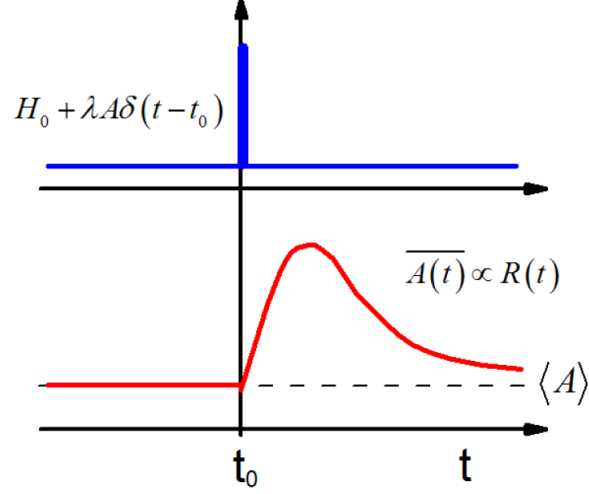


Figure 3: Equilibrium system undergoing an impulse perturbation

### 2.3 Frequency-Domain Representation

Let us also observe the behavior of the non-equilibrium system in the frequency domain as a spectral response function (susceptibility). We Fourier transform both sides of equation 7 to get:

$$\delta \overline{A(\omega)} = \int_{-\infty}^{\infty} dt \left[ \int_0^{\infty} d\tau R(\tau) f(t - \tau) \right] e^{i\omega t}. \quad (10)$$

We now insert  $1 = e^{-i\omega t} e^{i\omega t}$  into the right hand side to get:

$$\delta \overline{A(\omega)} = \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau R(\tau) f(t - \tau) e^{i\omega(t - \tau)} e^{i\omega \tau}. \quad (11)$$

$$\delta \overline{A(\omega)} = \int_{-\infty}^{\infty} dt' e^{i\omega t'} f(t') \int_0^{\infty} d\tau R(\tau) e^{i\omega \tau}. \quad (12)$$

Hence we can write  $\delta \overline{A(\omega)} = \tilde{f}(\omega) \chi(\omega)$ . Note that in equation 12, we have switched variables by setting  $t' = t - \tau$ .  $\tilde{f}(\omega)$  represents the complex part of the frequency domain representation of the driving force, which is retrieved after doing the Fourier transform on  $f(t')$ . The second term, i.e.,  $\chi(\omega)$  is the susceptibility which is the Fourier transform of the impulse response function. This is a frequency domain representation of the linear response function. We can switch between time and frequency domains to show that a convolution of the force and response in time leads to the product of the force and response in frequency. This is known as the convolution theorem, which states:

$$A(t) \otimes B(t) \equiv \int_{-\infty}^{\infty} d\tau A(t-\tau)B(\tau) = \int_{-\infty}^{\infty} d\tau A(\tau)B(t-\tau) = F^{-1}[\tilde{A}(\omega)\tilde{B}(\omega)], \quad (13)$$

where  $\tilde{A}(\omega) = F[A(t)]$  and  $F, F^{-1}$  is the Fourier and inverse Fourier transform respectively. It is important to be mindful of the fact that although  $R(\tau)$  is a real function depicting an observable,  $\chi(\omega)$  is complex:

$$\chi(\omega) = \chi'(\omega) + i\chi''(\omega), \quad (14)$$

as we have defined  $\chi(\omega)$  as:

$$\chi(\omega) = \int_0^{\infty} d\tau R(\tau)e^{i\omega\tau}. \quad (15)$$

We then have:

$$\chi' = \int_0^{\infty} d\tau R(\tau)\cos(\omega\tau) = \text{Re}[F(R(\tau))] \quad (16)$$

and

$$\chi'' = \int_0^{\infty} d\tau R(\tau)\sin(\omega\tau) = \text{Im}[F(R(\tau))], \quad (17)$$

where  $\chi'$  and  $\chi''$  are even and odd frequency functions. Hence we can say:

$$\chi'(\omega) = \chi'(-\omega), \quad (18)$$

$$\chi''(\omega) = -\chi''(-\omega), \quad (19)$$

such that:

$$\chi(-\omega) = \chi^*(\omega). \quad (20)$$

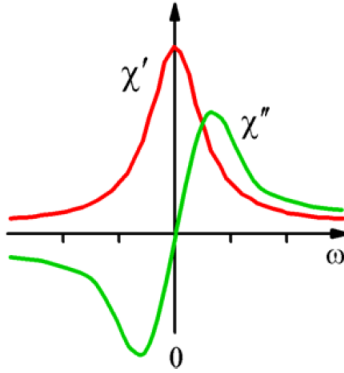


Figure 4: Graphical Representation of  $\chi'$  and  $\chi''$

## 2.4 Kramers-Krönig Relations

We can see that  $\chi'$  and  $\chi''$  are not truly independent of one another, given that they are sine and cosine transforms of the same function. We use Kramers-Krönig Relationships to equate the two:

$$\chi'(\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\chi''(\omega')}{\omega' - \omega} d\omega', \quad (21)$$

$$\chi''(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\chi'(\omega')}{\omega' - \omega} d\omega'. \quad (22)$$

The following equations can be acquired by substituting the inverse sine transform of equation 18 into equation 17:

$$\chi'(\omega) = \frac{1}{\pi} \int_0^{\infty} dt \cos(\omega t) \int_{-\infty}^{\infty} \chi''(\omega') \sin(\omega' t) d\omega', \quad (23)$$

$$\chi'(\omega) = \frac{1}{\pi} \lim_{L \rightarrow \infty} \int_{-\infty}^{\infty} d\omega' \chi''(\omega') \int_0^L \cos(\omega t) \sin(\omega' t) dt. \quad (24)$$

Using the identity:  $\cos(ax)\sin(bx) = \frac{1}{2}\sin(a+b)x + \frac{1}{2}\sin(b-a)x$ , we can rewrite the above equation as:

$$\chi'(\omega) = \frac{1}{\pi} \lim_{L \rightarrow \infty} P \int_{-\infty}^{\infty} d\omega' \chi''(\omega') \frac{1}{2} \left[ \frac{-\cos(\omega' + \omega)L + 1}{\omega' + \omega} - \frac{\cos(\omega' - \omega)L + 1}{\omega' - \omega} \right]. \quad (25)$$

The rapid oscillations of the cosine terms make us expect they will vanish when taking the limit  $L \rightarrow \infty$ . This is the same as averaging over a monochromatic field. On the other hand, we can also average over a single oscillation:  $L = 2\pi(\omega' - \omega)$  to acquire equation 21. All of this is only possible when we adhere to the concept of causality explained earlier, Kramers-Krönig relationships are bounded by the lower limit of  $t_{initial} = 0$  on the first integral evaluated above.

## 2.5 Quantum Linear Response Functions

Having developed a classical understanding of the Linear Response Theory, we turn to its quantum counterpart. To develop a quantum description of the linear response function, we observe that the response of a system to an applied external agent can be solved in the interaction picture where our time-dependent Hamiltonian is:

$$H(t) = H_0 - f(t)\hat{A} = H_0 + V(t). \quad (26)$$

Here  $H_0$  is the material Hamiltonian for the equilibrium system, and the external stimulus acts on the system through  $\hat{A}$ .  $\hat{A}$  is an operator in the system states with a time-dependency of  $f(t)$ . We treat this as a perturbation problem

by asserting that  $V(t)$  is small. Our goal is to describe the non-equilibrium response of  $\overline{A(t)}$ , which we will obtain by doing an ensemble average of the expectation value of  $\hat{A}$ . In the interaction picture, the pure state can be represented as:

$$\langle A(t) \rangle = \langle \Psi_I(t) | A_I(t) | \Psi_I(t) \rangle \quad (27)$$

$$\langle A(t) \rangle = \langle \Psi_0 | U_I^\dagger(t) A_I U_I(t) | \Psi_0 \rangle. \quad (28)$$

Let's also rewrite equation 26 in the interaction picture:

$$V_I(t) = U_0^\dagger(t) V(t) U_0(t), \quad (29)$$

$$V_I(t) = -f(t) A_I(t). \quad (30)$$

In order to calculate the ensemble average after applying the external stimulus, we observe that the non-equilibrium state of the system can be described by  $|\Psi_I(t)\rangle$  which is related to the initial equilibrium state  $|\Psi_0\rangle$ , as seen in equation 27 and 28. Hence the non-equilibrium expectation value can be acquired by an equilibrium averaging over the expectation value of  $U_I^\dagger A_I U_I$ :

$$\overline{A(t)} = \sum_n p_n \langle n | U_I^\dagger A_I U_I | n \rangle, \quad (31)$$

where  $|n\rangle$  are just the eigenstates of  $H_0$ . In our calculations, we will just work with the first-order solutions to  $U_I(t)$ :

$$U_I(t, t_0) = 1 + \frac{i}{\hbar} \int_{t_0}^t dt' f(t') A_I(t'). \quad (32)$$

We now plug in the value of the unitary time operator into  $A(t)$  and integrate it over the entire temporal history of the system once the external agent starts to interact with the equilibrium system.

$$A(t) = U_I^\dagger A_I U_I \quad (33)$$

$$A(t) = \{1 + \frac{i}{\hbar} \int_{t_0}^t dt' f(t') A_I(t')\} A_I(t) \{1 - \frac{i}{\hbar} \int_{t_0}^t dt' f(t') A_I(t')\} \quad (34)$$

Note that the  $f$  is the dependence of the external agent. It commutes with  $A$  and is not involved with the unperturbed Hamiltonian  $H$ . Since we are dealing with a linear theory, we retain the linear terms of  $f(t')$ .

$$A(t) \cong A_I(t) + \frac{i}{\hbar} \int_{t_0}^t dt' f(t') \{A_I(t) A_I(t') - A_I(t') A_I(t)\}, \quad (35)$$



$$A(t) = A_I(t) + \frac{i}{\hbar} \int_{t_0}^t dt' f(t') [A_I(t), A_I(t')]. \quad (36)$$

We set  $t_0$  equal to inf as our system is initially in equilibrium. We also switch variables to the time interval  $\tau = t - t'$  and utilize  $A_I(t) = U_0^\dagger A U_0(t)$  to obtain:

$$A(t) = A_I(t) + \frac{i}{\hbar} \int_0^\infty d\tau f(t - \tau) [A_I(\tau), A_I(0)]. \quad (37)$$

This allows us to calculate the expectation value of  $A$  by using the ensemble averaging method. Assuming the external stimulus applies force equally to all the particles in the ensemble, we get:

$$\overline{A(t)} = \langle A \rangle + \frac{i}{\hbar} \int_0^\infty d\tau f(t - \tau) \langle [A_I(\tau), A_I(0)] \rangle. \quad (38)$$

Note that the first term does not include any  $f$  term, which means it comes from the ensemble average of the equilibrium for the value of  $A$ . This naturally leads us to believe that  $\langle A \rangle$  is time-independent in our calculations:

$$\langle A(t) \rangle = \sum_n p_n \langle n | A_I | n \rangle = \langle A \rangle. \quad (39)$$

The second term is just an ensemble averaging done over the commutator in  $A_I(t)$ :

$$\langle [A_I(\tau), A_I(0)] \rangle = \sum_n p_n \langle n | [A_I(\tau), A_I(0)] | n \rangle. \quad (40)$$

Now we compare equation 38 with the expression of the linear response function to find the quantum linear response function:

$$R(\tau) = -\frac{i}{\hbar} \Theta(\tau) \langle [A_I(\tau), A_I(0)] \rangle. \quad (41)$$

Note that the step function has been added to ensure the causality property. The crucial idea here is that the time development of the system with the applied external potential is dictated by the dynamics of the equilibrium system (which was also our initial goal to show). The entire dependence in the response function is under  $H_0$ . Therefore, the linear response function is the sum of two correlation functions with the order of operators interchanged. This is the imaginary part of the correlation function depicted by  $C'''(\tau)$ .

$$R(\tau) = -\frac{i}{\hbar} \Theta(\tau) \{ \langle A_I(\tau) A_I(0) \rangle - \langle A_I(0) A_I(\tau) \rangle \}, \quad (42)$$

$$R(\tau) = -\frac{i}{\hbar} \Theta(\tau) (C_{AA}(\tau) - C_{AA}^*(\tau)) \quad (43)$$

,

$$R(\tau) = \frac{2}{\hbar} \Theta(\tau) C''(\tau). \quad (44)$$

As expected, the linear response function is real. If we express the correlation function in the eigenstate description, we get the following:

$$C(t) = \sum_{n,m} p_n |A_{mn}|^2 e^{-i\omega_{mn}t}, \quad (45)$$

which then becomes:

$$R(\tau) = \frac{2}{\hbar} \Theta(\tau) \sum_{n,m} p_n |A_{mn}|^2 \sin(\omega_{mn}t). \quad (46)$$

Note that  $R(\tau)$  can always be expanded in sines because it is an odd function of time. This means that the impulse response must have a value of 0 at  $t = t_0$  and move away from 0 at the point where the external potential is applied.

## 2.6 Liouville Equations

The Liouville theorem uses equations to describe the time evolution of the phase space distribution function. It is a fundamental equation commonly used in statistical mechanics with a wide range of applications in quantum mechanics. Consider a Hamiltonian system with canonical coordinates  $q_i$  and conjugate momenta  $p_i$ , where  $i = 1, \dots, n$ . Then the phase space distribution  $\rho(p, q)$  determines the probability of the system being found in the infinitesimal phase space volume  $d^n q d^n p$ . The Liouville Equation dictates the evolution of  $\rho(p, q; t)$  in time  $t$ :

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \sum_{i=1}^n \left( \frac{\partial \rho}{\partial q_i} \dot{q}_i + \frac{\partial \rho}{\partial p_i} \dot{p}_i \right) = 0. \quad (47)$$

The Hamiltonian of the system determines the time derivatives of  $q$  and  $p$ . The above equation shows the conservation of density in phase space. Liouville theorem states that the distribution function is constant along any trajectory in phase space. The proof of Liouville's theorem uses the n-dimensional divergence theorem. The proof is contingent on the fact that the evolution of  $\rho$  obeys an n-dimensional version of the continuity equation:

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^n \left( \frac{\partial(\rho \dot{q}_i)}{\partial q_i} + \frac{\partial(\rho \dot{p}_i)}{\partial p_i} \right) = 0. \quad (48)$$

This means that the tuple  $(\rho, \rho \dot{q}_i, \rho \dot{p}_i)$  is a conserved current. The only difference between the above equation and the Liouville equation is the terms where  $H$  is the Hamiltonian and the Hamiltonian's equations, and the conservation of the Hamiltonian along the flow, have been used. This is illustrated in the equation below:

$$\rho \sum_{i=1}^n \left( \frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} \right) = \rho \sum_{i=1}^n \left( \frac{\partial^2 H}{\partial q_i \partial p_i} - \frac{\partial^2 H}{\partial p_i \partial q_i} \right) = 0. \quad (49)$$

Viewing the motion through phase space as a 'fluid flow' of system points, the theorem that the convective derivative of the density is zero follows from the continuity equation by noting that the 'velocity field'  $(\dot{p}, \dot{q})$  has zero divergence. Similarly, since a conserved current exists, there is implied symmetry via Noether's theorem. This symmetry is invariant under time, and the symmetry's generator is the Hamiltonian of the system.

## 2.7 Quantum Liouville Equation

For our research, we are interested in the quantum mechanical formulation of the Liouville equation. In quantum mechanics, the Liouville theorem describes the time evolution of a mixed quantum state. Canonical quantization yields a quantum analog of the theorem, utilizing the Von Neumann equation. To do so, we describe a Hamiltonian using classical mechanics. The classical variables are then replaced by their analogous quantum operators, and commutators replace Poisson brackets. In our case, we get:

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar} [H, \rho], \quad (50)$$

where  $\rho$  is now the density matrix for the mixed state. When this equation is applied to the expectation value of the observable in question, the new equation is given by Ehrenfest's theorem and takes the form:

$$\frac{d}{dt} \langle A \rangle = \frac{1}{i\hbar} \langle [A, H] \rangle. \quad (51)$$

where  $A$  is our observable. The difference in sign follows from the assumption that the operator is stationary while the state is dependent on time.

## 3 Kubo Formulation

To derive the derive formulation we first look at the Schrodinger picture of pure states:

$$i \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle. \quad (52)$$

In order to generalize to mixed states, we can also express our system under the Liouville-von Neumann equation:

$$i \frac{\partial \rho}{\partial t} = [\hat{H}, \rho]. \quad (53)$$

The above equations tell us how to evolve a quantum state in time. In order to understand this we must be able to dissect the Hamiltonian involved in the

systems, however, for most complex systems solving the Hamiltonian analytically or computationally can be very tedious if not impossible.

Let us study a system under the interaction picture in which the system is initially in thermal equilibrium and then gently pushed out of equilibrium. The unperturbed Hamiltonian is called  $\hat{H}_0$  and is in thermal equilibrium in the Gibbs state:

$$\rho = \frac{1}{Z} e^{-\beta \hat{H}_0} \quad (54)$$

We can assume to have solved the eigen value problem for the Hamiltonian and can express our terms in the energy eigen basis:

$$\hat{H}_0 |E_k\rangle = E_k |E_k\rangle. \quad (55)$$

Thus the exponential term in equation 54 can be expanded as:

$$e^{-\beta \hat{H}_0} = \sum_m e^{-\beta E_m} |E_m\rangle \langle E_m|, \quad (56)$$

and the partition function as:

$$Z = \sum_m e^{-\beta E_m}. \quad (57)$$

The expectation value of some given observable  $A$  can be expressed as:

$$\langle A \rangle_{\beta,0} = \frac{1}{Z} \sum_m e^{-\beta E_m} \langle E_m | A | E_m \rangle. \quad (58)$$

The subscripted terms  $\beta$  and 0 indicate that the expectation value is a thermal average with respect to the Hamiltonian  $\hat{H}_0$  and this thermal average is being taken at the inverse temperature  $\beta$ . In the initial condition, our state  $\hat{\rho}$  as well as our observable  $A$  are time independent. However, at  $t > 0$  we introduce a time dependent external perturbation. Our new Hamiltonian then becomes:

$$H(t) = H_0 + \lambda V(t), \quad (59)$$

where  $\hat{H}_0$  is the free Hamiltonian and  $\lambda V(t)$  is our interacting Hamiltonian. We assume that  $\lambda \ll 1$ . Due to the perturbation, the energy eigen basis of the total Hamiltonian have been altered, hence:

$$H(t) |E_m\rangle \neq E_m |E_m\rangle. \quad (60)$$

In the Schrodinger picture, the eigen states of the free Hamiltonian evolve in time according to:

$$i \frac{\partial}{\partial t} |E_m(t)\rangle = H(t) |E_m(t)\rangle. \quad (61)$$

Expressing it in the Interaction Picture we get:

$$|E_m(t)\rangle = e^{-iH_0 t} |E_m(t)\rangle_I, \quad (62)$$

where  $|E_m(t)\rangle_I = U(t) |E_m(0)\rangle$ . Since it is the expression for the free Hamiltonian, we can just re-write it as:  $|E_m(t)\rangle_I = U(t) |E_m\rangle$ .

We now expand the time evolution operator in terms of the Dyson Series, up till the first order to obtain:

$$U(t) = 1 - i\lambda \int_0^t dt' V_I(t'), \quad (63)$$

where our external perturbation  $V_I(t)$  is given in the Schrodinger Picture as:

$$V_I(t) = e^{iH_0 t} V(t) e^{-iH_0 t}. \quad (64)$$

This implies that the time evolution of our perturbation Hamiltonian is dependent on the free Hamiltonian. The expectation value of our observable  $A$  in time becomes:

$$\langle A(t) \rangle = \frac{1}{Z} \sum_m e^{-\beta E_m} \langle E_m(t) | A | E_m(t) \rangle. \quad (65)$$

Expanding the time dependence of the free Hamiltonian's energy eigen state in the Heisenberg Picture, yields:

$$\langle A(t) \rangle = \frac{1}{Z} \sum_m e^{-\beta E_m} \langle E_m | U^\dagger(t) e^{iH_0 t} A e^{-iH_0 t} U(t) | E_m \rangle. \quad (66)$$

We can now re-write it in term of the interaction picture to obtain:

$$\langle A(t) \rangle = \frac{1}{Z} \sum_m e^{-\beta E_m} \langle E_m | U^\dagger(t) A_I(t) U(t) | E_m \rangle. \quad (67)$$

Plugging in the approximate expansion of the time evolution operator gives us:

$$\langle A \rangle_{\beta,0} - i\lambda \int_0^t dt' \frac{1}{Z} \sum_m e^{-\beta E_m} \langle E_m | (A_I(t) V_I(t') - V_I(t') A(t)) | E_m \rangle. \quad (68)$$

Note that the term " $A_I(t) V_I(t') - V_I(t') A(t)$ " is simply a commutation relation between  $A_I(t)$  and  $V_I(t)$  and can be expressed as the Kubo Formula:

$$\langle A(t) \rangle = \langle A \rangle_{\beta,0} - i\lambda \int_0^t dt' \langle [A_I(t), V_I(t')] \rangle_{\beta,0}. \quad (69)$$

This result indicates that we only need to be aware of the free Hamiltonian energy eigen values and eigen kets, and the time evolution of the observables in the interaction picture depend on the free Hamiltonian [4].

## 4 Master Equation Formulation

This section will introduce open quantum systems and decoherence in terms of the master equation formalism. The master equation approach allows us to express the time evolution of the reduced density matrix  $\hat{\rho}_S(t)$  for the open quantum system  $\mathcal{S}$  interacting with the environment  $\mathcal{E}$ . This means we can skip the tedious process of first determining the total system-environment combination followed by tracing out the degrees of freedom. Note that in studying open systems, we are only interested in the dynamics of the environment but rather the system and the system environment interaction. Also it is analytically impossible to determine the time evolution of the density matrix. Master equation formalism resolves both the concerns by only analyzing the influence of the environment onto the system and allows for certain approximation schemes to compute the time evolution [5].

### 4.1 General Formalism

The ordinary formula for decoherence in an open quantum systems in the reduced density matrix is as follows:

$$\hat{\rho}_S(t) = \text{Tr}_{\mathcal{E}}\{\hat{\rho}_{S\mathcal{E}}(t)\} \equiv \text{Tr}_{\mathcal{E}}\{\hat{U}(t)\hat{\rho}_{S\mathcal{E}}(0)\hat{U}^\dagger(t)\}, \quad (70)$$

where  $\hat{U}(t)$  is the standard time-evolution operator for the composite system  $\mathcal{SE}$ . To compute the time evolution, one must determine the dynamics of the density matrix of the total system before reaching a reduced description via the trace operation. This approach is more or less impossible for reasonably complex systems. However, in the Master-Equation approach we instead calculate  $\hat{\rho}_S(t)$  directly from the following expression:

$$\hat{\rho}_S(t) = \hat{V}(t)\hat{\rho}_S(0), \quad (71)$$

here the operator  $\hat{V}(t)$  represents the dynamical map which generates the evolution of  $\hat{\rho}_S(t)$ .  $\hat{V}(t)$  is known as a superoperator since it is an operator acting on another operator. Obviously, both the above equations are equivalent, and the master equation could be seen as a re-writing of the general equation form.

The master equation only becomes useful once we impose certain assumptions about the system-environment interaction and dynamics. These assumptions allow us to calculate an approximation of the time evolution of  $\hat{\rho}_{S\mathcal{E}}(t)$ . In this section, we will focus on local time first-order differential equations:

$$\frac{d}{dt}\hat{\rho}_S(t) = \hat{\mathcal{L}}[\hat{\rho}_S(t)] = -i[\hat{H}'_S, \hat{\rho}_S(t)] + \hat{\mathcal{D}}[\hat{\rho}_S(t)], \quad (72)$$

The time locality implies that a change in  $\hat{\rho}_S(t)$  at time  $t$  only depends on  $\hat{\rho}_S$  evaluated at  $t$  where  $t' \neq t$ . The superoperator  $\hat{\mathcal{L}}$  acts on  $\hat{\rho}_S(t)$  and is determined by the initial state of the environment and the Hamiltonian. The superoperator

is decomposed into a unitary part  $i[\hat{H}'_S, \hat{\rho}_S(t)]$  which is given by the Liouville-von Neumann commutator with the Hamiltonian  $\hat{H}'_S$  and the non-unitary part  $\hat{\mathcal{D}}[\hat{\rho}_S(t)]$  which represents our system's decoherence or dissipation.

Note that if the system is totally unitary then the decoherence term goes to zero and we are left with:

$$\frac{d}{dt}\hat{\rho}_S(t) = i[\hat{H}'_S, \hat{\rho}_S(t)]. \quad (73)$$

The above equation varies from the Liouville-von Neumann equation for closed quantum systems by the use of the environment shifted Hamiltonian  $\hat{H}'_S$  instead of the unperturbed Hamiltonian  $\hat{H}_S$ .

## 4.2 The Born-Markov Master Equation

The Born-Markov Master Equation allows one to combine multiple decoherence elements into one simple (often closed form) system. This master equation makes two major assumptions.

The first assumption known as the "Born Approximation", states that the system-environment coupling is sufficiently weak and the environment is reasonably large such that there is negligible changes in the density operator of the environment and that the system and environment stay in a product state at all times[6]:

$$\hat{\rho}(t) \approx \hat{\rho}_S(t) \otimes \hat{\rho}_E. \quad (74)$$

The second assumption known as the "Markov Approximation", states that the 'memory effects' of the environment are negligible in the sense that any self correction within the environment created by the coupling to the system decays very quickly compared to the timescale being used to observe variations in the system.

The interacting Hamiltonian can then be written in the following diagonal form:

$$\hat{H}_{\text{int}} = \sum_{\alpha} \hat{S}_{\alpha} \otimes \hat{E}_{\alpha}, \quad (75)$$

note that the operators for the system  $\hat{S}_{\alpha}$  and environment  $\hat{E}_{\alpha}$  are unitary but not necessarily Hermitian. Then the reduced density operator  $\hat{\rho}_S(t)$  becomes:

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}_S, \hat{\rho}_S(t)] - \sum_{\alpha} \left\{ [\hat{S}_{\alpha}, \hat{B}_{\alpha}\hat{\rho}_S(t)] + [\hat{\rho}_S(t)\hat{C}_{\alpha}, \hat{S}_{\alpha}] \right\}, \quad (76)$$

where the system operators  $\hat{B}_{\alpha}$  and  $\hat{C}_{\alpha}$  are defined as:

$$\hat{B}_{\alpha} \equiv \int_0^{\infty} d\tau \sum_{\beta} \mathcal{C}_{\alpha\beta}(\tau) \hat{S}_{\beta}^{(I)}(-\tau), \quad (77)$$

$$\hat{\mathcal{C}}_\alpha \equiv \int_0^\infty d\tau \sum_\beta \mathcal{C}_{\beta\alpha}(-\tau) \hat{S}_\beta^{(I)}(-\tau). \quad (78)$$

The term  $\mathcal{C}_{\alpha\beta}(\tau)$  is given by:

$$\mathcal{C}_{\alpha\beta}(\tau) \equiv \langle \hat{E}_\alpha(\tau) \hat{E}_\beta \rangle_{\hat{\rho}_\mathcal{E}}, \quad (79)$$

which signifies that the average is taken over the initial state  $\hat{\rho}_\mathcal{E}$  which remains relatively constant under the Born approximation. The  $\mathcal{C}_{\alpha\beta}(\tau)$  will henceforth be called the 'environment self-correction function' because it measures the degree to which the environment retains information about its interaction with the system over time.

To explicitly determine the quantities  $\hat{B}_\alpha$  and  $\hat{\mathcal{C}}_\alpha$  we would need to calculate the interaction picture operators  $\hat{S}_\alpha^{(I)}(\tau)$  and  $\hat{E}_\alpha^{(I)}(\tau)$  and the environment correlation functions. However, in most situations, where we have to consider only one observable which is being monitored by the environment, the master equation greatly simplifies and we are left with the following diagonal decomposition:

$$\hat{H}_{\text{int}} = \hat{S} \otimes \hat{E} \quad (80)$$

We will now derive the Born-Markov Master Equations from first principles. Let us decompose the total system-environment Hamiltonian in the interaction picture as:

$$\hat{H} = \hat{H}_S + \hat{H}_\mathcal{E} + \hat{H}_{\text{int}}. \quad (81)$$

In order to apply perturbation theory we can write the Hamiltonian as:

$$\hat{H}_0 \equiv \hat{H}_S + \hat{H}_\mathcal{E}, \quad (82)$$

where  $\hat{H}_0$  now represents the free Hamiltonian, allowing us to treat the interacting Hamiltonian  $\hat{H}_{\text{int}}$  as a perturbation. We can now write the density operator and the interacting Hamiltonian in the interaction picture as:

$$\hat{H}_{\text{int}}(t) = e^{i\hat{H}_0 t} \hat{H}_{\text{int}} e^{-i\hat{H}_0 t} \quad (83)$$

$$\begin{aligned} \hat{\rho}^{(I)}(t) &= e^{i\hat{H}_0 t} \hat{\rho}(t) e^{-i\hat{H}_0 t} \\ &= e^{i\hat{H}_0 t} e^{-i\hat{H} t} \hat{\rho} e^{i\hat{H} t} e^{-i\hat{H}_0 t} \end{aligned} \quad (84)$$

The time evolution of  $\hat{\rho}^{(I)}(t)$  can be determined by the Liouville-von Neumann equation in the interaction picture,

$$\frac{d}{dt} \hat{\rho}^{(I)}(t) = -i [\hat{H}_{\text{int}}(t), \hat{\rho}^{(I)}(t)] \quad (85)$$

Note that this means that the evolution of the interaction-picture density operator is completely dependent on just the system-environment coupling part



$\hat{H}_{\text{int}}$  of the full Hamiltonian.

Integrating the time evolution of the density operator, we get:

$$\hat{\rho}^{(I)}(t) = \hat{\rho}(0) - i \int_0^t dt' [\hat{H}_{\text{int}}(t'), \hat{\rho}^{(I)}(t')]. \quad (86)$$

We can now plug this back into the right hand side of equation 85 to obtain:

$$\begin{aligned} \frac{d}{dt} \hat{\rho}^{(I)}(t) &= -i \left[ \hat{H}_{\text{int}}(t), \left\{ \hat{\rho}(0) - i \int_0^t dt' [\hat{H}_{\text{int}}(t'), \hat{\rho}^{(I)}(t')] \right\} \right] \\ &= -i [\hat{H}_{\text{int}}(t), \hat{\rho}(0)] - \int_0^t dt' [\hat{H}_{\text{int}}(t), [\hat{H}_{\text{int}}(t'), \hat{\rho}^{(I)}(t')]]. \end{aligned} \quad (87)$$

Since we are able to write  $\hat{\rho}_S^{(I)}(t) = \text{Tr}_{\mathcal{E}} \{ \hat{\rho}^{(I)}(t) \}$ , we can transform the equation into an equation for the reduced density operator  $\hat{\rho}_S^{(I)}(t)$  by taking the trace over the environment:

$$\frac{d}{dt} \hat{\rho}_S^{(I)}(t) = -i \text{Tr}_{\mathcal{E}} [\hat{H}_{\text{int}}(t), \hat{\rho}(0)] - \int_0^t dt' \text{Tr}_{\mathcal{E}} [\hat{H}_{\text{int}}(t), [\hat{H}_{\text{int}}(t'), \hat{\rho}^{(I)}(t')]]. \quad (88)$$

Without the loss of generality, one can also assume that:

$$\text{Tr}_{\mathcal{E}} [\hat{H}_{\text{int}}(t), \hat{\rho}(0)] = 0, \quad (89)$$

which simplifies the time derivative of the density operator to:

$$\frac{d}{dt} \hat{\rho}_S^{(I)}(t) = - \int_0^t dt' \text{Tr}_{\mathcal{E}} [\hat{H}_{\text{int}}(t), [\hat{H}_{\text{int}}(t'), \hat{\rho}^{(I)}(t')]]. \quad (90)$$

All the above calculations have been done without any approximations. Now we need to add desirable features to equation 90 to make it standard for a master equation. Firstly note that equation 90 is not time local because the right hand side depends on the total system-environment density operator being evaluated from 0 to  $t$ . So we need to add two major properties to the equation.

First, we want to write down the master equation solely in terms of the reduced density operator  $\hat{\rho}_S^{(I)}(t)$  and the initial environment state. This means eliminating any terms pertaining to a time-dependent state of the environment. Second we would like to remove all dependencies of the change of  $\hat{\rho}_S^{(I)}(t)$  at time  $t$  on  $\hat{\rho}_S^{(I)}(t)$  calculated at times  $t' < t$ . In order to accomplish this we will now introduce the Born-Markov Approximations to the system. Before that please note that for a weakly coupled system-environment it can be assumed that there is an absence of initial correlations between the system and the environment, which can be expressed as:

$$\hat{\rho}(0) = \hat{\rho}^{(I)}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_{\mathcal{E}}(0) \quad (91)$$

### 4.2.1 Imposing the Born Approximation

The Born approximation assume that the density operator of the system-environment combination remains in a product form at all times and that the temporal changes in the density matrix of the environment can be ignored:

$$\hat{\rho}(t) \approx \hat{\rho}_S(t) \otimes \hat{\rho}_E \quad \forall t \geq 0. \quad (92)$$

In the interaction picture this is expressed as:

$$\hat{\rho}^{(I)}(t) \approx \hat{\rho}_S^{(I)}(t) \otimes \hat{\rho}_E \quad \forall t \geq 0. \quad (93)$$

In the Born approximation we use the intuition that the interaction between the system and environment is adequately weak, and that the environment is large in relation to the system in such a way that the density operator for the environment does not change by interacting with the system and the system and the environment stay in a separable state at all time. In real experiments this is often the case because usually the system is coupled to a very large environment which when viewed as a whole undergoes minuscule changes in the course of its interaction. Thus, we can re-write equation 90 using the born Approximation as:

$$\frac{d}{dt}\hat{\rho}_S^{(I)}(t) = - \int_0^t dt' Tr_E [\hat{H}_{\text{int}}(t), [\hat{H}_{\text{int}}(t'), \hat{\rho}_S^{(I)}(t') \otimes \hat{\rho}_E]]. \quad (94)$$

### 4.2.2 Imposing the Markov Approximation

We can now impose time locality onto equation 94 using the Markov Approximation. Let us begin by writing the interaction Hamiltonian in the diagonal form and transforming it into the interaction picture:

$$\begin{aligned} \hat{H}_{\text{int}}(t) &= e^{i\hat{H}_0 t} \hat{H}_{\text{int}} e^{-i\hat{H}_0 t} \\ &= \sum_{\alpha} (e^{i\hat{H}_S t} \hat{S}_{\alpha} e^{-i\hat{H}_S t}) \otimes (e^{i\hat{H}_E t} \hat{E}_{\alpha} e^{-i\hat{H}_E t}) \\ &= \sum_{\alpha} \hat{S}_{\alpha}(t) \otimes \hat{E}_{\alpha}(t) \end{aligned} \quad (95)$$

This allows us to express equation 94 as:

$$\frac{d}{dt}\hat{\rho}_S^{(I)}(t) = - \int_0^t dt' \sum_{\alpha\beta} Tr_E [\hat{S}_{\alpha}(t) \otimes \hat{E}_{\alpha}(t), [\hat{S}_{\beta}(t') \otimes \hat{E}_{\beta}(t'), \hat{\rho}_S^{(I)}(t') \otimes \hat{\rho}_E]], \quad (96)$$

where  $\mathcal{C}_{\alpha\beta}(t, t')$  is defined as:

$$\mathcal{C}_{\alpha\beta}(t, t') \equiv Tr_E \{ \hat{E}_{\alpha}(t) \hat{E}_{\beta}(t') \hat{\rho}_E \} = \langle \hat{E}_{\alpha}(t) \hat{E}_{\beta}(t') \rangle_{\hat{\rho}_E}. \quad (97)$$

Let us now propose that the system is in a stationary state in equilibrium,

$$[\hat{H}_{\mathcal{E}}, \hat{\rho}_{\mathcal{E}}] = 0, \quad (98)$$

which allows us to write:

$$\mathcal{C}_{\alpha\beta}(t, t') = \text{Tr}_{\mathcal{E}}\{\hat{E}_{\alpha}(t - t')\hat{E}_{\beta}\hat{\rho}_{\mathcal{E}}\} \equiv \mathcal{C}_{\alpha\beta}(t - t'). \quad (99)$$

Note that due to the assumption  $[\hat{H}_{\mathcal{E}}, \hat{\rho}_{\mathcal{E}}] = 0$ , the environment self-correlation functions no longer depend on absolute time but rather on the time interval between the results of the two identical measurements whose degree of correlation is obtained through equation 99.

We can now insert equation 99 into equation 96 to yield:

$$\begin{aligned} \frac{d}{dt}\hat{\rho}_{\mathcal{S}}^{(I)}(t) = & - \int_0^t dt' \sum_{\alpha\beta} \left\{ \mathcal{C}_{\alpha\beta}(t - t') [\hat{S}_{\alpha}(t)\hat{S}_{\beta}(t')\hat{\rho}_{\mathcal{S}}^{(I)}(t') - \hat{S}_{\beta}(t')\hat{\rho}_{\mathcal{S}}^{(I)}(t')\hat{S}_{\alpha}(t)] \right. \\ & \left. + \mathcal{C}_{\beta\alpha}(t' - t) [\hat{\rho}_{\mathcal{S}}^{(I)}(t')\hat{S}_{\beta}(t')\hat{S}_{\alpha}(t) - \hat{S}_{\alpha}(t)\hat{\rho}_{\mathcal{S}}^{(I)}(t')\hat{S}_{\beta}(t')] \right\}. \end{aligned} \quad (100)$$

In the above derivation we have used the cyclic invariance property of the trace acting on operators:

$$\text{Tr}_{\mathcal{E}}\{\hat{E}_{\alpha}\hat{E}_{\beta}\hat{\rho}_{\mathcal{E}}\} = \text{Tr}_{\mathcal{E}}\{\hat{\rho}_{\mathcal{E}}\hat{E}_{\alpha}\hat{E}_{\beta}\} = \text{Tr}_{\mathcal{E}}\{\hat{E}_{\alpha}\hat{\rho}_{\mathcal{E}}\hat{E}_{\beta}\}. \quad (101)$$

To further simplify our result, let us now apply the Markov Approximation. In most physical weakly coupled systems, the quantum correlations of dynamical systems are destroyed on a time scale correlation of ' $\tau_{\text{corr}}$ ' which is generally significantly smaller than the characteristic timescale ' $\tau_{\mathcal{S}}$ '. This allows for the Markov Approximation to hold and give sufficiently accurate results. This results in two major changes to our equation. First, since there is an insignificant change of the reduced interaction-picture density operator during the time interval of  $\tau_{\text{corr}}$  we can replace the retarded-time density operator  $\hat{\rho}_{\mathcal{S}}^{(I)}(t')$  by the current-time density operator  $\hat{\rho}_{\mathcal{S}}^{(I)}(t)$  in the integrand side of the right hand side of equation 100. Secondly, we can extend the lower limit of the integration to  $-\infty$  because the self correlation functions vanish for  $t' < t$ . Finally we can write the new equation under Markov Approximations and with the substitute  $t' \rightarrow \tau \equiv t - t'$  as:

$$\begin{aligned} \frac{d}{dt}\hat{\rho}_{\mathcal{S}}^{(I)}(t) = & - \int_0^{\infty} d\tau \sum_{\alpha\beta} \left\{ \mathcal{C}_{\alpha\beta}(\tau) [\hat{S}_{\alpha}(t)\hat{S}_{\beta}(t - \tau)\hat{\rho}_{\mathcal{S}}^{(I)}(t) - \hat{S}_{\beta}(t - \tau)\hat{\rho}_{\mathcal{S}}^{(I)}(t)\hat{S}_{\alpha}(t)] \right. \\ & \left. + \mathcal{C}_{\beta\alpha}(-\tau) [\hat{\rho}_{\mathcal{S}}^{(I)}(t)\hat{S}_{\beta}(t - \tau)\hat{S}_{\alpha}(t) - \hat{S}_{\alpha}(t)\hat{\rho}_{\mathcal{S}}^{(I)}(t)\hat{S}_{\beta}(t - \tau)] \right\}. \end{aligned} \quad (102)$$

### 4.2.3 Transformation to the Schrodinger Picture

To convert the density operator evolution equation into the Schrodinger picture, we can use the standard procedure:

$$\hat{\rho}_S^{(I)}(t) = e^{i\hat{H}_S t} \hat{\rho}_S(t) e^{-i\hat{H}_S t}, \quad (103)$$

from which immediately follows:

$$\frac{d}{dt} \hat{\rho}_S^{(I)}(t) = i[\hat{H}_S, \hat{\rho}_S^{(I)}(t)] + e^{i\hat{H}_S t} \left( \frac{d}{dt} \hat{\rho}_S(t) \right) e^{-i\hat{H}_S t}. \quad (104)$$

Now by using  $\hat{\rho}_S^{(I)}(t) = e^{i\hat{H}_S t} \hat{\rho}_S(t) e^{-i\hat{H}_S t}$ , we can rewrite the above equation as:

$$\frac{d}{dt} \hat{\rho}_S(t) = -i[\hat{H}_S, \hat{\rho}_S(t)] + e^{-i\hat{H}_S t} \left( \frac{d}{dt} \hat{\rho}_S^{(I)}(t) \right) e^{i\hat{H}_S t}. \quad (105)$$

Now lets apply this recipe to our Born-Markov Master equation. We insert expression 102 for  $\frac{d}{dt} \hat{\rho}_S^{(I)}$  into the right hand side of equation 105. We will also pull the time evolution operators into the square brackets and obtain:

$$\begin{aligned} e^{-i\hat{H}_S t} \hat{S}_\alpha(t) \hat{S}_\beta(t - \tau) \hat{\rho}_S^{(I)}(t) e^{i\hat{H}_S t} &= \hat{S}_\alpha \left( e^{-i\hat{H}_S \tau} \hat{S}_\beta e^{i\hat{H}_S \tau} \right) \hat{\rho}_S \\ &= \hat{S}_\alpha \hat{S}_\beta(-\tau) \hat{\rho}_S. \end{aligned} \quad (106)$$

This leads us to re-introducing the commutator notation and re-writing equation 102 as:

$$\frac{d}{dt} \hat{\rho}_S(t) = -i[\hat{H}_S, \hat{\rho}_S(t)] - \int_0^\infty d\tau \sum_{\alpha\beta} \left\{ \mathcal{C}_{\alpha\beta}(\tau) [\hat{S}_\alpha, \hat{S}_\beta(-\tau) \hat{\rho}_S(t)] + \mathcal{C}_{\beta\alpha}(-\tau) [\hat{\rho}_S(t) \hat{S}_\beta(-\tau), \hat{S}_\alpha] \right\}. \quad (107)$$

Note that the integral on the right hand side goes over the whole range of  $\tau$  which means that the time dependence of the environment self-correlation functions and the operators in the interaction picture can be integrated outside. This finally allows us to further simplify our expression and obtain the final form of the Born-Markov Master Equation:

$$\frac{d}{dt} \hat{\rho}_S(t) = -i[\hat{H}_S, \hat{\rho}_S(t)] - \sum_{\alpha} \left\{ [\hat{S}_\alpha, \hat{B}_\alpha \hat{\rho}_S(t)] + [\hat{\rho}_S(t) \hat{C}_\alpha, \hat{S}_\alpha] \right\}. \quad (108)$$

### 4.3 Lindblad Master Equation Form

The Lindblad form of the master equation is a subset of the Born-Markov Master Equations obtained by ensuring positivity of the reduced density matrix at all times:

$$\langle \psi | \hat{\rho}_S(t) | \psi \rangle \geq 0. \quad (109)$$

This condition of positivity is physically reasonable as we would want the elements of the reduced density matrix to represent the probabilities of the state a system can occupy. This condition naturally holds for an exact time evolution of the density matrix, however, it may not be the case for a reduced density matrix evolved through an approximation.

The most general form of the master equation that also ensure positivity is of the following form:

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}_S, \hat{\rho}_S(t)] + \frac{1}{2} \sum_{\alpha\beta} \gamma_{\alpha\beta} \left\{ [\hat{S}_\alpha, \hat{\rho}_S(t) \hat{S}_\beta^\dagger] + [\hat{S}_\alpha \hat{\rho}_S(t), \hat{S}_\beta^\dagger] \right\}, \quad (110)$$

where the operator  $\hat{S}_\alpha$  are the system operators present in the diagonal decomposition of the interacting Hamiltonian. Furthermore,  $\gamma_{\alpha\beta}$  are the time-independent coefficients capturing all the information regarding the physical parameters of the decoherence/dissipation process and can be used to define a coefficient matrix  $\Gamma \equiv (\gamma_{\alpha\beta})$ .

The Lindblad Master Equation is both Markovian and time local. In order to derive the equation from the Born-Markov Master Equation we use another approximation called the “rotating-wave approximation”. This is a commonly used approximation in Quantum Optics and is justified when the characteristic timescale  $\tau_S$  for the system is small compared to system’s relaxation timescale. We can simplify the Lindblad equation by diagonalizing the matrix  $\Gamma$  by the coefficients  $\gamma_{\alpha\beta}$ . This allows us to re-write in diagonal form as:

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}'_S, \hat{\rho}_S(t)] - \frac{1}{2} \sum_{\mu} \kappa_{\mu} \left\{ \hat{L}_{\mu}^\dagger \hat{L}_{\mu} \hat{\rho}_S(t) + \hat{\rho}_S \hat{L}_{\mu}^\dagger \hat{L}_{\mu} - 2 \hat{L}_{\mu} \hat{\rho}_S(t) \hat{L}_{\mu}^\dagger \right\}. \quad (111)$$

Here the  $\hat{H}'_S$  symbolizes the Lamb-shifted Hamiltonian of the system. The Lindblad operators  $\hat{L}_{\mu}$  are appropriate linear combinations of the original operators  $\hat{S}_{\alpha}$  whose coefficients can be obtained from the diagonalization of the matrix  $\Gamma$ .

If the operators  $\hat{S}_{\alpha}$  are hermitian we can write the equation in a double commutator form:

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}'_S, \hat{\rho}_S(t)] - \frac{1}{2} \sum_{\mu} \kappa_{\mu} \left[ \hat{L}_{\mu}, [\hat{L}_{\mu}, \hat{\rho}_S(t)] \right]. \quad (112)$$

In fact the standard equation of motion for environmental scattering,

$$\frac{\partial \rho_S(x, x', t)}{\partial t} = -\frac{i}{2m} \left( \frac{\partial^2}{\partial x'^2} - \frac{\partial^2}{\partial x^2} \right) \rho_S(x, x', t) - \Lambda(x - x')^2 \rho_S(x, x', t) \quad (113)$$

is also of the Lindblad form.

To visualize this, let us solve equation 112 with a single Lindblad Operator  $\hat{L} = \hat{x}$  and the free particle Hamiltonian  $\hat{H}_S = \hat{p}^2/2m$ ,

$$\frac{d}{dt}\hat{\rho}_S(t) = -\frac{i}{2m}[\hat{p}^2, \hat{\rho}_S(t)] - \frac{1}{2}\kappa[\hat{x}, [\hat{x}, \hat{\rho}_S(t)]]. \quad (114)$$

Expressing the equation in the position representation gives us:

$$\frac{\partial \rho_S(x, x', t)}{\partial t} = -\frac{i}{2m}\left(\frac{\partial^2}{\partial x'^2} - \frac{\partial^2}{\partial x^2}\right)\rho_S(x, x', t) - \frac{1}{2}\kappa(x - x')^2\rho_S(x, x', t), \quad (115)$$

which is almost identical to the equation of motion barring some coefficients that can be used to identify the Lindblad coefficients.

The Lindblad master equations give us a simple and intuitive method of representing the environmental monitoring of an open quantum system. If the Lindblad operators are chosen to be dimensionless then the coefficients  $\kappa_\mu$  can be viewed as one to one representation of decoherence rates. From equation 112 we can notice that if  $\hat{\rho}_S(t)$  commutes with each of the Lindblad operators  $\hat{L}_\mu$  for all times, i.e.,

$$[\hat{L}_\mu, \hat{\rho}_S(t)] = 0 \quad \forall \mu, t. \quad (116)$$

It can also be noted that since the Lindblad Operators are linear combinations of  $\hat{S}_\alpha$  they commute with the density matrix, i.e.,

$$[\hat{S}_\alpha, \hat{\rho}_S(t)] = 0 \quad \forall \alpha, t. \quad (117)$$

## 5 Limitations of the Standard Green Kubo Formula

To understand the limitations of the Kubo Formula, we will analyze a simple one-dimensional system coupled to two baths at its endpoints. The baths initially have different temperatures  $T$  and/or chemical potentials  $\mu$ , generating a current or a thermal flow. We wish to predict its steady-state dynamics by analyzing the steady-state currents flowing through the system. The system contains two “driving forces” which allow the steady-state charge/current to flow. The systems without any applied electric field can be called  $H_0$ , the unperturbed Hamiltonian. Applying a field (in this case, the electric field) gives rise to the term “ $V$ ”. The total Hamiltonian  $H$  can be expressed as  $H_0 + V$ . The second driving force is the gradient between the chemical potentials of the two baths connected at the system’s endpoints. This results in a non-equilibrium distribution function  $\rho$ . The steady-state expansion of the current would then be:

$$\langle J \rangle = Tr(\hat{J}\rho_\infty) \quad (118)$$

where  $\rho_\infty = \rho(t \rightarrow \infty)$  is the steady-state distribution to the non-equilibrium stationary state (NESS) after the system has been connected to both baths for a significant period of time. If the system is sufficiently large, it is possible to apply the above-studied approximations in the linear regime and assume that  $\rho_\infty \approx \rho_{eq}(H)$  which can then be used to calculate the current[7]. However, for systems with only one driving force (thermal currents): the non-equilibrium, it

becomes necessary to calculate  $\rho_\infty$ . A possible workaround is to assume gravitational potential or local equilibrium to introduce the potential  $V$ , which is how the standard Kubo Formula operates[1].

For finite-sized systems, it has been suggested that we can assume the reservoirs are coupled to the system through infinitely long, perfectly conducting wires to enable the total system to become infinite and allow us to apply the Kubo Formulation meaningfully. In cases where systems don't interact, it's been demonstrated that the Landauer formula becomes akin to substituting  $\rho_\infty$  with the presumption that states injected from the two leads follow the thermal distributions of their individual reservoirs[1]. Nevertheless, most investigations into conductance using the standard Kubo formula focus on infinitely uniform systems or extend findings from finite-sized systems to the limit of  $N \rightarrow \infty$ . In the latter scenario, once the eigenstates  $H_0 |m\rangle = \epsilon_m |m\rangle$  are determined, the formula becomes instrumental in computing various physical parameters. One notable example is the Drude weight equation[1]:

$$D = \frac{\pi\beta}{L} \sum_{\substack{m,n \\ \epsilon_m = \epsilon_n}} \frac{e^{-\beta\epsilon_m}}{Z} |\langle m | \hat{J} | n \rangle|^2. \quad (119)$$

The Drude weight equation is commonly used to discuss thermal or charge transport. We will first demonstrate that the standard Kubo formula does not give accurate results for the system connected to the two baths. We will use the Redfield Equational approach since they can correctly predict  $\rho_\infty = \rho_{eq}(H)$  for unbiased reservoirs. However, the Redfield Equations require a significant computational load to be solved fully, so we must apply it to small systems. Thankfully, researchers Jinshan Wu and Mona Berciu from the University of British Columbia have solved the system for  $N = 10$ ; we will use their work as a reference point. We will also be conducting our calculations under  $\hbar = 1$ .

As studied previously, the Liouville-von Neumann equation of motion for the density matrix in the close systems is as follows:

$$\frac{\partial \rho(t)}{\partial t} = L_H \rho(t) = -i[H, \rho]. \quad (120)$$

The stationary solutions of this equation are not unique. They contain an array of distributions, including  $\rho_{eq}(H) = \frac{1}{Z} e^{-\beta H}$ . If we look at  $H = H_0 + V$ , where take  $V$  as the static weak coupling to an external field, then we can utilize perturbation theory to obtain the  $t \rightarrow \infty$ , steady-state solution:

$$\delta \rho = \int_0^\infty dt e^{L_0 t - \eta t} L_V \rho_0, \quad (121)$$

where  $\eta \rightarrow 0^+$  and  $L_0 = L_{H_0}$ . Now, if we take  $\rho_0$  to be equal to  $\rho_{eq}(H_0)$ , then we just obtain the Green Kubo Formula as shown below:

$$\delta\rho = -i \int_0^\infty dt e^{-\eta t} \left[ V(-t), \frac{e^{-\beta H_0}}{Z} \right], \quad (122)$$

where  $V(t) = e^{iH_0 t} V e^{-iH_0 t}$ . We can rewrite the above formula by identity  $[V(-t), e^{-\beta H_0}] = -ie^{-\beta H_0} \int_0^\beta d\tau \dot{V}(-t - i\tau)$  to obtain:

$$\delta\rho = - \int_0^\infty dt e^{-\eta t} \int_0^\beta d\tau \rho_0 \dot{V}(-t - i\tau). \quad (123)$$

To express in terms of eigenvectors of  $H_0$ , we know that  $\langle m | \dot{V}(t) | n \rangle = i(\epsilon_m - \epsilon_n) V_{mn} e^{i(\epsilon_m - \epsilon_n)t}$  which converts the equation into:

$$\delta\rho = \sum_{\substack{m,n \\ \epsilon_m \neq \epsilon_n}} \frac{e^{-\beta\epsilon_m} - e^{-\beta\epsilon_n}}{Z} \frac{V_{mn}}{\epsilon_m - \epsilon_n - i\eta} |m\rangle \langle n|. \quad (124)$$

It should be noted that in the case where  $\epsilon_m = \epsilon_n$ ,  $\langle m | \dot{V}(t) | n \rangle = 0$ , which means the diagonal part of  $V$  does not contribute to the transport properties of the system. Now let's prove that the resulting  $\tilde{\rho} = \rho_{eq} H_0 + \delta\rho$  is indeed the first-order perturbation expansion of  $\rho_{eq} H$ . We assume that  $\langle m | V | n \rangle = 0$  if  $\epsilon_m = \epsilon_n$ . If that is not the case, we can eliminate the diagonal part of  $V$ , i.e.,  $V_0$ , and add  $H_0$ . This means that the eigenstates of the full Hamiltonian,  $H |\tilde{n}\rangle = \tilde{\epsilon}_n |\tilde{n}\rangle$ , to a first-order perturbation of the potential  $V$ . We can now also apply non-degenerative perturbation theory to all states to find that  $\tilde{\epsilon}_n = \epsilon_n + \mathcal{O}(V^2)$  and:

$$|\tilde{n}\rangle = |n\rangle + \sum_{m, \epsilon_m \neq \epsilon_n} \frac{\langle m | V | n \rangle}{\epsilon_n - \epsilon_m} |m\rangle + \mathcal{O}(V^2). \quad (125)$$

Which leads to  $\rho_{eq}(H) = \sum_n \frac{1}{Z} e^{-\beta \tilde{\epsilon}_n} |\tilde{n}\rangle \langle \tilde{n}| = \rho_{eq}(H_0) + \delta\rho + \mathcal{O}(V^2)$ , where  $\delta\rho$  is given by equation 124.

This confirms that the standard green-kubo formula predicts  $\rho_\infty \rightarrow \rho_{eq}(H)$ . This result can be troublesome because systems in systems where invariance to time symmetry remains unbroken, no steady state transport occurs as no currents are formed. Nonetheless, in a first-order perturbation, this may not be the case as the approximation of the NESS and  $\delta\rho$  may be the same or similar enough to encapsulate most of the system dynamics.

Before proceeding, it's essential to highlight an even more significant issue with the SKF as utilized in the literature, such as determining the Drude weight as described in equation 119. This issue is only naturally resolved for infinite or finite systems with periodic boundary conditions. A quick comparison of equations 119 and 124 reveals that while the former only accounts for contributions from degenerate states with  $n=m$ , the latter lacks such states altogether. To grasp the reason for this discrepancy, consider the derivation of equation 119 from equation 123, particularly for spinless fermions in a one-dimensional chain with a lattice constant of  $a=1$ .



$$H_0 = -t \sum_l (c_l^\dagger c_{l+1} + \text{h.c.}) + V_0 \sum_l n_l n_{l+1}, \quad (126)$$

where  $n_l = c_l^\dagger c_l$ , plus a static potential difference:

$$V = \sum_l V_l n_l \quad (127)$$

which is induced by a uniform electric field. We can now use the continuity equation to obtain:

$$\dot{V}(t) = \sum_l V_l \frac{d}{dt} n_l(t) = - \sum_l V_l [J_{l+1}(t) - J_l(t)], \quad (128)$$

where  $J_l = it(c_{l+1}^+ c_l - c_l^+ c_{l+1})$  is the local current operator. This equation can be reformed to:

$$- \sum_l [V_{l-1} J_l(t) - V_l J_l(t)] = -E J(t), \quad (129)$$

where  $J(t) = \sum_l J_l(t)$  is now the total current operator. We now utilize  $\dot{V}(t) = -E J(t)$  in equation 123 which gives us:

$$\delta\rho = E \int_0^\infty dt e^{-\eta t} \int_0^\beta d\tau \rho_0 J(-t - i\tau). \quad (130)$$

Hence, the DC conductivity is:

$$\sigma = \int_0^\infty dt e^{-\eta t} \int_0^\beta d\tau \langle J(-t - i\tau) J \rangle, \quad (131)$$

where  $\langle O \rangle = \text{Tr}[\rho_{eq}(H_0)]$ . The only controversial move in this derivation is the change:

$$\sum_l V_l J_{l+1}(t) \rightarrow \sum_l V_{l-1} J_l(t), \quad (132)$$

which changes the result from having no contribution from states with  $\epsilon_n = \epsilon_m$  to one whose contributions are only dictated by these states.

According to Wu and Berciu, this justification holds true only for an infinite system, where boundary effects are assumed to be negligible, or for a system with periodic boundary conditions and an external field exhibiting the same periodicity. Achieving the latter condition is only feasible for a charge current in an infinite system with periodic boundary conditions driven by a varying magnetic flux through the area enclosed by the system. However, this approach is bound to fail for a finite-size system (even one with periodic boundary conditions) subjected to a static applied electric field. The same holds for thermal transport, which cannot be experimentally induced in a system with

periodic boundary conditions. In both scenarios, it's challenging to grasp the physical relevance of the results obtained from equation 119. The problematic nature of using equation 119 and its equivalents for finite-size systems is further underscored by technical considerations. The spectrum of a finite-size system is always discrete, leading to any pair of degenerate eigenstates  $m = n$  contributing a delta function to the response functions. Such singular responses are physically unrealistic for finite-size systems. Various techniques have been proposed to mitigate these singular contributions to extract finite values, such as employing imaginary frequencies or averaging  $\sigma$  over a small range of frequencies  $\delta\omega$  and then approaching  $\delta\omega \rightarrow 0$ . Different approaches may yield different results, and the order in which various limits are approached, such as taking  $\eta \rightarrow 0$  before  $N \rightarrow \infty$  or vice versa, can also influence outcomes. All these nuances of the standard Kubo formula are intertwined with the potential divergence whenever  $m = n$ . In summary, utilizing the standard Kubo formula for finite-size systems is fraught with conceptual and technical challenges. We conclude that to describe a non-equilibrium steady state with a steady-state current flow in a finite-size system, one must go beyond considering the system as a closed entity and explicitly account for its connection to leads or baths[8].

## 6 Derivation of Kubo Formula for open finite-size systems

Now, we introduce an alternative deterministic formulation that explicitly incorporates the influence of thermal baths (heat transport) or coupling to leads (charge transport) on the system's state. This formulation is rooted in the Redfield equation (RE), which evaluates the evolution of the projected density matrix for the central system under consideration. This is obtained from the Liouville-von Neumann equation for the total density matrix describing the system plus reservoir after using a projection technique to trace the reservoirs. For the sake of understanding, let's assign an initial temperature to the initial left and right baths:  $T_{L/R} = T \pm \frac{\Delta T}{2}$ . Note that if  $\Delta \ll T$ , the system will just dissolve into a Kubo-like formula. We use the general form of the Redfield Equation[1]:

$$\frac{\partial \rho(t)}{\partial t} = [L_H + L_L(T_L) + L_R(T_R)]\rho(t), \quad (133)$$

where  $L_H \rho = -i[H, \rho]$  (akin to isolated systems), while  $L_{L/R}$  are the extra terms which describe the effects of the left and right thermal baths have on the system dynamics. The term  $L_{L/R}$  depends on the Hamiltonian  $H$  and its coupling to the baths. For example, if  $\Delta T \ll T$  then the Taylor expansion of  $L_{L/R}$  would lead to the following Redfield equation:

$$\frac{\partial \rho(t)}{\partial t} = [L_{H_0} + L_B(T) + L_P(\Delta T)]\rho(t) = L\rho(t), \quad (134)$$

where  $L_B(T) = L_L(T) + L_R(T)$  is the thermal bath input if they are kept at the same temperature while  $L_P(\Delta T)$  contains all the terms proportional to  $\Delta T$ . We assume thermal coupling does not induce a potential  $V$ , i.e.,  $H = H_0$ . We

are looking for the stationary-state solution  $\rho_\infty$  of the above equation, which satisfies

$$L\rho_\infty = 0, \quad (135)$$

and which we can assume to be unique for any given value of  $\Delta T$ . Wu and Berciu indicate that  $L$  must possess a non-degenerate zero eigenvalue, while all its other (transient) eigenvalues exhibit a negative real part. It's worth noting that  $L|_{\Delta T=0} = L_{H_0} + L_B(T)$  exhibits this characteristic. Furthermore, it can be demonstrated that under this condition, the solution as  $t$  approaches infinity converges to the anticipated thermal equilibrium for the system maintained at temperature  $T$ , denoted as  $\rho_\infty = \rho_{eq}(H_0)$ .

For small systems, equation 135 can be solved numerically to calculate the eigenstates corresponding to the zero eigenvalues. We term this solution  $\rho_{ex}$  and utilize it as a benchmark to validate the solutions obtained from different approximation schemes. A Kubo-like formula, potentially offering greater efficiency, can be derived using linear-response theory. The initial stage involves decomposing the Liouvillian  $L$  from equation 134 into a “small” and a “large” component. There exist two potential approaches:

$$\begin{cases} L_0^{(1)} = L_{H_0} + L_B(T), \\ \Delta L^{(1)} = L_P(\Delta T), \end{cases} \quad (136)$$

$$\begin{cases} L_0^{(2)} = L_{H_0}, \\ \Delta L^{(2)} = L_B(T) + L_P(\Delta T). \end{cases} \quad (137)$$

This paper will analyze the first approach since the second approach leads to a divergent solution that deviates from the exact numerical solution  $\rho_{ex}$  for quantities  $\langle m|A|n \rangle \neq 0$ [1]. We will assume that  $L_0^{(1)}$  has eigenvalues  $\{L_{0,\mu}^{(1)}\}$  and right/left eigenvectors  $\{|\mathcal{L}_\mu\rangle\}$  and  $\{|\mathcal{R}_\mu\rangle\}$ . As previously discussed, the unique steady-state solution of  $L_0^{(1)}$  will be  $\rho = \rho_{eq}(H_0)$ . The perturbation will produce a deviation  $\delta\rho_K^{(1)}$  just like we did in equation 121.

$$\begin{aligned} \delta\rho_K^{(1)} &= \sum_\mu \int_0^\infty dt e^{L_{0,\mu}^{(1)}t - \eta t} |\mathcal{R}_\mu\rangle \langle \mathcal{L}_\mu| \Delta L^{(1)} \rho_0 = \\ &= - \sum_\mu \frac{|\mathcal{R}_\mu\rangle \langle \mathcal{L}_\mu|}{L_{0,\mu}^{(1)} - \eta} \Delta L^{(1)} \rho_0 = - \sum_{\mu>0} \frac{|\mathcal{R}_\mu\rangle \langle \mathcal{L}_\mu|}{L_{0,\mu}^{(1)}} \Delta L^{(1)} \rho_0 \end{aligned} \quad (138)$$

It's worth noting that the sole divergent term, stemming from  $L_{0,0}^{(1)} = 0$ , vanishes due to  $(\mathcal{L}_0|\Delta L^{(1)}\rho_0 = (\rho_0|\Delta L^{(1)}\rho_0) = 0$ . Consequently, equation 138 comprises only regular contributions. Nonetheless, using equation 138 in actual practice proves challenging because determining all the eigenstates of  $L_0^{(1)}$  poses a formidable task unless the system boasts an exceedingly small Hilbert space. A

computationally more feasible solution arises when we combine the eigenequation  $L\rho_\infty = 0$  with the constraint  $Tr(\rho_\infty) = 1$ , yielding a regular system of coupled equations  $\bar{L}\bar{\rho}_\infty = v$ . In matrix notation,  $\bar{L}$  is constructed by substituting the first row of the equation  $L\rho_\infty = 0$  with  $Tr(\rho_\infty) = 1$ , rendering  $v$  a vector with its initial element as 1 and all others as 0. Consequently,  $det(\bar{L}) \neq 0$  while  $det(L) = 0$ . When solved numerically,  $\bar{L}\bar{\rho}_\infty = v$  yields the anticipated exact solution  $\rho_{ex}$ . Furthermore, we can resolve it to derive a Kubo-like formula by decomposing  $\bar{L}$  into  $\bar{L}_0^{(1)} + \Delta\bar{L}^{(1)}$ . We obtain:

$$\delta\bar{\rho}^{(1)} = -[\bar{L}_0^{(1)}]^{-1}\Delta\bar{L}^{(1)}\rho_0. \quad (139)$$

This approach is more convenient since it simplifies the process by inverting the non-singular matrix  $\bar{L}_0^{(1)}$ , which is simpler compared to finding all eigenstates of  $L_0^{(1)}$ , particularly for systems with up to  $N \approx 10$ . Researchers have confirmed that both methods yield identical outcomes for small  $N$ , where both can be executed[1]. Lastly, note that we express  $\rho_\infty^{(1)}$  as  $\rho_0 + \delta\bar{\rho}^{(1)}$ .

## 7 Conclusion

Through a strong fundamental understanding of Markovian Dynamics and Linear Response Theory, we demonstrated that the Green-Kubo Formula falls short in approximating the non-equilibrium stationary state, instead providing the first-order correction to the equilibrium state corresponding to the full Hamiltonian. Furthermore, we could see how employing the standard Kubo-Green formula on finite open systems typically results in unphysical divergences. However, by explicitly considering the coupling to baths, we resolve both issues and derive a well-behaved Kubo-like formula that can be applied to systems up to  $N \approx 10$ . While this is a promising result, it's still a relatively low number compared to practical system sizes. Therefore, more efficient methods must be extended to the Redfield equations to lessen the computational load required to reach numerical solutions. It should also be noted that although we could derive a Kubo-like formula for thermal heat transport in a two-reservoir system, the same physical assumptions may not hold for other quantum systems like the spin-fermionic system[9]. In this regard, researchers must adjust their physical parameters and initial conditions to match the system requirements and then apply the core principles discussed in this paper to obtain a generalized Green-Kubo formula for the system under study.

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