Different levels of approximations in Open Quantum Systems and their applications

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To those who believed in me when I doubted myself the most.

Abstract

Calculating the dynamics of a non-isolated system is generally computationally hard and sometimes even not feasible. Due to that reason, one needs to use different approximations that are detrimental to the accuracy of the results. However, in the majority of the current research papers, people tend to simply use the Markovian master equation (or GKLS.) While it is extremely simple to calculate and it is justified to use it in some circumstances one cannot always trust it as the final answer. This thesis aims to show that there are more ways to deal with open quantum system dynamics that are more reliable and easily implementable –for some systems– than the GKLS equation. Among those, we just focus on those that preserve the positivity of the state, i.e. the dynamics are completely positive.

The results will be presented in increasing order of precision. We begin with the results obtained from the familiar Markovian regime, followed by those obtained under non-Markovian approximations, such as the refined weak coupling approximation and a novel one introduced by us. Additionally, a fermionic resonant model has also been considered and we have shown that it can be solved exactly.

We have also applied the Markovian and non-Markovian dynamics to perform some desired tasks such as charging a quantum battery or estimating the temperature of a system. Finally, we compared the results from different approaches whenever possible.

Streszczenie

Obliczanie dynamiki nieizolowanego systemu jest generalnie trudne, a czasem nawet niewykonalne. Z tego powodu stosowane są różne przybliżenia, które niekorzystnie wpływają na dokładność wyników. W większości aktualnych prac badawczych wykorzystywane są Markowskie równania fundamentalne (GKLS). Chociaż podejście to jest proste obliczeniowo i użycie go jest uzasadnione w pewnych okolicznościach, jednakże nie zawsze można ufać uzyskanym wynikom i traktować ich jako pewnik. Ta praca ma na celu pokazanie, że istnieje więcej sposobów radzenia sobie z dynamiką otwartych systemów kwantowych. Sposoby te są bardziej niezawodne i łatwiejsze do wdrożenia (dla niektórych systemów) niż równanie GKLS. Wśród nich skupiamy się tylko na tych, które zachowują dodatnią określoność stanu, czyli na dynamice całkowicie dodatniej.

Wyniki zostaną przedstawione w kolejności rosnącej dokładności, począwszy od wyników uzyskanych z dobrze znanego reżimu Markowa, następnie uzyskanych przy przybliżeniach niemarkowskich, takich jak udoskonalone przybliżenie słabego sprzężenia, a kończąc na wprowadzonym przez nas nowym przybliżeniu. Dodatkowo rozważony został fermionowy model rezonansowy, dla którego zostało przedstawione ścisłe rozwiązanie.

Aby opisać pewne istotne zagadnienia fizyczne, takie jak ładowanie baterii kwantowej czy oszacowanie temperatury systemu użyta została zarówno dynamika Markowska jak i niemarkowska. W końcowym etapie pracy wyniki otrzymane dla różnych podejść zostały ze sobą porównane, tam gdzie było to możliwe.

Publications

This thesis will be based on our original works:

- [RAS+22]: Optimal quantum control of charging quantum batteries

  Rodríguez, RR and Ahmadi, B and Suárez, G and Mazurek, P and Barzanjeh, S and Horodecki, P

  arXiv preprint arXiv:2207.00094 (Sent to Physical Review Applied)

- [RRAM+22]: Catalysis in Charging Quantum Batteries

  Ravell Rodríguez, Ricard and Ahmadi, Borhan and Mazurek, Pawel and Barzanjeh, Shabir and Alicki, Robert and Horodecki, Pawel

  arXiv preprint arXiv:2205.05018 **(Accepted in Physical Review A)**

- [ARAH22] An approximation scheme and non-Hermitian re-normalization for description of atom-field system evolution

  Ahmadi, Borhan and Rodríguez, Ricard Ravell and Alicki, Robert and Horodecki, Michał

  arXiv preprint arXiv:2210.10345

- [RSH] *Rodríguez, Ricard Ravell and Suárez, Gerardo and Horodecki, Michał* in preparation

- [RMPLH] *Rodríguez, Ricard Ravell and Mehboudi, Mohammed and Perarnau-Llobet, Martí and Horodecki, Michał* in preparation

Another works that we did not use for the thesis:

- [BRH21] Edge of the set of no-signaling assemblages

  Banacki, Michał and Rodríguez, Ricard Ravell and Horodecki, Paweł

  Physical Review A, 103(5), 052434.

- [RBRRH22] Single trusted qubit is necessary and sufficient for quantum realization of extremal no-signaling correlations

  Ramanathan, Ravishankar and Banacki, Michał and Rodríguez, Ricard Ravell and Horodecki, Paweł

  npj Quantum Information, 8(1), 119.

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Notation

During the whole thesis we shall omit the hats on the operators and set $\hbar = K_B = 1$.

Contents

Chapter 1

Introduction

Quantum mechanics has revolutionized our understanding of the microscopic world on the atomic and subatomic levels. However, quantum systems are often described in isolation, assuming that they are completely separated from their environment [Sak06, Sha12]. In reality, almost all physical systems are open and interact with their surroundings, leading to complex quantum dynamics that is challenging to model and simulate [BP02, RH12, Lid19, Sch14].

The study of open quantum systems has gained significant attention in recent years due to its practical applications in quantum computing, quantum communication, and quantum sensing [Mer07, GT07, DRC17]. Open quantum systems are characterized by the interaction between the system and its environment, which results in a loss of coherence and the emergence of decoherence effects [BP02].

As commonly said, physics is the art of doing approximations and, I would humbly add that this is especially true when working with open quantum systems. There exists a plethora of methods and the list keeps growing day by day. The reason is that in general, it is very computationally demanding to calculate the dynamics of an open quantum system without using any approximation.

One of the most notorious among them is the so-called Markovian approximation. It assumes that the environment does not have any memory, so the dynamics after the present time t does not depend on the past, i.e. times before t. It is very helpful and simplifies the calculations a lot, but it only works in some regimes. In general, most processes in nature have memory and are not Markovian. This non-Markovianity is useful to perform some desired tasks such as systematic quantum control [RKK15], and perfect mixed state teleportation [LBP14].

If one would like to account for these memory effects, one may try to get the dynamics using other approximations. For that matter, we will resort to the so-called refined weak coupling [Riv17], first introduced by Alicki [Ali89] and later by Schaller and Brandes [SB08]. In this case, one does not end up with a master equation but rather with an exponent that gives the evolution. In that sense, we may call it the refined weak coupling equation. It is interesting because it ensures that the dynamics is completely positive while being non-Markovian, which is a property that any physical evolution should have.

Another way to deal with memory effects is employing the Bloch-Redfield equation [Red57, Blo57]. The drawback of using it is the fact that its dynamics is not completely positive and one may get non-physical states (given by non-positive matrices). However, there are some techniques to avoid this non-positivity [GN99, Whi08] Yet it is used in current research and especially in the field of Quantum Chemistry [JIP+15, CLAFLO+23]

This thesis aims to understand better the different approximations –specifically we will focus on the class of them that preserve complete positivity of the dynamics–when dealing with an open quantum system and see their range of validity. However, the dynamics of some systems are too complex to be accurately described by some given approximations so

one needs to pay the price of losing accuracy and keep approximating. Because of that, for some systems and platforms, we are not able to get the exact solution or the dynamics under the refined weak coupling approximation. Thus, we present different results obtained using Gorini-Kossakowski-Lindblad-Sudarshan (GKLS) master equation [GKS76, Lin76, CP17], the refined weak coupling equation [Ali89, SB08, Riv17], and exact dynamics. We apply these solutions for interesting tasks such as charging a quantum battery or estimating the temperature of the system. Additionally, we compare the results obtained under different regimes, whenever it is applicable.

To that end, this thesis is organized into four chapters. First, we introduce the dynamics of an open quantum system, we derive the GKLS master equation and the refined evolution equation. The next chapter presents the results obtained in a quantum battery setting introduced in [AFM$^+$18] using the GKLS master equation. The results of this chapter are based on our papers [RAS$^+$22, RRAM$^+$22]. and aim to improve the charging procedure of open quantum batteries. Later, in the third chapter, we show non-Markovian results obtained using the refined weak coupling and an approach derived by us [ARAH22]. Moreover, we benchmark the results obtained in the refined weak coupling approximation with the ones obtained using the GKLS equation in the aforementioned battery setting. This benchmark is based on a work by us that is not yet published [RSH]. In the last chapter, we present an exact solution of the resonant level model, namely without the need for any master equation or any kind of approximation as in the other chapters. This aims to improve the description of the "Spin-boson" model in the fermionic case. We apply the solution of the system to estimate its temperature and compare it to what one obtains when using the Markovian master equation. In addition, we benchmark the dynamics obtained exactly with the ones obtained using the GKLS master equation. This chapter is again based on one work that is in preparation [RMPLH].

The results presented in the thesis are structured in increasing order of accuracy. Namely, we start with the most difficult scenarios –the cases in which we had to resort to more approximations and hence the results are not that accurate–, and continue until the easiest model that we solved in an exact way, which gives us the most accurate results.

Chapter 2

Open Systems Dynamics

We are all familiar with the dynamics that a closed system undergoes, namely those given by the von Neumann equation [BP02]

$$\frac{\partial \rho(t)}{\partial t} = -i[H(t), \rho(t)], \tag{2.1}$$

where $\rho(t)$ and $H(t)$ are the state and the Hamiltonian of the system, respectively. For convenience, one can rewrite it as

$$\frac{\partial \rho(t)}{\partial t} = \mathcal{L}(t)\rho(t), \tag{2.2}$$

where $\mathcal{L}(t)$ is the Liouvillian super operator. Eq. (2.2) can readily be solved as

$$\rho(t) = \mathcal{T} \exp\left[\int_{t_0}^{t} ds \mathcal{L}(s)\right] \rho(t_0) \tag{2.3}$$

where $\mathcal{T}$ is the time-ordering operator that orders the products of time-dependent operators in such a way that the first acting on the right is the one evaluated at the smallest value of t.

In most cases, our system of interest (let us call it S) interacts with the environment/bath (B) and we are solely interested in the reduced state ρ_S. In that situation, one could compute $\rho_{SB}(t)$ using Eq. (2.3) and then trace out the degrees of freedom of the subsystem B. In real cases though, this turns out to be impracticable. Then, one typically traces out the subsystem B from Eq. (2.1) and then applies some approximations to get the dynamics for $\rho_S(t)$. As now $\rho_S(t)$ is no longer a closed system (remember that interacts with some degrees of freedom of B) its dynamics correspond to the dynamics of an open system [AL07, BP02, RH12, Sch14, Lid19]. These dynamics are no longer unitary and one needs to resort to some approximations to solve them.

In the first section of the chapter, we present the microscopic derivation of the GKLS master equation –which is of wide interest because describes a Markovian evolution [AL07, Nor97, BP02, RH12]–, explain in which regimes the approximations used to obtain it work, enumerate some properties of the steady state, and describe the global and local approach to calculate GKLS.

In the last section, we present the refined weak coupling evolution to derive a way to compute the dynamics and account for memory effects. Moreover, we show that the dynamics obtained under the refined weak coupling evolution tends to be those obtained using the global approach when time goes to infinity.

2.1 Microscopic derivation of GKLS master equation

Before starting the derivation of the Markovian master equation we would like to note that the GKLS equation is a general form to compute the dynamics of open quantum systems and is often used phenomenologically. However, Davies proposed a microscopic derivation of the GKLS master equation [Dav74, Dav76] that we present here. Hence, throughout the thesis, we deal with the GKLS-Davies equation.

Consider now that we start with a scenario analogous to the one depicted in Fig. (2.1). In that case, we have that the total system $(S+B)$ lives in the Hilbert space $\mathcal{H}_T = \mathcal{H}_S \otimes \mathcal{H}_B$ where $\mathcal{H}_S$ and $\mathcal{H}_B$ represent the Hilbert space for the system and the environment, respectively. We assume that the Hamiltonian of the system $(S+B)$ can be expressed as

$$H = H_S \otimes \mathbb{I}_B + \mathbb{I}_S \otimes H_B + V, \tag{2.4}$$

where V accounts for the interaction between the system and the bath. For simplicity, let us call $H_S \otimes \mathbb{I}_B$ as H_S and the same for the environment.

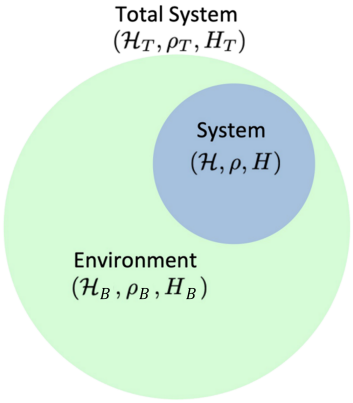


Figure 2.1: Pictorical representation of an open quantum system. The calligraphy letters represent the Hilbert spaces in which the Hamiltonians and states "live". Figure based on [Man20].

We start from the von Neumann equation for the total system in the interaction picture with respect to the free Hamiltonians H_S and H_B

$$\frac{\partial \tilde{\rho}_{SB}(t)}{\partial t} = -i[\tilde{V}(t), \tilde{\rho}_{SB}(t)], \tag{2.5}$$

where $\tilde{A} = U^\dagger(t) A U(t)$ and $U(t) = e^{-i(H_S + H_B)t}$. One can integrate the differential equation to get[1]

$$\rho_{SB}(t) = \rho_{SB}(0) - i \int_0^t ds[V(t), \rho_{SB}(t)]. \tag{2.6}$$

It is convenient for us to inject Eq. (2.6) back into Eq. (2.5) and trace out B to obtain

$$\frac{\partial}{\partial t}\rho_S(t) = -i \operatorname{Tr}_B[V(t), \rho_{SB}(0)] - \int_0^t ds \operatorname{Tr}_B \left[V(t), [V(s), \rho_{SB}(s)]\right]. \tag{2.7}$$

We now assume that the initial state of the system is a product state of the form $\rho_{SB}(0) = \rho_S(0) \otimes \rho_B(0)$. Furthermore, we note that any interaction Hamiltonian V (in

[1] We omit tildes from now on during this chapter, and all the operators are in the interaction if we do not say otherwise.

Schrodinger picture) acting on $\mathcal{H}_S \otimes \mathcal{H}_B$ can be written as (see [RH12] for the proof)

$$V = \sum_k A_k \otimes B_k, \tag{2.8}$$

where $A_k^\dagger = A_k$ and $B_k^\dagger = B_k$.

Keeping that in mind, we can compute

$$\mathrm{Tr}_B(V(t)\rho_{SB}(0)) = \mathrm{Tr}_B\left(\sum_k A_k(t) \otimes B_k(t)\rho_S(0) \otimes \rho_B(0)\right) = \sum_k A_k(t)\rho_S(0)\,\mathrm{Tr}_B(B_k(t)\rho_B(0)) = 0, \tag{2.9}$$

where we used that $\mathrm{Tr}_B(B_k(t)\rho_B(0)) = 0$ which is always a mild assumption as long as $[H_B, \rho_B] = 0$ [KCK08]. That is usually the case because one considers that the bath starts in thermal equilibrium and is given by the Gibbs state

$$\rho_B(0) = \frac{e^{-\beta H_B}}{\mathrm{Tr}(e^{-\beta H_B})}, \tag{2.10}$$

where β is the inverse temperature of the bath. Moreover, $A_k(t) = e^{iH_S t}A_k e^{-iH_S t}$ and $B_k(t) = e^{iH_B t}B_k e^{-iH_B t}$. With this, we now have

$$\frac{\partial}{\partial t}\rho_S(t) = -\int_0^t ds\,\mathrm{Tr}_B\left[V(t), [V(s), \rho_{SB}(s)]\right]. \tag{2.11}$$

If the bath is sufficiently larger than the system and the coupling between them is small (weak-coupling approximation), one could consider that the system of the system will not affect the system of the bath during the whole evolution and write the state of the system as $\rho_{SB}(t) \approx \rho_S(t) \otimes \rho_B(0)$. This is called the Born approximation. Even though we present it as an approximation, it may be more accurate to treat it as an ansatz to solve the equations.[2] In that way we get

$$\frac{\partial}{\partial t}\rho_S(t) = -\int_0^t ds\,\mathrm{Tr}_B\left[V(t), [V(s), \rho_S(s) \otimes \rho_B(0)]\right] = -\int_0^t d\tau\,\mathrm{Tr}_B\left[V(t), [V(t-\tau), \rho_S(t-\tau) \otimes \rho_B(0)]\right], \tag{2.12}$$

where we perform a change of variables in the integrand because it will be useful later.

This equation is non-local in time, the dynamics at time t depend on the states at all the previous times. To simplify the matters, we take the so-called Markov approximation and consider that the "short-memory" of the bath only keeps track of the events within the time range $[0, \tau_B]$, where τ_B is the relaxation time of the bath and it is related to the correlation functions of the reservoir. Thus, we substitute $\rho_S(t-\tau)$ by $\rho_S(t)$ and get

$$\frac{\partial \rho_S(t)}{\partial t} = -\int_0^t d\tau\,\mathrm{Tr}_B\left[V(t), [V(t-\tau), \rho_S(t) \otimes \rho_B(0)]\right]. \tag{2.13}$$

This approximation is justified if the integrand becomes almost zero for $t >> \tau_B$. In addition, one considers that the coupling between the bath and the system g obeys $g << 1/\tau_B$. Finally, assuming again that the correlation function of the reservoir is negligible for $t >> \tau_B$, we can send the limit of the integral to infinity as[3]

$$\frac{\partial \rho_S(t)}{\partial t} = -\int_0^\infty d\tau\,\mathrm{Tr}_B\left[V(t), [V(t-\tau), \rho_S(t) \otimes \rho_B(0)]\right], \tag{2.14}$$

which is the Bloch-Redfield equation[4] [Red57, Blo57]. It is generally not completely positive (CP) and therefore it can make the state non-positive (some techniques try to circumvent

[2] See [RH12] for a very interesting discussion about this.

[3] For a rigorous proof, see [ABLZ12].

[4] Some people define Eq. (2.13) as the Bloch-Redfield equation (see for example [Whi18, Lid19, BP02].)

the issue [GN99, Whi08].)[5] As mentioned before, there is a caveat here, the dynamics described by (2.14) are only meaningful for times bigger than the relaxation time τ_B.

Eq. (2.14) is still non-CP and it can lead to unphysical states. To obtain CP dynamics, one has to resort to an extra approximation, the so-called secular approximation. To do so, let us rewrite Eq. (2.14) using Eq. (2.8) for $V(t)$,

$$\frac{\partial \rho_S(t)}{\partial t} = -\sum_{k,k'} \int_0^\infty d\tau \, \mathrm{Tr}_B \left[A_k(t) \otimes B_k(t), [A_{k'}(t-\tau) \otimes B_{k'}(t-\tau), \rho_S(t) \otimes \rho_B(0)]\right]. \tag{2.15}$$

To be as explicit as possible, we will expand the double commutator as

$$\begin{aligned}
&\mathrm{Tr}_B \left[A_k(t) \otimes B_k(t), [A_{k'}(t-\tau) \otimes B_{k'}(t-\tau), \rho_S(t) \otimes \rho_B(0)]\right] && (2.16)\\
&= A_k(t)A_{k'}(t-\tau)\rho_S(t) \, \mathrm{Tr}\left[B_k(t)B_{k'}(t-\tau)\rho_B(0)\right] && (2.17)\\
&- A_{k'}(t-\tau)\rho_S(t)A_k(t) \, \mathrm{Tr}\left[B_{k'}(t-\tau)\rho_B(0)B_k(t)\right] && (2.18)\\
&- A_k(t)\rho_S(t)A_{k'}(t-\tau) \, \mathrm{Tr}\left[\rho_B(0)B_{k'}(t-\tau)B_k(t)\right] && (2.19)\\
&+ \rho_S(t)A_k(t-\tau)A_{k'}(t) \, \mathrm{Tr}\left[B_k(t)\rho_B(0)B_{k'}(t-\tau)\right]. && (2.20)
\end{aligned}$$

It is useful to define now the two-point correlation functions of the bath as

$$\begin{aligned}
\mathcal{B}_{kk'}(t, t-\tau) &= \mathrm{Tr}\left[B_k(t)B_{k'}(t-\tau)\rho_B(0)\right] && (2.21)\\
&= \mathrm{Tr}\left[e^{iH_B t}B_k e^{-iH_B t}e^{iH_B(t-\tau)}B_{k'}(t-\tau)e^{-iH_B(t-\tau)}\rho_B(0)\right] && (2.22)\\
&= \mathrm{Tr}\left[e^{iH_B \tau}B_k e^{-iH_B \tau}B_{k'}(t-\tau)\rho_B(0)\right] = \mathrm{Tr}\left[B_k(\tau)B_{k'}\rho_B(0)\right] && (2.23)\\
&= \mathcal{B}_{kk'}(\tau, 0) \equiv \mathcal{B}_{kk'}(\tau), && (2.24)
\end{aligned}$$

where we consider that ρ_B is a stationary state and thus commutes with H_B.

The correlation functions of the bath do not depend on the time t and without loss of generality, we can set $t = 0$. Following similar calculations, one can show that $\mathcal{B}^*_{kk'}(\tau) = \mathcal{B}_{kk'}(-\tau)$. Using these properties, we can simplify the Eq. (2.15) as

$$\frac{\partial \rho_S(t)}{\partial t} = -\sum_{k,k'} \int_0^\infty d\tau \mathcal{B}_{kk'}(\tau)\big([A_k(t), A_{k'}(t-\tau)\rho_S(t)] + h.c.\big), \tag{2.25}$$

where h.c. stands for the hermitian conjugate. The next step is moving the operators to the frequency domain. For that matter, let us assume that the spectrum of the Hamiltonian of the system is discrete, $H_S = \sum_\varepsilon \varepsilon|\varepsilon\rangle\langle\varepsilon|$. Hence

$$A_k(t) = e^{iH_S t}A_k e^{-iH_S t} = \sum_{\varepsilon,\varepsilon'} e^{-i(\varepsilon'-\varepsilon)t}|\varepsilon\rangle\langle\varepsilon|A_k|\varepsilon'\rangle\langle\varepsilon'| = \sum_\omega A_k(\omega)e^{-i\omega t}, \tag{2.26}$$

where $\omega = \varepsilon' - \varepsilon$ (it is called Bohr frequency) and $A_k(\omega) = \sum_{\omega=\varepsilon'-\varepsilon}\langle\varepsilon|A_k|\varepsilon'\rangle|\varepsilon\rangle\langle\varepsilon'|$. They are called jump operators (or eigenoperators) of the system and they fulfill the following properties

$$\begin{aligned}
A_k(\omega) &= A_k^\dagger(-\omega) && (2.27)\\
\sum_\omega A_k(\omega)e^{-i\omega t} &= \sum_\omega A_k^\dagger(\omega)e^{i\omega t}. && (2.28)
\end{aligned}$$

[5] In this sense, even if some people call it a Markovian equation, it is not strict Markovian because Markovian dynamics should preserve the positivity of the states. Thus, we will call the Markovian master equation the one obtained after performing the secular approximation and ensuring CP dynamics. In other words, the GKLS equation. As this subject is indeed an ongoing research discussion, we recommend the reader to take a look at [RHP14] to know more.

Let us now calculate the two terms of the commutator in Eq. (2.25)

$$A_k(t)A_{k'}(t-\tau)\rho(t) = \sum_{\omega\omega'} e^{i\omega' t}e^{-i\omega(t-\tau)}A_k^\dagger(\omega')\,A_{k'}(\omega)\rho(t) = \sum_{\omega\omega'} e^{i\omega\tau}e^{i(\omega'-\omega)t}A_k^\dagger(\omega')\,A_{k'}(\omega)\rho(t), \tag{2.29}$$

$$A_{k'}(t-\tau)\rho(t)A_k(t) = \sum_{\omega\omega'} e^{-i\omega(t-\tau)}e^{i\omega' t}A_{k'}(\omega)\rho(t)A_k^\dagger(\omega') = \sum_{\omega\omega'} e^{i\omega\tau}e^{i(\omega'-\omega)t}A_{k'}(\omega)\rho(t)A_k^\dagger(\omega')\,. \tag{2.30}$$

We can now define

$$\Gamma_{kk'}(\omega) = \int_0^\infty d\tau e^{i\omega\tau}\mathcal{B}_{kk'}(\tau), \tag{2.31}$$

which is the one-sided Fourier transform of the autocorrelation functions of the bath $\mathcal{B}_{kk'}$. So, in the frequency domain, Eq. (2.25) reads

$$\frac{\partial\rho_S(t)}{\partial t} = -\sum_{k,k'}\sum_{\omega,\omega'}\Big(\Gamma_{kk'}(\omega)e^{i(\omega'-\omega)t}\left[A_k^\dagger(\omega'),A_{k'}(\omega)\rho_S(t)\right]\Big) + h.c. \tag{2.32}$$

Now we can finally move on to perform the secular approximation –which is done in the spirit of the rotating wave approximation in quantum optics [GZZ04, BF05, LP00]–. To do that, we eliminate the crossed terms $\omega \neq \omega'$ assuming that they are rapidly oscillating if $t >> |\omega-\omega'|^{-1}$, and thus they average to zero. Before we also made the assumption that $t >> \tau_B$, so the secular approximation is only valid if $|\omega-\omega'|^{-1} > \tau_B$ for all $\omega \neq \omega'$. Therefore, one can summarize all the approximations as

$$g << 1/\tau_B < \min_{\omega\neq\omega'}|\omega-\omega'|. \tag{2.33}$$

With this, we have

$$\frac{\partial\rho_S(t)}{\partial t} = -\sum_{k,k'}\sum_{\omega}\Big(\Gamma_{kk'}(\omega)\left[A_k^\dagger(\omega'),A_{k'}(\omega)\rho_S(t)\right]\Big) + h.c. \tag{2.34}$$

However, it is convenient to still do some simplifications in the formula to get the final GKLS equation. We first define the Fourier transform of the autocorrelation functions as

$$\gamma_{kk'}(\omega) = \int_{-\infty}^\infty d\tau e^{i\omega\tau}\mathcal{B}_{kk'}(\tau), \tag{2.35}$$

which fulfills $\gamma^*_{kk'}(\omega) = \gamma_{k'k}(\omega)$. Hence,

$$\Gamma_{kk'}(\omega) = \int_0^\infty d\tau e^{i\omega\tau}\mathcal{B}_{kk'}(\tau) = \int_0^\infty d\tau e^{i\omega\tau}\frac{1}{2\pi}\int_{-\infty}^\infty d\omega' e^{-i\omega'\tau}\gamma_{kk'}(\omega') \tag{2.36}$$

$$= \frac{1}{2\pi}\int_{-\infty}^\infty d\omega'\gamma_{kk'}(\omega')\int_0^\infty d\tau e^{i(\omega-\omega')\tau}, \tag{2.37}$$

where we used the inverse Fourier transform for $\mathcal{B}_{kk'}(\tau)$. With the help of the mathematical identity

$$\int_0^\infty d\tau e^{i\omega\tau} = \pi\delta(\omega) + i\mathcal{P}\left(\frac{1}{\omega}\right), \tag{2.38}$$

where $\mathcal{P}(x)$ denotes the Cauchy principal value and can be calculated for a function f as

$$\left[\mathcal{P}\left(\frac{1}{\omega}\right)\right](f) = \lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon} d\omega\frac{f(\omega)}{\omega}. \tag{2.39}$$

Thus

$$\Gamma_{kk'}(\omega) = \frac{1}{2}\gamma_{kk'}(\omega) + iS_{kk'}(\omega), \tag{2.40}$$

where

$$S_{kk'}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega' \gamma_{kk'}(\omega')\mathcal{P}\left(\frac{1}{\omega-\omega'}\right). \tag{2.41}$$

As $S_{kk'}(\omega) = S^*_{k'k}(\omega)$, we can rewrite

$$\gamma_{kk'}(\omega) = \Gamma_{kk'}(\omega) + \Gamma^*_{k'k}(\omega) \tag{2.42}$$

$$S_{kk'}(\omega) = \frac{1}{2i}\left(\Gamma_{kk'}(\omega) - \Gamma^*_{k'k}(\omega)\right), \tag{2.43}$$

which after some tedious but straightforward calculations (see [Lid19] for details) allows us to obtain the GKLS equation

$$\frac{d\rho_S(t)}{dt} = -i\left[H_{\rm LS}, \rho_S(t)\right] + \sum_{\omega}\sum_{kk'}\gamma_{kk'}(\omega)\left(A_{k'}(\omega)\rho_S(t)A^\dagger_k(\omega) - \frac{1}{2}\left\{A^\dagger_k(\omega)A_{k'}(\omega), \rho_S(t)\right\}\right), \tag{2.44}$$

where

$$H_{\rm LS} = \sum_{\omega}\sum_{kk'} S_{kk'}(\omega)A^\dagger_k(\omega)A_{k'}(\omega), \tag{2.45}$$

is the so-called Lambshift Hamiltonian –we call it Hamiltonian because it is Hermitian by construction– and it commutes with the Hamiltonian of the system, i.e. $[H_{\rm LS}, H_S] = 0$. This Hamiltonian accounts for the shifts in the energies of the system produced by the interaction with the bath. The other term of the dynamics

$$\mathcal{D}(\rho_S(t)) = \sum_{\omega}\sum_{kk'}\gamma_{kk'}(\omega)\left(A_{k'}(\omega)\rho_S(t)A^\dagger_k(\omega) - \frac{1}{2}\left\{A^\dagger_k(\omega)A_{k'}(\omega), \rho_S(t)\right\}\right), \tag{2.46}$$

accounts for the dissipation (or incoherent evolution) and is usually called the dissipator. $\gamma_{kk'}(\omega)$ are called the decaying rates and we will see later that one can rewrite them as $\gamma_{kk'}(\omega) = 2\pi\,\mathrm{Tr}\left[B_k(\omega)B_{k'}\rho_B(0)\right]$.

We would like to note that Eq. (2.44) is in the interaction picture with respect to the free Hamiltonians of the system. However, due to the construction of the jump operators, it is straightforward to get the dynamics in the Schrödinger picture as

$$\frac{d\rho_S(t)}{dt} = -i\left[H_S + H_{\rm LS}, \rho_S(t)\right] + \sum_{\omega}\sum_{kk'}\gamma_{kk'}(\omega)\left(A_{k'}(\omega)\rho_S(t)A^\dagger_k(\omega) - \frac{1}{2}\left\{A^\dagger_k(\omega)A_{k'}(\omega), \rho_S(t)\right\}\right), \tag{2.47}$$

where the only new term is the Hamiltonian of the system H_S and we note that $\rho_S(t)$ is now in the Schrödinger picture.

The above equation gives CP dynamics as long as $\gamma(\omega)$ is a semidefinite positive matrix. The proof of that follows from Bochner's theorem [RS$^+$80, RS$^+$75] that states that the Fourier transform of a function is positive if the function is of a positive type. A function $f(x)$ is of a positive type if the matrix $f_{mn} = f(x_m - x_n)$ is positive semidefinite for any x_m and x_n. In our case, $f(x) = \mathcal{B}_{kk'}(\tau) = \mathrm{Tr}[B_k(\tau)B_{k'}\rho_B(0)]$ which can be proven to be of positive type (see [RH12] for the proof.)

To finish, we would like to note that the evolution of ρ_S will be given as

$$\rho_S(t) = e^{\mathcal{L}t}\rho_S(0), \tag{2.48}$$

where

$$\mathcal{L}(\cdot) = -i\left[H_S + H_{LS}, (\cdot)\right] + \sum_{\omega}\sum_{kk'}\gamma_{kk'}(\omega)\left(A_{k'}(\omega)(\cdot)A^\dagger_k(\omega) - \frac{1}{2}\left\{A^\dagger_k(\omega)A_{k'}(\omega), (\cdot)\right\}\right) \tag{2.49}$$

is the action of the Liouvillian (or generator of the dynamics) superoperator to any operator.[6]

2.1.1 Steady state properties

The steady state of a general evolution is given by

$$\frac{\partial \rho_{st}}{\partial t} = \mathcal{L}\rho_{st} = 0. \tag{2.50}$$

Nonetheless, it is not always the case that any initial state relaxes to a steady state, namely

$$\lim_{t\to\infty} \rho(t) = \rho_{st}. \tag{2.51}$$

To fulfill this, the only eigenoperator of the adjoint Liouvillian $\mathcal{L}^\dagger$ with null eigenvalue should be proportional to the identity [AL07]. In other words, the only operator that commutes with all the jump operators of the system and its Hamiltonian is again proportional to the identity [AFH09]. These are called the ergodicity conditions.[7]

The Gibbs state with respect to the system's Hamiltonian H_S and with the same temperature T as the bath, i.e.

$$\tau_S = \frac{e^{-\beta H_S}}{\mathrm{Tr}(e^{-\beta H_S})}, \tag{2.52}$$

is a steady state for the GKLS master equation. Let us prove it. First, note that starting with the bath at the thermal state we have

$$\langle B_a(t)B_b(0)\rangle = \mathrm{Tr}(\tau_B e^{iH_B t}B_a e^{-iH_B t}B_b) = \frac{1}{\mathrm{Tr}(e^{-\beta H_B})}\mathrm{Tr}(B_b e^{i(t+i\beta)H_B}B_a e^{-iH_B t}) \tag{2.53}$$

$$= \frac{1}{\mathrm{Tr}(e^{-\beta H_B})}\mathrm{Tr}(B_b e^{i(t+i\beta)H_B}B_a e^{-i(t+i\beta)H_B}e^{-\beta H_B}) = \langle B_b(0)B_a(t+i\beta)\rangle, \tag{2.54}$$

which is called Kubo-Martin-Schwinger (KMS) condition [Kub57, MS59]. Second, we have

$$\gamma_{ab}(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau}\,\mathrm{Tr}(B_a(\tau)B_b\tau_B) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau}\,\mathrm{Tr}(B_b B_a(\tau+i\beta)\tau_B). \tag{2.55}$$

We can now rewrite $B_a(\tau)$ as we did in Eq. (2.26) and then $B_a(\tau) = \sum_\omega e^{-i\omega\tau}B_a(\omega)$. However, this has the problem that the correlation functions will be periodic and when integrating them from zero to infinite, the integral will diverge [RH12]. The only way to solve this problem is to consider that the spectrum of the bath is continuous and in that case, $B_a(\tau) = \int_{-\omega_{max}}^{\omega_{max}} d\omega e^{-i\omega\tau}B_a(\omega)$ where ω_{max} is the maximum eigenfrequency of the bath (it can be infinite.)

In that case

$$\gamma_{ab}(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau}\,\mathrm{Tr}(B_b B_a(\tau+i\beta)\tau_B) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau}\int_{-\omega_{max}}^{\omega_{max}} d\omega' e^{-i\omega'(\tau+i\beta)}\,\mathrm{Tr}(B_b B_a(\omega')\tau_B) \tag{2.56}$$

$$= \int_{-\omega_{max}}^{\omega_{max}} d\omega' e^{\beta\omega'}\int_{-\infty}^{\infty} d\tau e^{i\tau(\omega-\omega')}\,\mathrm{Tr}(B_b B_a(\omega')\tau_B) = \int_{-\omega_{max}}^{\omega_{max}} d\omega' e^{\beta\omega'}2\pi\delta(\omega-\omega')\,\mathrm{Tr}(B_b B_a(\omega')\tau_B) \tag{2.57}$$

$$= 2\pi e^{\beta\omega}\,\mathrm{Tr}(B_b B_a(\omega)\tau_B) = 2\pi e^{\beta\omega}[\mathrm{Tr}(B_a^\dagger(\omega)B_b\tau_B)]^* \tag{2.58}$$

$$= 2\pi e^{\beta\omega}[\mathrm{Tr}(B_a(-\omega)B_b\tau_B)]^* = e^{\beta\omega}\gamma_{ab}^*(-\omega) = e^{\beta\omega}\gamma_{ba}(-\omega), \tag{2.59}$$

[6] The notation $(\cdot)$ indicates that this is where the operator is in the formula.

[7] This is indeed an interesting topic and we defer the reader to [Spo77, Fri77, Fri78] for more details.

where we used the definition of Dirac's delta and assumed that ω was in the spectrum of the bath, i.e. $\omega \in \{-\omega_{max}, \omega_{max}\}$.[8] In addition, we used that $\gamma_{ab}(\omega) = 2\pi \operatorname{Tr}(B_a(\omega)B_b\tau_B)$ which can be easily obtained performing analogous calculations. Finally, we have

$$\tau_A A_a(\omega) = e^{\beta\omega} A_a(\omega)\tau_A \tag{2.60}$$

$$\tau_A A_a^\dagger(\omega) = e^{-\beta\omega} A_a^\dagger(\omega)\tau_A. \tag{2.61}$$

With all these properties, we can calculate the stationarity of the thermal state as

$$\frac{\partial\tau_S}{\partial t} = \sum_\omega \sum_{a,b} \gamma_{ab}(\omega) \left[A_b(\omega)\tau_S A_a^\dagger(\omega) - \frac{1}{2}\left\{ A_a^\dagger(\omega)A_b(\omega), \tau_S \right\} \right] \tag{2.62}$$

$$= \sum_\omega \sum_{a,b} \gamma_{ab}(\omega) \left[e^{-\beta\omega} A_b(\omega)A_a^\dagger(\omega)\tau_S - A_a^\dagger(\omega)A_b(\omega)\tau_S \right] \tag{2.63}$$

$$= \sum_\omega \sum_{a,b} \left[\gamma_{ab}(\omega)e^{-\beta\omega} A_b^\dagger(-\omega)A_a(-\omega) - \gamma_{ab}(\omega)A_a^\dagger(\omega)A_b(\omega) \right] \tau_S \tag{2.64}$$

$$= \sum_\omega \sum_{a,b} \left[\gamma_{ba}(-\omega) A_b^\dagger(-\omega)A_a(-\omega) - \gamma_{ab}(\omega)A_a^\dagger(\omega)A_b(\omega) \right] \tau_S = 0. \tag{2.65}$$

We defer the reader to reference [Lid19] for more detailed calculations.

Nonetheless, the steady state should be the partial trace of the Gibbs state of the total Hamiltonian (system plus bath) up to some corrections in the strength of the coupling between the system and the bath [TMCA22, ŁWS+22]. This has been extensively discussed and it is an active area in the field. So, even when the dynamics given by the GKLS are CP, there are some problems with it such as its failure to describe the dynamics if the levels of the system are nearly degenerated (one can see [TR08] for a method to deal with continuous Hamiltonians and preserve CP dynamics), and giving the incorrect steady state [Ali89]. In the case of an almost degenerate spectrum, according to Alicki and Lendi [AL07], one may still use the GKLS equation, derived for the degenerate levels, and add splitting as a Hamiltonian perturbation. This is the so-called local approach that we will introduce in the next subsection.

On the other hand, although the Bloch-Redfield equation [Blo57, Red57] is not CP, it has been shown that in some cases [FC11, TWH12, CA21, PGM+20, TDKP22] one obtains the expected steady state.

To sum up, the drawbacks and advantages of using each equation and the range of their validity as well as coming up with better and more refined approximations are still exciting ongoing research problems.

Finally, before concluding this section we talk about two approaches, local and global, to deal with more complex systems in which our system of interest is made of interacting subsystems that do not interact directly with the bath.

2.1.2 Local and global approach

We shall now examine how the GKLS-Davies equation works in presence of degeneracy and show how it leads to the so-called "local-global" problem. We shall explain this through an example. We explain this section using an example. Consider a Hamiltonian of this form

$$H = H_A + H_C + gH_{AC} + H_B + V_{AB}, \tag{2.66}$$

[8] The aforementioned property, $\gamma_{ab}(\omega) = e^{\beta\omega}\gamma_{ba}(-\omega)$, it is very important and it is used to prove the detailed balance condition and to obtain the Pauli master equation [Lid19, BP02], which gives the evolution of the populations. As an example, this is interesting for adiabatic quantum computing and quantum annealing in which all the important information is contained in the ground state [AL18].

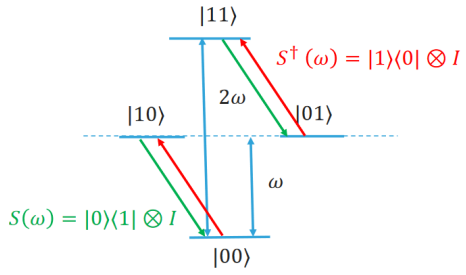
where

$$H_A = H_C = \omega|1\rangle\langle 1|, \tag{2.67}$$
$$V_{AB} = \sigma_{x,A} \otimes B, \tag{2.68}$$
$$H_{AC} = \frac{1}{2}\left(\sigma^+ \otimes \sigma^- + \sigma^- \otimes \sigma^+\right), \tag{2.69}$$

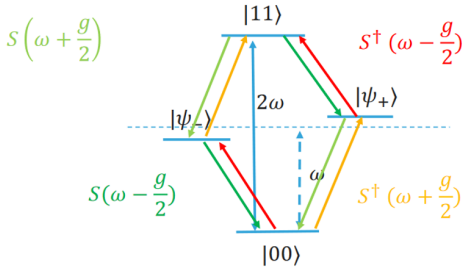
with B being a bath operator that we do not need to specify and $\sigma^+ = \sigma^{-\dagger} = |0\rangle\langle 1|$. Both H_A and H_C correspond to two-level systems. If we consider $g = 0$, we will have that the jump operators[9] will only connect the following states

$$|00\rangle \longleftrightarrow |10\rangle, |11\rangle \longleftrightarrow |01\rangle, \tag{2.70}$$

as seen in Fig. (2.2(a)).



(a) g=0



(b) $g \neq 0$

Figure 2.2: Jumps between the energies of the system for both $g = 0$ and $g \neq 0$.

Nevertheless, the situation is completely different even if one moves away from $g = 0$ infinitesimally and breaks the degeneracy. In that case ($g \neq 0$ and fixed), to compute the jump operators, one needs to first diagonalize the whole Hamiltonian $H_A + H_C + gH_{AC}$. Doing so, one gets that the eigenfrequencies are $\omega \pm g/2$ which respectively correspond to the eigenvectors $|\psi_+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$ and $|\psi_-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$, and 2ω and zero for excited and the ground state respectively ($|11\rangle$ and $|00\rangle$.) This translates to the following jump operators

$$S\left(\omega + \frac{g}{2}\right) = \frac{1}{\sqrt{2}}\left(|\psi_-\rangle\langle 11| + |00\rangle\langle\psi_+|\right), \tag{2.71}$$
$$S\left(\omega - \frac{g}{2}\right) = \frac{1}{\sqrt{2}}\left(|\psi_+\rangle\langle 11| - |00\rangle\langle\psi_-|\right), \tag{2.72}$$

and the transpose of them (see Fig. (2.2(b)) for a pictorical representation.)

[9] They are simply given by $S(\omega) = |0\rangle\langle 1| \otimes \mathbb{I}_C$ and $S(-\omega) = |1\rangle\langle 0| \otimes \mathbb{I}_C$.

This discontinuity is non-physical since one would not expect the jump operators to differ so much for small g's. This problem stems from the fact that the GKLS equation works only for times $t >> \frac{1}{\Delta\omega}$ (secular approximation) where $\Delta\omega$ is the smallest difference of frequencies in H_A. In our case, $\Delta\omega = g$.

To treat this, one uses the local approach –where one treats the interaction H_{AC} as a perturbation, and gets the jump operators as in the case with null g – and keeps in mind that it is valid for $t << \frac{1}{g}$. And the global approach (analogous to the case with $g \neq 0$) for $t >> \frac{1}{g}$.

Moreover, there exists a general rule exposed in [AL07, Ali89, BF05]. Namely, that for any Hamiltonian $H = H_0 + V$ one can get the GKLS equation for the whole H, that is the global approach, or instead derive it for H_0 and add V in the Hamiltonian part of the final GKLS form (local approach.) The global scheme is valid for $t >> 1/\Delta\omega$, where ω corresponds to the frequencies of H. The local one is justified for times that are both $t >> 1/\Delta\omega$ for ω's in H_0 and $t << 1/\Delta\omega$ for ω's in V. Therefore, when we say that we treat something as a perturbation, it explicitly means that we apply the local approach as introduced here.

In this thesis, we deal with one bath. Nevertheless, we would like to point out that the problem has also been studied for two baths. It was first highlighted in [LK14]. In [HPLM$^+$17], the authors showed that for two baths if the interaction between the subsystems g is smaller than the natural frequencies of the systems that interact with the bath, the local approach is justified. On the other hand, if g is bigger than the decaying rate of the systems one should use the global approach. Besides, we defer the reader to [SAC21, GCN$^+$17, DCLH$^+$18] to see the validity and issues with the local approach as well as for the comparison between the two approaches in detail.

2.2 Refined weak coupling

In reference, [Riv17] the refined weak coupling was used to calculate the spin-boson model. This approach has the advantage that it both accounts for non-Markovian effects and describes CP dynamics. Thus, in [Riv17] some non-Markovian effects were described. Here we present its derivation.

As before, we consider a Hamiltonian of the form

$$H = H_S + H_B + V, \tag{2.73}$$

and the initial condition $\rho(0) = \rho_S(0) \otimes \rho_B$ where $[H_B, \rho_B] = 0$. We again move to the interaction picture with respect to H_A and H_B. Thus, the state of the subsystem S fulfills

$$\tilde{\rho}_S(t) = \mathrm{Tr}_B[U(t)\rho_S(0) \otimes \rho_B U^\dagger(t)], \tag{2.74}$$

where $U(t) = \mathcal{T} e^{-i\int_0^t \tilde{V}(s)ds}$ and $\tilde{A} = e^{-i(H_S+H_B)t} A e^{i(H_S+H_B)t}$. $\mathcal{T}$ is the time-ordering operator.

Expanding the unitary $U(t)$ in Eq. (2.74), we get

$$\tilde{\rho}_S(t) = \rho_S(0) - \frac{1}{2}\mathcal{T}\int_0^t dt_1 \int_0^t dt_2 \,\mathrm{Tr}_B\left[\tilde{V}(t_1), \left[\tilde{V}(t_2), \rho_S(0) \otimes \rho_B\right]\right] + \mathcal{O}(\tilde{V}^3), \tag{2.75}$$

where we used that the first order term is zero, i.e. $\mathrm{Tr}[\tilde{V}(t)\rho_B] = 0$. As we explained in chapter (2), we can always assume that as long as ρ_B is a stationary state of H_B.

Now, we calculate

$$\mathcal{T}\int_0^t dt_1\int_0^t dt_2\,\mathrm{Tr}_B\left[\tilde{V}(t_1),\left[\tilde{V}(t_2),\rho_S(0)\otimes\rho_B\right]\right]=\int_0^t dt_1\int_0^t dt_2\theta(t_1-t_2)\,\mathrm{Tr}_B\left[\tilde{V}(t_1),\left[\tilde{V}(t_2),\rho_S(0)\otimes\rho_B\right]\right] \tag{2.76}$$

$$+\int_0^t dt_1\int_0^t dt_2\theta(t_2-t_1)\,\mathrm{Tr}_B\left[\tilde{V}(t_2),\left[\tilde{V}(t_1),\rho_S(0)\otimes\rho_B\right]\right], \tag{2.77}$$

where $\theta(x)$ is the Heaviside step function and is defined

$$\theta(x):=\begin{cases}1, & x>0\\ 0. & x\leq 0\end{cases} \tag{2.78}$$

We can compute the double commutator terms as

$$\int_0^t dt_1\int_0^t dt_2\theta(t_1-t_2)\,\mathrm{Tr}_B\left[\tilde{V}(t_1),\left[\tilde{V}(t_2),\rho_S(0)\otimes\rho_B\right]\right]=\int_0^t dt_1\int_0^t dt_2\theta(t_1-t_2)\,\mathrm{Tr}_B\left(\tilde{V}(t_1)\tilde{V}(t_2)\rho_S(0)\otimes\rho_B\right) \tag{2.79}$$

$$-\int_0^t dt_1\int_0^t dt_2\theta(t_1-t_2)\,\mathrm{Tr}_B\left(\tilde{V}(t_1)\rho_S(0)\otimes\rho_B\tilde{V}(t_2)\right)-\int_0^t dt_1\int_0^t dt_2\theta(t_1-t_2)\,\mathrm{Tr}_B\left(\tilde{V}(t_2)\rho_S(0)\otimes\rho_B\tilde{V}(t_1)\right) \tag{2.80}$$

$$+\int_0^t dt_1\int_0^t dt_2\theta(t_1-t_2)\,\mathrm{Tr}_B\left(\rho_S(0)\otimes\rho_B\tilde{V}(t_2)\tilde{V}(t_1)\right), \tag{2.81}$$

and analogously

$$\int_0^t dt_1\int_0^t dt_2\theta(t_2-t_1)\,\mathrm{Tr}_B\left[\tilde{V}(t_2),\left[\tilde{V}(t_1),\rho_S(0)\otimes\rho_B\right]\right]=\int_0^t dt_1\int_0^t dt_2\theta(t_2-t_1)\,\mathrm{Tr}_B\left(\tilde{V}(t_2)\tilde{V}(t_1)\rho_S(0)\otimes\rho_B\right) \tag{2.82}$$

$$-\int_0^t dt_1\int_0^t dt_2\theta(t_2-t_1)\,\mathrm{Tr}_B\left(\tilde{V}(t_2)\rho_S(0)\otimes\rho_B\tilde{V}(t_1)\right)-\int_0^t dt_1\int_0^t dt_2\theta(t_2-t_1)\,\mathrm{Tr}_B\left(\tilde{V}(t_1)\rho_S(0)\otimes\rho_B\tilde{V}(t_2)\right) \tag{2.83}$$

$$+\int_0^t dt_1\int_0^t dt_2\theta(t_2-t_1)\,\mathrm{Tr}_B\left(\rho_S(0)\otimes\rho_B\tilde{V}(t_1)\tilde{V}(t_2)\right). \tag{2.84}$$

Now, knowing that $\theta(x)=\frac{1+sgn(x)}{2}$ and defining $W(t)\equiv\int_0^t\tilde{V}(s)ds$ we notice that we can arrange all the terms in three different expressions (after some algebra)

$$\mathcal{Z}_1[\rho_S(0)]=-\,\mathrm{Tr}_B[W(t)\rho_S(0)\otimes\rho_B W(t)], \tag{2.85}$$

$$\mathcal{Z}_2[\rho_S(0)]=\mathrm{Tr}_B[W^2(t)\rho_S(0)\otimes\rho_B]+\int_0^t dt_1\int_0^t dt_2\theta(t_1-t_2)\,\mathrm{Tr}_B\left[\left[\tilde{V}(t_1),\tilde{V}(t_2)\right]\rho_S(0)\otimes\rho_B\right] \tag{2.86}$$

and

$$\mathcal{Z}_3[\rho_S(0)]=\mathrm{Tr}_B[\rho_S(0)\otimes\rho_B W^2(t)]-\int_0^t dt_1\int_0^t dt_2\theta(t_1-t_2)\,\mathrm{Tr}_B\left[\rho_S(0)\otimes\rho_B\left[\tilde{V}(t_1),\tilde{V}(t_2)\right]\right]. \tag{2.87}$$

Finally, $\tilde{\rho}_S(t)=\rho_S(0)+\mathcal{Z}(t)[\rho_S(0)]+\mathcal{O}(\tilde{V}^3)$ where

$$\mathcal{Z}(t)[\rho_S(0)]=-\frac{1}{2}\left(2\mathcal{Z}_1[\rho_S(0)]+\mathcal{Z}_3[\rho_S(0)]+\mathcal{Z}_2[\rho_S(0)]\right) \tag{2.88}$$

$$=-i[\Lambda(t),\rho_S(0)]+\mathrm{Tr}_B\left[W(t)\rho_S\otimes\rho_B W(t)-\frac{1}{2}\{W^2(t),\rho_S\otimes\rho_B\}\right]. \tag{2.89}$$

In addition, $\Lambda(t)$ is an hermitian operator and reads

$$\Lambda(t) = \frac{1}{2i}\int_0^t dt_1 \int_0^t dt_2 \theta(t_1 - t_2)\,\mathrm{Tr}_B\left[\left[\tilde{V}(t_1), \tilde{V}(t_2)\right]\rho_B\right]. \tag{2.90}$$

If we write ρ_B in its eigenbasis and perform the trace, we can see that the for any fixed t, the coefficients will be positive and $\mathcal{Z}(t)$ will have GKLS form. Then, as up to the second order we have $\rho_S(t) = (\mathbb{I} + \mathcal{Z}(t))\rho_S(0) + \mathcal{O}(\tilde{V}^3) \simeq e^{\mathcal{Z}(t)}\rho_S(0)$, the dynamics will be completely positive and will approach the exact one for short times.

It is possible to express all the quantities that appear in $\mathcal{Z}(t)$ in terms of the jumping operators introduced in Eq. (2.26). We just state the results and defer the reader to [Riv17] to see all the details. The hermitian operator $\Lambda(t)$ reads

$$\Lambda(t) = \sum_{\omega,\omega'}\sum_{k,l} \Xi_{kl}\left(\omega, \omega', t\right) A_k^\dagger(\omega) A_l\left(\omega'\right) \tag{2.91}$$

with

$$\Xi_{kl}\left(\omega, \omega', t\right) = \frac{1}{2i}\int_0^t dt_1 \int_0^t dt_2\, \mathrm{sgn}\left(t_1 - t_2\right) e^{i\left(\omega t_1 - \omega' t_2\right)}\,\mathrm{Tr}\left[\tilde{B}_k\left(t_1 - t_2\right) B_l \rho_B\right] \tag{2.92}$$

and the whole exponent

$$\mathcal{Z}(t)\left[\rho_S(0)\right] = -i\left[\Lambda(t), \rho_S(0)\right] + \sum_{\omega,\omega'}\sum_{k,l}\Gamma_{kl}\left(\omega, \omega', t\right)\left[A_l\left(\omega'\right)\rho_S(0)A_k^\dagger(\omega) - \frac{1}{2}\left\{A_k^\dagger(\omega)A_l\left(\omega'\right), \rho_S(0)\right\}\right], \tag{2.93}$$

where

$$\Gamma_{kl}\left(\omega, \omega', t\right) = \int_0^t dt_1 \int_0^t dt_2 e^{i\left(\omega t_1 - \omega' t_2\right)}\,\mathrm{Tr}\left[\tilde{B}_k\left(t_1 - t_2\right) B_l \rho_B\right]. \tag{2.94}$$

The same result could be obtained if one used the expression for the second order cumulant $K^{(2)}(t)$ exposed in [MABL13].

Finally, the next subsection shows how the refined weak coupling approach tends to the global GKLS equation for long times.

2.2.1 Global GKLS equation from long time limit in refined weak coupling

Here we argue that for long times the dynamics obtained by the refined weak coupling approximation match those obtained in the weak coupling limit and after applying the Born, Markov, and secular approximation. In other words,

$$\lim_{t\to\infty}\frac{\mathcal{Z}(t)}{t} \to \mathcal{L}_G \tag{2.95}$$

where $\mathcal{L}_G$ is the Liouvillian for the global GKLS.

To do so, we start with the dissipation rates

$$\frac{\Gamma_{kl}\left(\omega, \omega', t\right)}{t} = \frac{1}{t}\int_0^t dt_1 \int_0^t dt_2 e^{i\left(\omega t_1 - \omega' t_2\right)}\,\mathrm{Tr}\left[\tilde{B}_k\left(t_1 - t_2\right) B_l \rho_B\right] \tag{2.96}$$

$$= \frac{1}{t}\int dv \int_0^t dt_1 \int_0^t dt_2 e^{i\left[(\omega - v)t_1 - \left(\omega' - v\right)t_2\right]}\,\mathrm{Tr}\left[B_k(v) B_l \rho_E\right], \tag{2.97}$$

where in the last line we decomposed B_k in terms of the bath's jump operators $B_k(\omega)$ as $B_k = \int d\nu B_k(\nu)$. If we now perform the integration over t_1 and t_2 we get

$$\frac{\Gamma_{kl}\left(\omega, \omega', t\right)}{t} = \int dv t \exp\left[i\frac{(\omega - \omega')\,t}{2}\right]\mathrm{sinc}\left[\frac{(\omega - v)t}{2}\right]\mathrm{sinc}\left[\frac{(\omega' - v)\,t}{2}\right]\mathrm{Tr}\left[B_k(v) B_l \rho_E\right]. \tag{2.98}$$

Using the lemma from [Riv17], namely

$$\lim_{t\to\infty}\int_I f(\omega)t\,\mathrm{sinc}\left[\frac{(\omega+a)t}{2}\right]\mathrm{sinc}\left[\frac{(\omega+b)t}{2}\right]d\omega = 2\pi\delta_{a,b}f(-a), \tag{2.99}$$

if $a \in I$ and zero otherwise (for sufficiently well-behaved functions $f(\omega)$), we get

$$\lim_{t\to\infty}\frac{\Gamma_{kl}\left(\omega,\omega',t\right)}{t} = 2\pi\delta_{\omega,\omega'}\,\mathrm{Tr}\left[B_k(\omega)B_l\rho_E\right], \tag{2.100}$$

where the Kronecker delta takes care of the secular approximation and $2\pi\,\mathrm{Tr}\left[B_k(\omega)B_l\rho_E\right]$ corresponds to the Markovian decaying rate. Thus, the dissipator of the refined weak coupling approach tends to be the dissipator of the global GKLS master equation. One could also derive the same for the lamb shift Hamiltonian but it is a little bit more involving (see [Riv17] for the proof.) This proof is not completely rigorous because one does the following

$$\lim_{t\to\infty}\mathcal{Z}(t) = \lim_{t\to\infty}t\frac{\mathcal{Z}(t)}{t} = t\lim_{t\to\infty}\frac{\mathcal{Z}(t)}{t} \approx t\mathcal{L}_G. \tag{2.101}$$

Taking out t of this limit cannot be always justified. Fortunately, we will see some numerical results that support the result. Not only that but also there has been some theoretical work done to prove this limit more rigorously[mar]. Hence, we can now state that $\lim_{t\to\infty}\mathcal{Z}(t)/t = \mathcal{L}_G$ and so the dynamics are the same for both approaches for long times because $e^{\mathcal{Z}(t)} \approx e^{\mathcal{L}_G t}$.

Chapter 3

Markovian dynamics

In this chapter, all the presented results have been obtained using GKLS [GKS76, Lin76, BP02] equation. As mentioned in chapter 2, to get this type of master equation one should use several assumptions and approximations. Whilst this can be seen as a drawback, the easiness of the calculations and the fact that in a plethora of circumstances, the use of master equations can be justified [RPHP10], makes them very appealing.

During this chapter, we talk about our results when charging quantum batteries where their dynamics are modeled by Markovian master equations. Before moving to our original results, we first talk about quantum batteries in general and the known results in the literature.

3.1 Quantum Batteries

Batteries are ubiquitous in almost every aspect of our lives. They are useful because they store energy that can be used for future tasks. Essentially, a quantum battery [BD21] is a battery that due to its dimensions is subject to the laws of quantum physics.

A priori, one could think about whether studying them is meaningful at all. Some papers [AF13, HPLHA13, BVMG15, CPB+17] showed a quantum advantage in collectively charging many-body systems and therefore, positively answered the question. Since then, the area has seen a growing interest from the physics community. A lot of different models have been studied to see if one can use them as quantum batteries. To name a few: spin chains [LLM+18], quantum dots and superconducting qubits [FCA+18a], qubits in an optical cavity [AKM+19a], and disordered chains [CCDWGPH20, ZDZ22].

Treating a quantum battery as an open system is necessary if one wants to encapsulate noise effects, which always appear in laboratories. In this situation, different methods have been proposed to get improvements in charging processes. To give some examples: in [SÇCZ19, QM20], a passive method was introduced to charge qutrit batteries through the so-called dark states, and in [GCCB20] measurements empowered by linear feedback schemes [MGP21] obtained better results in charging than considering the system to be isolated.

In this thesis, we will consider the charger-mediated approach that was introduced in [AFM+18]. See Fig. (3.1) for a visual description. The charger is the only component of the system that interacts with the bath. Then, during the whole charging process, it dissipates energy into the environment. In this setting, using the local[1] GKLS master equation [HPLM+17] comes in handy and makes the calculations easier than resorting to the global one. Since the interaction between the charger and the battery will be weak, it is reasonable to do so. As the charger interacts with the battery (typically they both are qubits or oscillators), the setting allows for the pumping of energy from the pulse to the

[1] See subsection (2.1.2) for more details about the local approach and global approach.

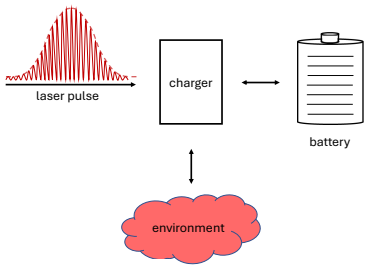


Figure 3.1: Charger-mediated approach. A classical electromagnetic field pumps the charger while this interacts with a battery and an environment. Picture taken from our paper [RAS+22].

battery, while at the same time keeping the battery partially isolated, which improves the quality of the stored energy.

Because we are interested in the useful energy stored in the battery, the figure of merit will be the ergotropy [ABN04]. Let us first define the internal energy of the system as $E(\rho) = \mathrm{Tr}(\rho H)$, where ρ is the state of the system and H its Hamiltonian. In a cyclic unitary process, where the Hamiltonian of the system is the same at the beginning and the end of the process, one can define ergotropy $\mathcal{E}(\rho)$ as

$$\mathcal{E}(\rho) := E(\rho) - E(\rho_p), \tag{3.1}$$

where ρ_p is the so-called passive state and its relationship with ρ is $\rho_p = \min_U U\rho U^\dagger$, where one minimizes over all the unitaries. If one deals with pure states, the passive state will always be the ground state of the system. Then, when trying to maximize ergotropy is convenient that the final state will be pure.

In the literature [FCA+18b, FAM+19, AKM+19b, AKM+19a, JFSR+20], people investigated how one could benefit from quantum correlations and quantum coherence of the initial state when charging a quantum battery in the charger-mediated approach. This has the inconvenience of the energy costs needed to prepare the initial state in a specific way. In our works, however, we relaxed these requirements –the initial state being in the ground state, which is experimentally friendly– and we obtained better results in terms of energy and ergotropy stored in the battery, and also in the energy cost from the field[2] in two different paradigms. In the first one, we use tools of Optimal Control Theory, specifically, Krotov's method [KF83, Kro88, Kro95, KK99]. In the last one, we see how injecting an ancillary system –we call it a catalyst because it barely stores energy during the process– helps boost the final energy stored in the battery. The results are shown in the following subchapters.

3.1.1 Optimal charging of quantum batteries

One can distinguish between two ways of performing a desired transformation of a quantum system: autonomous and non-autonomous.

For the first approach, one prepares an extra quantum system that interacts with the main one through a time-independent coupling. This coupling can activate additional interactions between the parts of the main system. To calculate the energy costs of the process, one needs to account for the preparation and the dynamics of the additional system. The autonomous paradigm is used for describing thermal machines [WH19, Mit19].

On the other hand, in the non-autonomous paradigm, one controls the system actively. This is the case of driving the system through a time-dependent pulse, or in feedback

[2] The explicit definition will be later introduced.

schemes, which depend on measurements and operations performed when needed and can be based on both quantum and classical information processing [Llo00].

In this thesis, we use an external classical (laser) drive, with no feedback mechanism whatsoever. The reason is that we do not expect to get any improvements from the interaction with the bath. Therefore, we use the open-loop approach (no information about the system is retrieved during the process) to describe the field. This is the minimal non-autonomous model possible and is motivated by its simplicity to be studied in experiments. The assumption of the laser being classical is justified if one considers the weak back-reaction that the system imposes on the laser.

As we are in the charger-mediated approach, the laser does not interact directly with the battery. Therefore, the charger mediates the interaction between them. This setting does not allow one to study settings made of many chargers that are charged in a synchronized way. In [ASFM22] similar scenarios were studied in which there was no drive, and they concluded that coherence shared between the chargers (oscillators) improved the energy and ergotropy stored on the battery.

Nevertheless, the method proposed here can be extended to many control fields that interact with many chargers. Unfortunately, one can see that the optimization becomes less efficient when finding the optimal field when having more batteries [RAS+22].

Next, we explain Krotov's method and outline the results obtained.

Krotov's method

In any charging scheme, one desires that the dynamics corresponding to the process evolve from a given initial state –usually the ground state of the battery– to a target state –the excited state of the battery– in a given time, τ. To make the calculations the most general and realistic possible, we will be only concerned with the evolution of an open quantum system given by

$$\frac{d\rho}{dt} = \mathcal{L}\rho, \quad \rho(t_0) = \rho_0, \tag{3.2}$$

where ρ_0 is the initial state and $\mathcal{L}$ the Liouvillian. Within this evolution, if one wants to drive the initial state of the system to some desired state while bounding the energy injected into the charger by the field, one can use Krotov's method [KF83, Kro88, Kro95, KK99] –that relies on an iterative numerical tool [ZR98, WG07, Goe19] and it is been used extensively in the literature [TKO92, RNK12, SKT93, BKT97, ST02]– to minimize a general functional[3]

$$J\left[\rho^{(i)}(\tau), \varepsilon^{(i)}(t)\right] = J_\tau\left(\rho^{(i)}(\tau)\right) + \int_0^\tau g_a\left(\varepsilon^{(i)}(t)\right) \mathrm{d}t, \tag{3.3}$$

where $\rho^{(i)}(\tau)$ represents the state of the system at the final time τ steered by the electrical field of iteration i, $\varepsilon^{(i)}(t)$. J_τ corresponds to $J_\tau = 1 - \mathcal{F}^i(\tau)$, where $\mathcal{F}^i(\tau) = \mathrm{tr}\left[\rho^{\mathrm{tgt}\,\dagger}\rho^i(\tau)\right]$ is the fidelity between the states $\rho^i(\tau)$ and ρ^{tgt}, and ρ^{tgt} is the target or desired state.

The last part of the functional takes into account the energy cost of the drive:

$$g_a\left(\varepsilon^{(i)}(t)\right) = \frac{\lambda_a}{S(t)}\left(\varepsilon^{(i)}(t) - \varepsilon^{(i-1)}(t)\right)^2 \tag{3.4}$$

$$= \frac{\lambda_a}{S(t)}\left(\Delta\varepsilon^{(i)}(t)\right)^2, \tag{3.5}$$

where $\lambda_a > 0$ is a numerical parameter that enters in the optimization –the smaller the λ_a the faster the optimization is– and $S(t) \in [0, 1]$ allows for the control of the shape of the

[3] This functional can be easily generalized to having n different fields and target states. See [kro, GBGE+19] for more details on this and also on a comparison between Krotov's and other optimization methods.

pulse. During the thesis $S(t)$ has the form

$$S(t) = \begin{cases} \sin^2\left(\frac{\pi}{2}\frac{t}{t_{\text{on}}}\right) & \text{for} \quad 0 \leq t \leq t_{\text{on}} \\ 1 & \text{for} \quad t_{\text{on}} < t < \tau - t_{\text{off}} \\ \sin^2\left(\frac{\pi}{2}\frac{(t-\tau)}{t_{\text{off}}}\right) & \text{for} \quad \tau - t_{\text{off}} \leq t \leq \tau, \end{cases} \tag{3.6}$$

where $t_{\text{on}} = t_{\text{off}} = 0.005\tau$ and it takes into account the turning off and on of the field which may disturb the system in a non-trivial way. It also makes our results more experimentally feasible. We model the initial field (guess field) as $\varepsilon^{(i=0)}(t) = S(t)\kappa$. In our numerical simulations, we choose κ big enough to ensure fast convergence. However, κ should not be too large to obtain optimized pulses that are not energetically costly. The term $\left(\Delta\varepsilon^{(i)}(t)\right)^2$ accounts for the difference in the shape of the pulse in two consequent iterations.

We did not choose $S(t)$ and $\varepsilon^{(i=0)}(t)$ arbitrarily. We did it in such a way as to ensure that at the initial and final times, the field has small values. Minimizing the difference between the field in one iteration and the next guarantees that there will not be substantial modifications of the field in the aforesaid regime. Thus, turning on and off the optimized field would be done smoothly.

The optimization consists of finding a way to produce a diminution of the value of the functional when increasing the iterations, i.e.

$$J\left[\rho^{(i+1)}(\tau), \varepsilon^{(i+1)}(t)\right] \leq J\left[\rho^{(i)}(\tau), \varepsilon^{(i)}(t)\right]. \tag{3.7}$$

This is achieved when the classical field is updated as [ZR98]

$$\Delta\varepsilon^{(i)}(t) = \frac{S(t)}{\lambda_a} \operatorname{Im}\left[\operatorname{Tr}\left(\sigma^{(i-1)}(t)\left(\frac{i\partial\mathcal{L}}{\partial\varepsilon(t)}\Big|_{(i)}\right)\rho^{(i)}(t)\right)\right]. \tag{3.8}$$

where ρ and σ correspond to the density matrix of the so-called forward and backward states respectively. Above, we used a shorthand notation for

$$\frac{\partial\mathcal{L}}{\partial\varepsilon(t)}\Big|_{(i)} = \frac{\partial\mathcal{L}}{\partial\varepsilon(t)}\Big|_{\varepsilon(t)=\varepsilon^{(i)}(t)}. \tag{3.9}$$

This derivative is not always easy to calculate. Not only that but sometimes the fact that it may depend on $\varepsilon(t)$ itself could lead to numerical instabilities. The reason is that in that case, the derivative should be evaluated in the control field from the preceding iteration. Fortunately, for the case at hand, the Liouvillian is linear in the control field $\varepsilon(t)$, making the derivative simple enough to get an analytic form.

The backward states σ evolve according to [GRK14]

$$\frac{d\sigma}{dt} = -\mathcal{L}^\dagger\sigma, \quad \sigma(\tau) = \rho^{\text{tgt}}, \tag{3.10}$$

where the time goes backward. $\mathcal{L}^\dagger$ is the adjoint Liouvillian and it will be explicitly written in the next sections. The initial condition $\sigma(\tau) = \rho^{\text{tgt}}$ is not the most general one. Nevertheless, for the sake of this thesis and the calculations presented here it is sufficient.

Now that we have defined all the ingredients and components, we can explain the algorithm. To make matters simpler, we will consider that $\frac{\partial\mathcal{L}}{\partial\varepsilon(t)}$ does not depend on time, that is also our case. We construct a grid made of $N+1$ time points to discretize it. The initial time is, as usual, $t = 0$ and the final is $t = \tau$. We denote dt as the difference between two points in the grid. The states are only defined at the points of the grid.

We denote $\varepsilon^{(i=1)}(t)$ as the initial guess of the control field. Firstly, for the iteration i we compute $\sigma^{(i-1)}(t)$ by propagating the backward states σ as in Eq. (3.10) with field $\varepsilon^{(i)}(t)$ from $t = \tau$ to $t = 0$ along the whole time grid. Now, to calculate the change in the field,

Eq. (3.8) can be discretized and used to get the update of the field with our initial state ρ_0 as follows

$$\Delta\varepsilon^{(i)}(\bar{t}) = \frac{S(\bar{t})}{\lambda_a}\,\mathrm{Im}\left[\mathrm{Tr}\left(\sigma^{(i-1)}(t)\left(\frac{i\partial\mathcal{L}}{\partial\varepsilon(t)}\Big|_{(i)}\right)\rho^{(i)}(t)\right)\right], \tag{3.11}$$

with the main difference being that the update is now calculated for time $\bar{t} = t + dt/2$ instead of t. This solves the problem with Eq. (3.8) where the field is calculated at time t using the states at also time t. However, to get the states at this time, one needs to propagate them with the field from (3.8). Hence, the solution for this is calculating the field at $\bar{t}$ so, the update does only depend on the information from past points in the grid. In fact, (3.8) is just the continuous version of (3.11) when the distance between two-time points goes to zero. In addition, it is important to note that convergence is only mathematically guaranteed in the continuous limit.

With this new field, we can propagate the forward states ρ while sequentially updating the field for all time points. One then obtains $\rho^{(i)}(t)$ and $\varepsilon^{(i)}(t)$. The way to do this is extending the field values calculated at $\bar{t}$ to $t + dt$, with the assumption that doing this discretization does not produce rapidly oscillating fields –if that were the case, one can always make dt smaller–.

Finally, we go to the next iteration, $i+1$, where now the guess field will be the updated field of the iteration i. We then repeat the procedure until we reach the convergence of the functional from Eq. (3.3).

Results

We investigate the setting in which the charger and the battery are both quantum harmonic oscillators (QHO) and the dissipation is modeled by the local GKLS equation. We will compare the case in which the classical field is oscillatory (see [AFM+18] for the explicit form)[4] with the one in which we optimize the control field $\varepsilon(t)$. In the latter, the Hamiltonian reads[5]

$$H = H_A + H_B + H_{AB} - \mu\varepsilon(t)(a + a^\dagger) \otimes \mathbb{I}_B, \tag{3.12}$$

with

$$H_A = \omega a^\dagger a, \quad H_B = \omega b^\dagger b, \quad H_{AB} = g(a^\dagger b + a b^\dagger), \tag{3.13}$$

and μ the coupling strength between the charger and the field.

The operators a and b are bosonic annihilation operators acting on the charger and the battery respectively and fulfill the commutation relationships $[a, a^\dagger] = [b, b^\dagger] = 1$. The dissipation from the charger to the bath is accounted for through the Lindblad superoperator

$$\mathcal{D}_T[\rho] = \gamma(n+1)\mathcal{D}_a[\rho] + \gamma n\mathcal{D}_{a^\dagger}[\rho], \tag{3.14}$$

where $\mathcal{D}_c(\cdot) = c(\cdot)c^\dagger - 1/2\{c^\dagger c, \cdot\}$ for any operator c, $n = \frac{1}{e^{\omega/T}-1}$ corresponds to the occupation number of the mode with frequency ω of the bosonic bath, and γ is the decaying rate.

In this setting, as we are performing an optimization over the control field $\varepsilon(t)$, another figure of merit is

$$\mathcal{W}_\tau = \int_0^\tau dt\ |\varepsilon(t)|^2, \tag{3.15}$$

where τ is the final time of the evolution. It can be understood as the energy cost of the field. In addition, apart from the ergotropy stored in the battery and the energy spent by

[4] In this chapter, we are comparing the results with those from [AFM+18]. Then, we used the same parameters as them. In the next chapter, as we rigorously benchmark and test the global, local, and the refined weak coupling equation, we pay more attention to the parameters for which the local approach is justified. This validity is explained in subsection (2.1.2).

[5] As the reader may notice, we are now dealing with an external driving that is time-dependent. We will consider it as a perturbation (μ is small) and we assume that the influence of this term only appears in the commutator part in the GKLS equation [RPHP10]. We will also assume this for the catalytic evolution. This is again the local approach with respect to the field term as mentioned in subsection (2.1.2).

the field, we are also interested in describing the efficiency of the optimized procedure. To quantify it, we will define the quality factors as

$$\alpha_{\mathcal{E}} =: \left(\frac{\mathcal{E}_{opt}(\rho)}{\mathcal{E}_{osc}(\rho)} - 1\right) \times 100\%, \tag{3.16}$$

$$\alpha_{\mathcal{W}} =: \left(\frac{\mathcal{W}_{osc}(\rho)}{\mathcal{W}_{opt}(\rho)} - 1\right) \times 100\% \tag{3.17}$$

where all the values will be evaluated at the final time τ and the subindices represent if we optimized the field (opt) or not (osc).

The Hamiltonian of Eq. (3.12) is quadratic on the bosonic operators so the evolution preserves the gaussianity of the initial state. Since our initial state is on the ground state, and hence it is Gaussian, all the information of the state at any time t is encoded in the first and second moments of the operators [Ser17]. This simplifies the problem because no one has to perform the optimization over a low-dimensional space. Thus, we need to rewrite the evolution of the forward and backward states, and the update of the field as a function of the first and second moments.

To do so, we first define a vector of operators

$$\mathbf{r} = (x_1, x_2, p_1, p_2)^T, \tag{3.18}$$

where $x_j = \sqrt{\frac{1}{2\omega}}(a_j + a_j^\dagger)$ and $p_j = i\sqrt{\frac{\omega}{2}}(a_j^\dagger - a_j)$ with $j = 1, 2$.[6] As mentioned before, the operators from the vector fulfill the bosonic commutation relations, and this translates to $[\mathbf{r}, \mathbf{r}^T] = iJ$, with $J = \begin{pmatrix} 0_2 & \mathbb{I}_2 \\ -\mathbb{I}_2 & 0_2 \end{pmatrix}$, where $\mathbb{I}_2$ and 0_2 are the identity matrix and the zero matrices, respectively. In full generality, any state of the system can be described by its statistical moments

$$\langle \mathbf{r}_1 \dots \mathbf{r}_4 \rangle = \operatorname{Tr} \rho \mathbf{r}_1 \dots \mathbf{r}_4. \tag{3.19}$$

In the case that the state is Gaussian, the first and second moments are enough to fully describe the state. So we construct the vector $|r\rangle$ of the first moments

$$|r\rangle = \sum_{i=1}^{4} \langle \mathbf{r}_i \rangle |i\rangle, \tag{3.20}$$

as well as the second moment's matrix:

$$V = \frac{1}{2} \sum_{i,j=1}^{4} \langle \{\mathbf{r}_i, \mathbf{r}_j\} \rangle |i\rangle\langle j|. \tag{3.21}$$

Consequently, to perform the optimization via Krotov's method, we need to arrange all the elements of $|r\rangle$ and V in a vector-like object ψ and perform the whole procedure on it. As V is symmetric by construction, we just need the elements from the upper triangular part.

[6] Here we used the mass of the oscillators $m = 1$.

Thus, we have

$$\psi = \begin{pmatrix} c \\ |r\rangle_1 \\ |r\rangle_2 \\ |r\rangle_3 \\ |r\rangle_4 \\ V_{11} \\ V_{12} \\ V_{13} \\ V_{14} \\ V_{22} \\ V_{23} \\ V_{24} \\ V_{33} \\ V_{34} \\ V_{44} \end{pmatrix}, \tag{3.22}$$

where c is an independent parameter needed to linearize the equations of motion.

The evolution of the state ρ reads[7]

$$\frac{d\rho}{dt} = -i[H,\rho] + \mathcal{D}_T(\rho). \tag{3.23}$$

From this, we can compute the expectation values for the desired operators via Heisenberg equations. Accordingly, for any operator O one has

$$\frac{d\langle O\rangle}{dt} = i\langle[H,O]\rangle + \langle\mathcal{D}_T^\dagger(O)\rangle, \tag{3.24}$$

where $\mathcal{D}_T^\dagger(O)$ is the adjoint dissipator and reads

$$\begin{aligned} \mathcal{D}_T^\dagger(O) &= \gamma(n+1)\left(a^\dagger O a - \frac{1}{2}\{a^\dagger a, O\}\right) \\ &+ \gamma n\left(aOa^\dagger - \frac{1}{2}\{aa^\dagger, O\}\right). \end{aligned} \tag{3.25}$$

Computing Eq. (3.24) for all the components of ψ we can express the evolution as

$$\frac{\partial\psi}{\partial t} = A_f\psi, \tag{3.26}$$

which will be the forward equation of motion with the initial constraint $\psi(t=0) = \varphi_i$, where φ_i is the vector-like object of Eq. (3.22) for the initial state. A_f is given by

$$A_f = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{\gamma}{2} & 0 & 1 & \frac{g}{w} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{g}{w} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\sqrt{2w}\mu\varepsilon(t) & -w^2 & -gw & -\frac{\gamma}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -gw & -w^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{\gamma\left(n+\frac{1}{2}\right)}{w} & 0 & 0 & 0 & 0 & -\gamma & 0 & 2 & \frac{2g}{w} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{\gamma}{2} & \frac{g}{w} & 1 & 0 & 1 & \frac{g}{w} & 0 & 0 & 0 \\
0 & \sqrt{2w}\mu\varepsilon(t) & 0 & 0 & 0 & -w^2 & -gw & -\gamma & 0 & 0 & 0 & 0 & 1 & \frac{g}{w} & 0 \\
0 & 0 & 0 & 0 & 0 & -gw & -w^2 & 0 & -\frac{\gamma}{2} & 0 & 0 & 0 & 0 & 1 & \frac{g}{w} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{2g}{w} & 2 & 0 & 0 & 0 & 0 \\
0 & 0 & \sqrt{2w}\mu\varepsilon(t) & 0 & 0 & 0 & -w^2 & 0 & 0 & -gw & -\frac{\gamma}{2} & 0 & \frac{g}{w} & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -gw & 0 & 0 & -w^2 & 0 & 0 & 0 & \frac{g}{w} & 1 \\
\gamma w\left(n+\frac{1}{2}\right) & 0 & 0 & 2\sqrt{2w}\mu\varepsilon(t) & 0 & 0 & 0 & -2w^2 & 0 & 0 & -2gw & 0 & -\gamma & 0 & 0 \\
0 & 0 & 0 & 0 & \sqrt{2w}\mu\varepsilon(t) & 0 & 0 & -gw & -w^2 & 0 & -w^2 & -gw & 0 & -\frac{\gamma}{2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2gw & 0 & 0 & -2w^2 & 0 & 0 & 0
\end{pmatrix}. \tag{3.27}$$

[7] It is the GKLS master equation, as we said at the beginning of the chapter.

Analogously, the backward evolution should be computed from the adjoint Liouvillian dynamics (see Eq. (3.10))

$$\frac{d\langle O\rangle}{dt} = i\langle[H,O]\rangle + \langle\mathcal{D}_T(O)\rangle, \tag{3.28}$$

where

$$\begin{aligned}\mathcal{D}_T(O) &= \gamma(n+1)\left(aOa^\dagger - \frac{1}{2}\{a^\dagger a, O\}\right)\\ &+ \gamma n\left(a^\dagger O a - \frac{1}{2}\{aa^\dagger, O\}\right)\end{aligned} \tag{3.29}$$

is the usual dissipator. Again, we can rewrite our Gaussian formalism as

$$\frac{\partial\chi}{\partial t} = A_b\chi, \tag{3.30}$$

where it should be noted that the time runs backward. In this case, the boundary condition is $\chi(\tau) = \varphi_{tar}$, where φ_{tar} corresponds to the target state and τ is the final time of the evolution. Defining $M = A_f - A_b$, we have

$$M = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{2\gamma\left(n+\frac{1}{2}\right)}{w} & 0 & 0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma & 0 & 0 & 0\\
2\gamma w\left(n+\frac{1}{2}\right) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma
\end{pmatrix}, \tag{3.31}$$

which is more compact that both A_f and A_b.

The last element needed to perform the optimization is the update of the field. It is given in Eq. (3.8) and for the iteration i is

$$\Delta\varepsilon^i(t) = \frac{S(t)}{\lambda_a}\mathrm{Im}\left[\mathrm{Tr}\left(\sigma^{i-1}(t)\frac{i\partial\mathcal{L}}{\partial\varepsilon(t)}\Big|_{(i)}\rho^i(t)\right)\right] = -\frac{S(t)}{\lambda_a}\mathrm{Im}\left[\mathrm{Tr}\left(\sigma^{i-1}(t)\left[\mu(a_1+a_1^\dagger),\rho^i(t)\right]\right)\right], \tag{3.32}$$

where ρ and σ are the usual density matrices for the forward and backward states, respectively. For the same reasoning as before, this update can be calculated as a function of the elements in ψ and χ. We defer the reader to our paper [RAS+22] to see the explicit version.

The optimization results are compared with those from [AFM+18] in Fig. (3.2). It is easy to see that the values of the energy and the ergotropy are higher in the optimized case. Not only there is an advantage on these values, but also on the energy used by the field: for the optimized field is 30.73, and for the oscillatory pulse is 31.41. This results in a quality factor $\alpha_{\mathcal{W}} = 2.2\%$. While the improvement is not very big, it is quite relevant in terms of the ergotropy extraction $\alpha_{\mathcal{E}} = 25\%$. Moreover, it is clear from Fig. (3.2)(b) that more energy is transferred to the battery for both optimized and non-optimized cases for longer times. It is worth noting that if we allow more time to charge the battery, the quality factor would be better than before, especially in the energy cost ($\alpha_{\mathcal{W}} = 157\%$ and $\alpha_{\mathcal{E}} = 28\%$.)

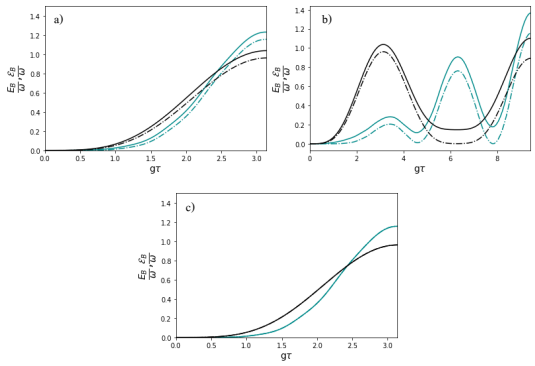


Figure 3.2: Energy (solid line) and ergotropy (dotted line) are plotted versus $g\tau$ where the green color indicates the case of optimizing the field and the black color when pumping the charger with the oscillatory field given in [FAM+19]. In a), the final time is the time in which the energy and ergotropy have the maximum values in the non-optimized case. In b), we doubled the final time. We set $g = 0.2\omega$, $\gamma = 0.01\omega$, $F = \mu = 0.1\omega$, $n = 1$ and $\kappa = 0.01$. c) shows that in the zero temperature regime $n = 0$, the state remains pure, and thus ergotropy and energy are the same. These values are those from plot a).

Whether the initial state for the system is $|0\rangle_C \otimes |0\rangle_B$ and the driving $\varepsilon(t)$ is fixed at temperature T, the ergotropy will be independent of the temperature. Truly, one can separate the energy as

$$E_{\varepsilon(t),T} = E_{\varepsilon(t),T=0} + E_{\varepsilon(t)=0,T} \tag{3.33}$$

and prove that

$$\mathcal{E}_{\varepsilon(t),T} = E_{\varepsilon(t),T=0} = E_{\varepsilon(t),T} - E_{\varepsilon(t)=0,T}. \tag{3.34}$$

To prove Eq. (3.34), one follows an analogous procedure to the one in [FAM+19]. In their case though, the driving was sinusoidal. The aforementioned proof makes use of the fact that under the evolution of a quadratic Hamiltonian plus a lossy channel at temperature $T = 0$, the state remains coherent and product at all times [Ser17].

To sum up, our algorithm is useful for finding a battery's optimal driving. We can choose the target state in such a way as to get the amount of energy of any other resource we can think of. Even though we used the method for pure states, it can be also used for mixed-state evolution. This can lead to physically realistic settings such as having some noise in the initial state. Finally, we would like to note that even though the results here are not Markovian in the most strict sense (see [RHP14] for a detailed review) because we have a time-dependent term in the Hamiltonian (the field), we put them in this chapter because we got them from using the GKLS equation and manually adding this time-dependent term in the master equation.

3.1.2 Catalytic charging of quantum batteries

We start by investigating the framework considered before where the charger and battery are both oscillators with the same frequency and the whole dynamics are modeled by the local GKLS equation [AFM+18]. For the sake of completeness, we write explicitly the Hamiltonian of the system (taken from [AFM+18])

$$H = \omega a^\dagger a + \omega b^\dagger b + g(ab^\dagger + ba^\dagger) + F\left(e^{i\omega_f t}a + e^{-i\omega_f t}a^\dagger\right), \tag{3.35}$$

where the interaction between the charger and the pulse has been computed using the dipole approximation and the rotating wave approximation (RWA) [LP00]. We again use the local

GKLS which in the interaction picture with respect to the charger and the battery reads

$$\dot{\rho} = \mathcal{L}[\rho] = -i[g(ab^\dagger + ba^\dagger) + F\left(e^{i\Delta_{af}t}a + e^{-i\Delta_{af}t}a^\dagger\right), \rho] + \gamma(n+1)\mathcal{D}_a[\rho] + \gamma n\mathcal{D}_{a^\dagger}[\rho], \quad (3.36)$$

where $\Delta_{af} = \omega_f - \omega$ is often zero i.e. the frequency is the laser is the same as the natural frequency of the battery and the charger and the dissipators are defined in the same way as before. In that case, we can see in Fig. (3.3) the energy and ergotropy dynamics for some parameters shown in the caption. Whether the bath is at zero temperature ($n = 0$) the Markovian evolution preserves the coherent nature of the state because our model is a quantum harmonic oscillator linearly coupled to the bath [Kos72]. So, we start with the whole system being in the ground state (a coherent state) and the dynamics will preserve the purity and then ergotropy will be the same as the energy.[8]

Interestingly, in Fig. (3.3) we can see the bounds on the available ergotropy. For all temperature regimes this bound holds. Truly, bounds exist on the energy stored in the charger and the battery. They are of the order $(F/g)^2$, in the case of not having noise ($n = 0$) and with an oscillating frequency of the order g. Having local noise ($n \neq 0$) suppresses these oscillations. This is the case because, even when the frequency of the laser is the same as the natural frequency of the charger and the battery, the whole system is off-resonant.

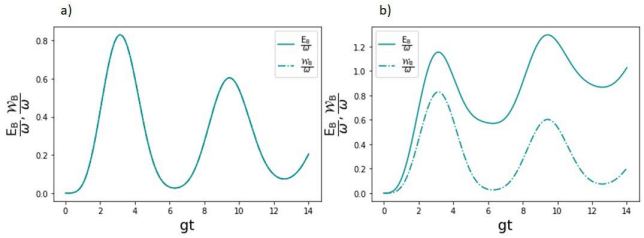


Figure 3.3: Off-resonant charging. Energy E_B/ω (solid line) and ergotropy $\mathcal{W}_B/\omega$ (dotted line) stored on a quantum battery B, charged by the interaction with A (the quantum charger) as a function of gt. The parameters are: $g = 0.2\omega$, $F = 0.1\omega$, $\gamma = 0.05\omega$ and $\Delta_{af} = 0$. In **a**), $n = 0$ and **b**), $n = 1$.

To note this off-resonance, we define a new pair of operators as

$$C_\pm = \frac{1}{\sqrt{2}}(a \pm b). \quad (3.37)$$

If we rewrite Eq. (3.35) in terms of C_+ and C_- we obtain

$$H = \omega_+ C_+^\dagger C_+ + \omega_- C_-^\dagger C_- + \frac{F}{\sqrt{2}}\left(e^{-i\omega_f t}C_+ + e^{i\omega_f t}C_+^\dagger\right) + \frac{F}{\sqrt{2}}\left(e^{-i\omega_f t}C_- + e^{i\omega_f t}C_-^\dagger\right), \quad (3.38)$$

where $\omega_\pm = \omega \pm g$. Then, the global frequencies $\omega_\pm$ are different that the frequency of the laser ω_f and this system is off-resonant. The stronger the coupling g, the further from the resonance the system is. Of course, one can avoid this problem by tuning ω_f to be the same as one of the global frequencies. Indeed, in Fig. (3.4) we can see that the energy keeps increasing in that case. This setting has the caveat of needing to know the coupling constant g or having the experimental capability of tuning the laser to all the spectrum of frequencies.

On the other hand, one could get similar by adding a qubit "between" the charger and the battery. The Hamiltonian is now

[8] That is the case because the ground state has zero energy.

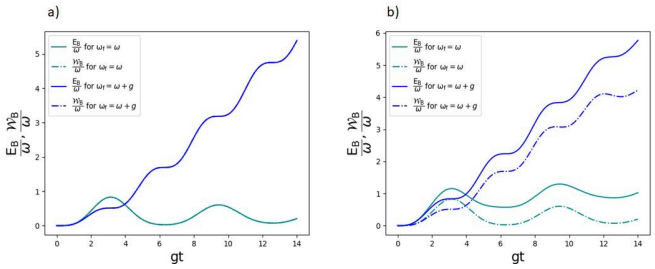


Figure 3.4: On-resonant charging. Energy E_B/ω (dashed line) and ergotropy $\mathcal{W}_B/\omega$ (dotted line) of the quantum battery B charged through the interaction with the quantum charger A versus gt and $\omega_f = \omega_+ = \omega + g$ (the same results hold for ω_-), $g = 0.2\omega$, $F = 0.1\omega$ and $\gamma = 0.05\omega$. In **a**) $n = 0$, and in **b**) $n = 1$.

$$H = \omega a^\dagger a + \omega_q q^\dagger q + \omega b^\dagger b + g_{aq}(aq^\dagger + a^\dagger q) + g_{bq}(bq^\dagger + b^\dagger q) + F\left(e^{i\omega_f t}a + e^{-i\omega_f t}a^\dagger\right) \quad (3.39)$$

where $q = \sigma_x - i\sigma_y$ with σ_x and σ_y being the Pauli matrices. Following a similar procedure as before, we can define the super-mode operators

$$C_+ = \sin\theta\, a + \cos\theta\, b, \quad (3.40)$$

$$C_- = \cos\theta\, a - \sin\theta\, b, \quad (3.41)$$

where

$$\sin\theta = \frac{g_{aq}}{\sqrt{g_{aq}^2 + g_{bq}^2}}, \qquad \cos\theta = \frac{g_{bq}}{\sqrt{g_{aq}^2 + g_{bq}^2}}, \quad (3.42)$$

and rewrite Eq. (3.39) as

$$H = \omega_+ C_+^\dagger C_+ + \omega_- C_-^\dagger C_- + \omega_q q^\dagger q + g(C_+ q^\dagger + C_+^\dagger q) + F\sin\theta(e^{-i\omega_f t}C_+ + e^{i\omega_f t}C_+^\dagger) + F\cos\theta(e^{-i\omega_f t}C_- + e^{i\omega_f t}C_-^\dagger), \quad (3.43)$$

where, now $\omega_\pm = \omega$ and $g = \sqrt{g_{aq}^2 + g_{bq}^2}$. The laser field is now in resonance with the mode C_- (and C_+) of the charger-battery system. As before, when one has no noise, there is an unbounded transfer of energy to C_- mode that neither depends on the coupling constants g_{aq} and g_{bq} or the energy gap w_q of the catalyst, which may be unknown or fluctuate during the time. In the noise case, there is still an improvement in the energy that would depend on the dissipation rate.

The energy stored on the qubit is logically bounded by ω_q. Considering the energy splitting in the ancillary qubit to be equal to $\omega_q = \omega$ and also $\omega_f = \omega = \omega_q$ we can write the evolution of the system in the interaction picture with respect to the free Hamiltonians of the battery and the charger as

$$\dot\rho = -i\left[g(aq^\dagger + qa^\dagger + bq^\dagger + qb^\dagger) + F\left(a + a^\dagger\right), \rho\right] + \gamma\Big((n+1)\mathcal{D}_a[\rho] + n\mathcal{D}_{a^\dagger}[\rho]\Big). \quad (3.44)$$

where we consider that the qubit is isolated ($\gamma_q = 0$.) Of course, one can consider that the qubit suffers from dissipation (see [RRAM+22] for the results.) As displayed in Fig. (3.5) numerical results show the unbounded growth in energy and ergotropy extraction. Remarkably, the energy of the qubit is near zero during the whole charging process. Because of that, we call the qubit catalyst [LBS21a, LBS21b, Tur07]. Furthermore, the catalyst does not get significantly entangled with any component of the system. Accordingly, one could reset it and apply it for further charging procedures with no energy cost.

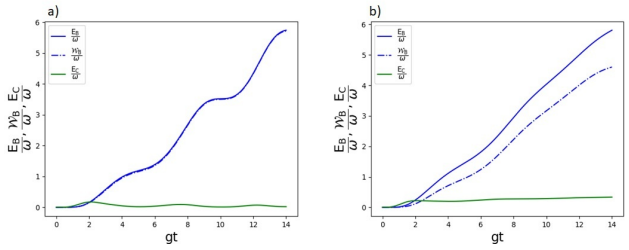


Figure 3.5: Catalyst charging. Plot of energy stored in the battery E_B/ω (dashed line), ergotropy extraction $\mathcal{W}_B/\omega$ (dotted line), and energy of the catalyst $E_C(t)$ (green) as a function of gt where $g_{aq} = g_{bq} = 0.2\omega$, $F = 0.1\omega$, $\gamma_a = 0.05\omega$ and $\Delta_{af} = 0$. In **a)** $n = 0$ and in **b)** $n = 1$.

The catalyst charging has the advantage of not depending on probing the coupling strength and its fluctuations. As a final comment, we note that the current proposal is experimentally feasible with the current superconducting technology [UTC+21]. Nowadays, with the available techniques for nano-fabrication of quantum circuits, it is possible to design qubits and resonators in the strong-coupling regime $g_{aq} \sim \omega_q$ [BGGW21]. So it is possible to observe these effects experimentally [KQC+17]. For more on experimental realizations of the results presented in this chapter, please see [RRAM+22, RAS+22].

Chapter 4

Non-Markovian dynamics

Until this chapter, we have presented results in the Markovian regime. Nevertheless, the majority of the process that happens in nature is non-Markovian. The treatment of non-Markovian dynamics is far more complex than the Markovian one. If the system is simple enough, e.g. the resonant level model [Sch14], or preserves Gaussian states [RPHP10], one can resort to an exact treatment. However, in this chapter, we tackle some ways to solve the Liouvillian dynamics, under some assumptions and approximations, but without resorting to the Markovian one. More precisely, we use the refined weak coupling approximation and one novel approximation that we will later introduce. Therefore, our results contain non-Markovian effects.

First, we compare the results obtained in the battery setting introduced before in three schemes: using the global approach, local, and the refined weak coupling equation. Finally, we show our novel non-Markovian approximation [ARAH22] and apply it to some cases.

4.1 Benchmark in the battery setting

In the battery setting, our system of interest consists of two interacting subsystems, the charger, and the battery. Hence, as introduced in chapter 2, one can derive the GKLS equation in two different ways: one can treat the interaction between the subsystems as a perturbation or not. We shall compute the dynamics in both cases and compare them with the refined weak coupling scheme.

In our benchmark, we use the equations from [AFM$^+$18] for the local approach. Therefore, we just need to compute the dynamics equations for the global and the refined case. Let us start with the global.

The Hamiltonian reads

$$\begin{aligned} H &= \omega_0 a^\dagger a + \omega_0 b^\dagger b + g(ab^\dagger + a^\dagger b) + F(e^{-i\omega_0 t}a^\dagger + e^{i\omega t}a) \\ &+ \int_0^\infty d\omega \omega b_\omega^\dagger b_\omega + \int_0^\infty d\omega h(\omega)(ab_\omega^\dagger + a^\dagger b_\omega) = H_S + H_B + H_{SB}. \end{aligned} \tag{4.1}$$

Moreover, as explained in subsection (2.1.2), we consider the field as a perturbation in our three approaches so it will only produce energy shifts. This is valid as long as $F << \omega_0$, and $F << g$. Again, the Hamiltonian is quadratic and if one starts with a Gaussian state it will preserve its gaussianity. Therefore, one only needs to calculate the first and second moments of the operators.

For the global case, as mentioned before, one needs to diagonalize the whole system (battery+charger) to construct the eigenoperators. For our case, we have that the free Hamiltonian H_0 can be rewritten as

$$H_0 = \omega_0 a^\dagger a + \omega_0 b^\dagger b + g(ab^\dagger + a^\dagger b) = \Omega_+ c_1^\dagger c_1 + \Omega_- c_2^\dagger c_2, \tag{4.2}$$

where $c_1 = \frac{1}{\sqrt{2}}(a+b)$, $c_2 = \frac{1}{\sqrt{2}}(a-b)$ and $\Omega_\pm = \omega_0 \pm g$. So the whole Hamiltonian reads

$$H = \Omega_+ c_1^\dagger c_1 + \Omega_- c_2^\dagger c_2 + \frac{1}{\sqrt{2}}\int_0^\infty d\omega h(\omega)(c_1 b_\omega^\dagger + c_1^\dagger b_\omega) + \frac{1}{\sqrt{2}}\int_0^\infty d\omega h(\omega)(c_2 b_\omega^\dagger + c_2^\dagger b_\omega) \tag{4.3}$$

$$+ \int_0^\infty d\omega \omega b_\omega^\dagger b_\omega. \tag{4.4}$$

With this, we can construct our new jump operators as

$$A_1(\Omega_{+,-}) = \frac{1}{\sqrt{2}} c_{1,2} = A_1^\dagger(-\Omega_{+,-}) \tag{4.5}$$

$$A_2(\Omega_{+,-}) = \frac{-i}{\sqrt{2}} c_{1,2} = A_2^\dagger(-\Omega_{+,-}) \tag{4.6}$$

$$B_1(\Omega_{+,-}) = \frac{h(\Omega_{+,-}) b_{\Omega_{+,-}}}{2} = B_1^\dagger(-\Omega_{+,-}) \tag{4.7}$$

$$B_2(\Omega_{+,-}) = \frac{-ih(\Omega_{+,-}) b_{\Omega_{+,-}}}{2} = B_2^\dagger(-\Omega_{+,-}). \tag{4.8}$$

Following the same procedure as in [RH12] (see the examples) and after some algebra[1], one gets the final master equation in Schrödinger's picture

$$\frac{d}{dt}\rho_S(t) = -i\Omega_+ \left[c_1^\dagger c_1, \rho_S(t)\right] - i\Omega_- \left[c_2^\dagger c_2, \rho_S(t)\right] \tag{4.9}$$

$$+ \left[\frac{\gamma(\Omega_+)}{2}\left[n(\Omega_+)+1\right]\right]\left(c_1\rho_S(t)c_1^\dagger - \frac{1}{2}\left\{c_1^\dagger c_1, \rho_S(t)\right\}\right) \tag{4.10}$$

$$+ \left[\frac{1}{2}\gamma(\Omega_+)\, n(\Omega_+)\right]\left(c_1^\dagger\rho_S(t)c_1 - \frac{1}{2}\left\{c_1 c_1^\dagger, \rho_S(t)\right\}\right) \tag{4.11}$$

$$+ \left[\frac{1}{2}\gamma(\Omega_-)\left[n(\Omega_-)+1\right]\right]\left(c_2\rho_S(t)c_2^\dagger - \frac{1}{2}\left\{c_2^\dagger c_2, \rho_S(t)\right\}\right)$$

$$+ \left[\frac{1}{2}\gamma(\Omega_-)\, n(\Omega_-)\right]\left(c_2^\dagger\rho_S(t)c_2 - \frac{1}{2}\left\{c_2 c_2^\dagger, \rho_S(t)\right\}\right) \tag{4.12}$$

where $\gamma(\Omega_\pm) = 2\pi J(\Omega_\pm)$. Now, following the arguments exposed in the subsection (2.1.2), we have the field term appearing on the master equation in the part with the commutator. Thus, if we move to the interaction picture with respect to $H = \omega_0 a^\dagger a + \omega_0 b^\dagger b$ and write c_i in terms of a and b, the master equation finally reads[2]

$$\frac{d}{dt}\rho_S(t) = -i\left[F\left(a_1 + a_1^\dagger\right) + g\left(a_1 a_2^\dagger + a_2 a_1^\dagger\right), \rho_S\right] + \sum_{j,k}^{2} K_{j,k}^{(1)}\left[a_j\rho(t)a_k^\dagger - \frac{1}{2}\left\{a_k^\dagger a_j, \rho_S(t)\right\}\right] \tag{4.13}$$

$$+ \sum_{j,k}^{2} K_{j,k}^{(2)}\left[a_j^\dagger\rho(t)a_k - \frac{1}{2}\left\{a_k a_j^\dagger, \rho_S(t)\right\}\right] \tag{4.14}$$

[1] We discarded the Lamb shift.

[2] We defined $a \equiv a_1$ and $b \equiv a_2$ just to write this equation in a compact form. For the rest of the chapter, we stick to a for the charger and b for the battery.

where

$$K_{11}^{(1)} = \frac{1}{4}[\gamma_+(n(\Omega_-)+1) + \gamma_-(n(\Omega_-)+1)] = K_{22}^{(1)}, \tag{4.15}$$

$$K_{12}^{(1)} = \frac{1}{4}[\gamma_+(n(\Omega_+)+1) - \gamma_-(n(\Omega_-)+1)] = K_{22}^{(1)}, \tag{4.16}$$

$$K_{11}^{(2)} = \frac{1}{4}[\gamma_+ n(\Omega_+) + \gamma_- n(\Omega_-)] = K_{22}^{(2)}, \tag{4.17}$$

$$K_{12}^{(2)} = \frac{1}{4}[\gamma_+ n(\Omega_+) - \gamma_- n(\Omega_-)] = K_{21}^{(2)}, \tag{4.18}$$

where $\gamma_\pm = \gamma(\Omega_\pm)$. Using that for any operator $\mathcal{O}$ we have $\frac{d}{dt}\langle\mathcal{O}\rangle = Tr(\mathcal{O}\frac{d}{dt}\rho_S(t))$[3] we obtain the following equations of motion

$$\begin{cases} \langle\dot{a}\rangle = -i(g\langle b\rangle + F) - \frac{1}{8}\langle a\rangle(\gamma_+ + \gamma_-) - \frac{1}{8}\langle b\rangle(\gamma_+ - \gamma_-) \\ \langle\dot{b}\rangle = -ig\langle a\rangle - \frac{1}{8}\langle a\rangle(\gamma_+ - \gamma_-) - \frac{1}{8}\langle b\rangle(\gamma_+ + \gamma_-) \end{cases} \tag{4.19a}$$

$$\begin{cases} \left\langle a\dot{b}^\dagger \right\rangle = i\left[g\left(\langle a^\dagger a\rangle - \left\langle b^\dagger b\right\rangle\right) - F\langle b\rangle^*\right] - \frac{1}{4}\left\langle ab^\dagger\right\rangle(\gamma_+ + \gamma_-) - \frac{1}{8}\left(\langle a^\dagger a\rangle + \langle b^\dagger b\rangle\right)(\gamma_+ - \gamma_-) \\ \quad + \frac{1}{4}(\gamma_+ n_+ - \gamma_- n_-) \\ \left\langle b^\dagger\dot{b}\right\rangle = 2g\,\mathrm{Im}\left\langle ab^\dagger\right\rangle - \frac{\langle b^\dagger b\rangle}{4}(\gamma_+ + \gamma_-) - \frac{\mathrm{Re}(\left\langle ab^\dagger\right\rangle)}{4}(\gamma_+ - \gamma_-) + \frac{n_+\gamma_+}{4} + \frac{n_-\gamma_-}{4} \\ \left\langle a^\dagger\dot{a}\right\rangle = -2\,\mathrm{Im}\left[g\left\langle ab^\dagger\right\rangle + F\langle a\rangle\right] - (\gamma_+ + \gamma_-)\frac{\langle a^\dagger a\rangle}{4} - \frac{\mathrm{Re}(\left\langle ab^\dagger\right\rangle)}{4}(\gamma_+ - \gamma_-) + \frac{n_+\gamma_+}{4} + \frac{n_-\gamma_-}{4} \end{cases} \tag{4.19b}$$

$$\begin{cases} \left\langle \dot{a^2}\right\rangle = -2i(g\langle ab\rangle + F\langle a\rangle) - \frac{\langle a^2\rangle}{4}(\gamma_+ + \gamma_-) - \frac{\langle ab\rangle}{4}(\gamma_+ - \gamma_-) \\ \langle\dot{ab}\rangle = -i\left[g\left(\left\langle a^2\right\rangle + \left\langle b^2\right\rangle\right) + F\langle b\rangle\right] - \frac{\langle a^2\rangle}{8}(\gamma_+ - \gamma_-) - \frac{\langle b^2\rangle}{8}(\gamma_+ - \gamma_-) - \frac{\langle ab\rangle}{4}(\gamma_+ + \gamma_-) \\ \left\langle \dot{b^2}\right\rangle = -2ig\langle ab\rangle - \frac{\langle b^2\rangle}{4}(\gamma_+ + \gamma_-) - \frac{\langle ab\rangle}{4}(\gamma_+ - \gamma_-) \end{cases} \tag{4.19c}$$

Where we defined $n_\pm = n(\Omega_\pm)$. For the sake of completeness, the local equations read [AFM+18] (in a different interaction picture

$$\begin{cases} \langle\dot{a}\rangle = -i(g\langle b\rangle + F) - \dfrac{\gamma}{2}\langle a\rangle \\ \langle\dot{b}\rangle = -ig\langle a\rangle \end{cases} \tag{4.20a}$$

$$\begin{cases} \langle a\dot{b}^\dagger\rangle = i\left[g(\langle a^\dagger a\rangle - \langle b^\dagger b\rangle) - F\langle b\rangle^*\right] - \dfrac{\gamma}{2}\langle ab^\dagger\rangle \\ \langle b^\dagger\dot{b}\rangle = 2g\ \mathrm{Im}\langle ab^\dagger\rangle \\ \langle a^\dagger\dot{a}\rangle = -2\ \mathrm{Im}[g\langle ab^\dagger\rangle + F\langle a\rangle] - \gamma\langle a^\dagger a\rangle + \gamma n \end{cases} \tag{4.20b}$$

$$\begin{cases} \langle\dot{a^2}\rangle = -2i(g\langle ab\rangle + F\langle a\rangle) - \gamma\langle a^2\rangle \\ \langle\dot{ab}\rangle = -i[g(\left\langle a^2\right\rangle + \left\langle b^2\right\rangle) + F\langle b\rangle] - \dfrac{\gamma}{2}\langle ab\rangle \\ \langle\dot{b^2}\rangle = -2ig\langle ab\rangle \end{cases} \tag{4.20c}$$

where now γ and n correspond to the frequency ω_0.

[3] Actually, this is not mathematically true because we are in an interaction picture and then the operators evolve. However, in this specific picture, their evolution is encoded in a phase, and for the quantity that we will calculate $\omega_0\left(\langle a^\dagger a\rangle + \langle b^\dagger b\rangle\right)$, it does not make any difference. See [NB22] for a very clear explanation.

The remaining part of this subchapter is devoted to calculating the refined weak coupling equations for analogous quantities to those presented before. The refined weak coupling generator $\mathcal{Z}(t)$ has the same form of the master equation obtained for the global approach, with the difference being the decay rates and the Lamb shift. Hence, for the interaction picture with respect to the free Hamiltonian of the global modes ($H = \Omega_+ c_1^\dagger c_1 + \Omega_- c_2^\dagger c_2$), we get [SHW]

$$\mathcal{Z}(t)[\rho_S(0)] = -i[\xi^+(t)c_1^\dagger c_1 + \xi^-(t)c_2^\dagger c_2 + F\left((a+a^\dagger)\cos(gt) - i(b-b^\dagger)\sin(gt)\right), \rho_S(0)] \tag{4.21}$$

$$+ \frac{\gamma_1^+}{2}\left(c_1\rho_S(0)c_1^\dagger - \frac{\{c_1^\dagger c_1, \rho_S(0)\}}{2}\right) + \frac{\gamma_2^+}{2}\left(c_1^\dagger\rho_S(0)c_1 - \frac{\{c_1 c_1^\dagger, \rho_S(0)\}}{2}\right) \tag{4.22}$$

$$+ \frac{\gamma_1^-}{2}\left(c_2\rho_S(0)c_2^\dagger - \frac{\{c_2^\dagger c_2, \rho_S(0)\}}{2}\right) + \frac{\gamma_2^-}{2}\left(c_2^\dagger\rho_S(0)c_2 - \frac{\{c_2 c_2^\dagger, \rho_S(0)\}}{2}\right), \tag{4.23}$$

where

$$\xi^{+,-}(t) = \frac{1}{4\pi}\int_0^\infty d\varphi t^2\Big[\operatorname{sinc}^2\left(\frac{\Omega_{+,-}-\varphi}{2}t\right)\mathcal{P}\int_0^\infty d\nu\frac{J(\nu)(n_\nu+1)}{\varphi-\nu} + \operatorname{sinc}^2\left(\frac{\Omega_{+,-}+\varphi}{2}t\right)\mathcal{P}\int_0^\infty d\nu\frac{J(\nu)n_\nu}{\varphi+\nu}\Big], \tag{4.24}$$

$$\gamma_1^{+,-} = \int_0^\infty J(\nu)t^2\operatorname{sinc}^2\left(\frac{\Omega_{+,-}-\nu}{2}t\right)(n_\nu+1)d\nu, \tag{4.25}$$

$$\gamma_2^{+,-} = \int_0^\infty J(\nu)t^2\operatorname{sinc}^2\left(\frac{\Omega_{+,-}-\nu}{2}t\right)n_\nu d\nu, \tag{4.26}$$

$$n_\nu = \frac{1}{e^{\nu/T}-1}. \tag{4.27}$$

We added the field term in the corresponding interaction picture in the Hamiltonian part as usual.

As we are interested in the evolution of the first and second moments, we should go to the Heisenberg picture using

$$\langle A\rangle(t) = \operatorname{Tr}\left(A(0)\rho(t)\right) = \operatorname{Tr}\left(A(0)e^{\mathcal{L}t}\rho(0)\right) = \operatorname{Tr}\left(e^{\mathcal{L}^\dagger t}[A(0)]\rho(0)\right). \tag{4.28}$$

Therefore, our adjoint generator is

$$\mathcal{Z}^\dagger(t)[\rho_S(0)] = \frac{\gamma_1^+}{2}\left(c_1^\dagger\rho_S(0)c_1 - \frac{\left\{\rho_S(0), c_1^\dagger c_1\right\}}{2}\right) + \frac{\gamma_1^-}{2}\left(c_2^\dagger\rho_S(0)c_2 - \frac{\left\{\rho_S(0), c_2^\dagger c_2\right\}}{2}\right) \tag{4.29}$$

$$+ \frac{\gamma_2^+}{2}\left(c_1\rho_S(0)c_1^\dagger - \frac{\left\{\rho_S(0), c_1 c_1^\dagger\right\}}{2}\right) + \frac{\gamma_2^-}{2}\left(c_2\rho_S(0)c_2^\dagger - \frac{\left\{\rho_S(0), c_2 c_2^\dagger\right\}}{2}\right) \tag{4.30}$$

$$+ i\left[F\left((a+a^\dagger)\cos(gt) - i(b-b^\dagger)\sin(gt)\right) + \xi^+ c_1^\dagger c_1 + \xi^- c_2^\dagger c_2, \rho_S(0)\right]. \tag{4.31}$$

Now we can apply it to the operators that are interesting to us and we get[4]

$$\mathcal{Z}^\dagger(t)[a] = -iF\cos(gt) + (\frac{1}{2}\gamma_2^+ - \frac{1}{2}\gamma_1^+ - 2i\xi_+)\left(\frac{a}{4}+\frac{b}{4}\right) + (\frac{1}{2}\gamma_2^- - \frac{1}{2}\gamma_1^- - 2i\xi_-)\left(\frac{a}{4}-\frac{b}{4}\right) \tag{4.32}$$

$$\mathcal{Z}^\dagger(t)[a^\dagger] = iF\cos(gt) + (\frac{1}{2}\gamma_2^+ - \frac{1}{2}\gamma_1^+ + 2i\xi^+)\left(\frac{a^\dagger}{4}+\frac{b^\dagger}{4}\right) + (\frac{1}{2}\gamma_2^- - \frac{1}{2}\gamma_1^- + 2i\xi^-)\left(\frac{a^\dagger}{4}-\frac{b^\dagger}{4}\right) \tag{4.33}$$

$$\mathcal{Z}^\dagger(t)[b] = F\sin(gt) + (\frac{1}{2}\gamma_2^+ - \frac{1}{2}\gamma_1^+ - 2i\xi_+)\left(\frac{a}{4}+\frac{b}{4}\right) + (\frac{1}{2}\gamma_1^- - \frac{1}{2}\gamma_2^- + 2i\xi_-)\left(\frac{a}{4}-\frac{b}{4}\right) \tag{4.34}$$

$$\mathcal{Z}^\dagger(t)[b^\dagger] = F\sin(gt) + (\frac{1}{2}\gamma_2^+ - \frac{1}{2}\gamma_1^+ + 2i\xi^+)\left(\frac{a^\dagger}{4}+\frac{b^\dagger}{4}\right) + (\frac{1}{2}\gamma_1^- - \frac{1}{2}\gamma_2^- - 2i\xi^-)\left(\frac{a^\dagger}{4}-\frac{b^\dagger}{4}\right) \tag{4.35}$$

$$\mathcal{Z}^\dagger(t)[a^\dagger a] = -iF\cos(gt)\left(-a+a^\dagger\right) + \frac{1}{2}\gamma_1^+\left(-\frac{ab^\dagger}{4}-\frac{a^\dagger a}{2}-\frac{a^\dagger b}{4}\right) + \frac{1}{2}\gamma_1^-\left(\frac{ab^\dagger}{4}-\frac{a^\dagger a}{2}+\frac{a^\dagger b}{4}\right) \tag{4.36}$$

$$+\frac{1}{2}\gamma_2^+\left(\frac{1}{2}+\frac{ab^\dagger}{4}+\frac{a^\dagger a}{2}+\frac{a^\dagger b}{4}\right) + \frac{1}{2}\gamma_2^-\left(\frac{1}{2}-\frac{ab^\dagger}{4}+\frac{a^\dagger a}{2}-\frac{a^\dagger b}{4}\right) + i(\xi^+-\xi^-)\left(-\frac{ab^\dagger}{2}+\frac{a^\dagger b}{2}\right) \tag{4.37}$$

$$\mathcal{Z}^\dagger(t)[b^\dagger b] = F(b+b^\dagger) + \frac{1}{2}\gamma_1^+\left(-\frac{ab^\dagger}{4}-\frac{a^\dagger b}{4}-\frac{b^\dagger b}{2}\right) + \frac{1}{2}\gamma_1^-\left(\frac{ab^\dagger}{4}+\frac{a^\dagger b}{4}-\frac{b^\dagger b}{2}\right) \tag{4.38}$$

$$+\frac{1}{2}\gamma_2^+\left(\frac{1}{2}+\frac{ab^\dagger}{4}+\frac{a^\dagger b}{4}+\frac{b^\dagger b}{2}\right) + \frac{1}{2}\gamma_2^-\left(\frac{1}{2}-\frac{ab^\dagger}{4}-\frac{a^\dagger b}{4}+\frac{b^\dagger b}{2}\right) - i(\xi^+-\xi^-)\left(\frac{ab^\dagger}{2}-\frac{a^\dagger b}{2}\right) \tag{4.39}$$

$$\mathcal{Z}^\dagger(t)\left[\frac{a^\dagger b + b^\dagger a}{2}\right] = \frac{F}{2}\left(\sin(gt)\left(a+a^\dagger\right) + i\cos(gt)\left(b-b^\dagger\right)\right) + \frac{1}{2}\gamma_1^+\left(-\frac{ab^\dagger}{4}-\frac{a^\dagger a}{4}-\frac{a^\dagger b}{4}-\frac{b^\dagger b}{4}\right) \tag{4.40}$$

$$+\frac{1}{2}\gamma_1^-\left(-\frac{ab^\dagger}{4}+\frac{a^\dagger a}{4}-\frac{a^\dagger b}{4}+\frac{b^\dagger b}{4}\right) + \frac{1}{2}\gamma_2^+\left(\frac{1}{2}+\frac{ab^\dagger}{4}+\frac{a^\dagger a}{4}+\frac{a^\dagger b}{4}+\frac{b^\dagger b}{4}\right) \tag{4.41}$$

$$+\frac{1}{2}\gamma_2^-\left(-\frac{1}{2}+\frac{ab^\dagger}{4}-\frac{a^\dagger a}{4}+\frac{a^\dagger b}{4}-\frac{b^\dagger b}{4}\right) \tag{4.42}$$

$$\mathcal{Z}^\dagger(t)\left[\frac{a^\dagger b - b^\dagger a}{2}\right] = \frac{F}{2}\left(\sin(gt)\left(a-a^\dagger\right) + i\cos(gt)\left(b+b^\dagger\right)\right) + \frac{1}{2}\gamma_1^+\left(\frac{ab^\dagger}{4}-\frac{a^\dagger b}{4}\right) + \frac{1}{2}\gamma_1^-\left(\frac{ab^\dagger}{4}-\frac{a^\dagger b}{4}\right) \tag{4.43}$$

$$+\frac{1}{2}\gamma_2^+\left(-\frac{ab^\dagger}{4}+\frac{a^\dagger b}{4}\right) + \frac{1}{2}\gamma_2^-\left(-\frac{ab^\dagger}{4}+\frac{a^\dagger b}{4}\right) - i\xi_+\left(\frac{a^\dagger a}{2}-\frac{b^\dagger b}{2}\right) - i\xi_-\left(-\frac{a^\dagger a}{2}+\frac{b^\dagger b}{2}\right), \tag{4.44}$$

As we are interested in calculating $e^{\mathcal{Z}^\dagger(t)}$, it is more convenient to see the action of the

[4] During this section if we do not specify the label, all the operators are evaluated at t zero, namely $a \equiv a(0)$.

superoperator as a linear transformation. Thus, if we construct a vector of operators as

$$\vec{O} = \begin{pmatrix} a \\ a^\dagger \\ b \\ b^\dagger \\ a^\dagger a \\ b^\dagger b \\ \frac{a^\dagger b + b^\dagger a}{2} \\ \frac{a^\dagger b - b^\dagger a}{2} \end{pmatrix}, \tag{4.45}$$

therefore we can translate the action of $\mathcal{Z}^\dagger(t)$ to a transformation of the vector $\vec{O}$ to a new one $\vec{O}'$.

This new vector $\vec{O}'$ is given by $\vec{O}' = M\vec{O} + \vec{b}$ where

$$M = \begin{pmatrix} \Gamma_+ - \Xi_+ & 0 & \Gamma_- - \Xi_- - ig & 0 & 0 & 0 & 0 & 0 \\ 0 & \Gamma_+ + \Xi_+ & 0 & \Gamma_- + \Xi_- + ig & 0 & 0 & 0 & 0 \\ \Gamma_- - \Xi_- - ig & 0 & \Gamma_+ - \Xi_+ & 0 & 0 & 0 & 0 & 0 \\ 0 & \Gamma_- + \Xi_- + ig & 0 & \Gamma_+ + \Xi_+ & 0 & 0 & 0 & 0 \\ iF\cos(gt) & -iF\cos(gt) & 0 & 0 & 2\Gamma_+ & 0 & 2\Gamma_- & -2\Xi_- - 2ig \\ 0 & 0 & F & F & 0 & 2\Gamma_+ & 2\Gamma_- & 2\Xi_- + 2ig \\ \frac{F}{2}\sin(gt) & \frac{F}{2}\sin(gt) & \frac{iF}{2}\cos(gt) & -\frac{iF}{2}\cos(gt) & \Gamma_- & \Gamma_- & 2\Gamma_+ & 0 \\ \frac{F}{2}\sin(gt) & -\frac{F}{2}\sin(gt) & \frac{iF}{2}\cos(gt) & \frac{iF}{2}\cos(gt) & -\Xi_- - ig & \Xi_- + ig & 0 & 2\Gamma_+ \end{pmatrix} \tag{4.46}$$

and

$$\vec{b} = \begin{pmatrix} -iF\cos(gt) \\ iF\cos(gt) \\ F\sin(gt) \\ F\sin(gt) \\ \frac{\gamma_2^+}{4} + \frac{\gamma_2^-}{4} \\ \frac{\gamma_2^+}{4} + \frac{\gamma_2^-}{4} \\ \frac{\gamma_2^+}{4} - \frac{\gamma_2^-}{4} \\ 0 \end{pmatrix}, \tag{4.47}$$

where we defined

$$\Gamma_+ = \frac{-\gamma_1^+ - \gamma_1^- + \gamma_2^+ + \gamma_2^-}{8}, \tag{4.48}$$

$$\Gamma_- = \frac{-\gamma_1^+ + \gamma_1^- + \gamma_2^+ - \gamma_2^-}{8}, \tag{4.49}$$

$$\Xi_+ = i\frac{(\xi_+ + \xi_-)}{2}, \tag{4.50}$$

$$\Xi_- = i\frac{(\xi_+ - \xi_-)}{2}. \tag{4.51}$$

Ξ_+ and Ξ_- correspond to the Lamb shift terms.

Now we can use that

$$\vec{O}' = \mathcal{Z}^\dagger(t)[\vec{O}] = M\vec{O} + \vec{b}. \tag{4.52}$$

As $\mathcal{Z}^\dagger(t)[I] = 0$ then we have:

$$\mathcal{Z}^{\dagger 2}(t)[\vec{O}] = \mathcal{Z}^\dagger(t)[M\vec{O} + \vec{b}] = M(M\vec{O} + \vec{b}), \tag{4.53}$$

and iterating we get

$$\mathcal{Z}^{\dagger n}(t)[\vec{O}] = M^{n-1}(M\vec{O} + \vec{b}). \tag{4.54}$$

Thus, finally, the whole evolution is given by [SHW]

$$\vec{O}(t) = e^{\mathcal{Z}(t)}[\vec{O}] = \vec{O} + \sum_{n=1}^{\infty} \frac{M^{n-1}(M\vec{O} + \vec{b})}{n!} \tag{4.55}$$

$$= \vec{O} - (\vec{O} + M^{-1}\vec{b}) + \sum_{n=0}^{\infty} \frac{M^n \vec{O}}{n!} + \sum_{n=0}^{\infty} \frac{M^{n-1}\vec{b}}{n!} \tag{4.56}$$

$$= \vec{O} - (\vec{O} + M^{-1}\vec{b}) + e^M \vec{O} + e^M M^{-1}\vec{b} \tag{4.57}$$

$$= (e^M - \mathbb{I})M^{-1}\vec{b} + e^M \vec{O}. \tag{4.58}$$

From it, we can compute the expectation values of the operators as in Eq. (4.28)

$$\langle \vec{O}(t) \rangle = (e^M - \mathbb{I})M^{-1}\vec{b} + e^M \langle \vec{O} \rangle \tag{4.59}$$

where

$$\langle \vec{O} \rangle = \begin{pmatrix} \langle a(0) \rangle \\ \langle a^\dagger(0) \rangle \\ \langle b(0) \rangle \\ \langle b^\dagger(0) \rangle \\ \langle a^\dagger a(0) \rangle \\ \langle b^\dagger b(0) \rangle \\ \langle \frac{a^\dagger b + b^\dagger a(0)}{2} \rangle \\ \langle \frac{a^\dagger b - b^\dagger a}{2}(0) \rangle \end{pmatrix}. \tag{4.60}$$

It is important to keep in mind that the calculation of local and global equations for the observables has been performed in a different interaction picture from the one used in the refined weak coupling. To address this issue, we note that for the latter case, we computed the expectation value in the intermediate picture as

$$\langle A \rangle_I(t) = \mathrm{Tr}\left(A\rho_I(t)\right) = \mathrm{Tr}\left(U_S(t) A U_S^\dagger(t)\rho(t)\right) \tag{4.61}$$

where $U_S = e^{-i\left(\Omega_+ c_1^\dagger c_1 + \Omega_- c_2^\dagger c_2\right)t}$. We are interested in the "real" expectation value of the operator, namely $\langle A \rangle(t) = \mathrm{Tr}\left(A\rho(t)\right)$. Thus, we have:

$$\langle a^\dagger a \rangle_I(t) = \mathrm{Tr}\left(U_S(t) a^\dagger a U_S^\dagger(t)\rho(t)\right) = \mathrm{Tr}\left(\left[\cos(gt)a^\dagger + ib^\dagger \sin(gt)\right]\left[\cos(gt)a - ib\sin(gt)\right]\rho(t)\right) \tag{4.62}$$

$$= \cos^2(gt)\langle a^\dagger a \rangle(t) + \sin^2(gt)\langle b^\dagger b \rangle(t) - 2\sin(gt)\cos(gt)\,\mathrm{Im}\left(\langle a^\dagger b \rangle(t)\right), \tag{4.63}$$

and

$$\langle b^\dagger b \rangle_I(t) = \mathrm{Tr}\left(U_S(t) b^\dagger b U_S^\dagger(t)\rho(t)\right) = \mathrm{Tr}\left(\left[i\sin(gt)a^\dagger + b^\dagger \cos(gt)\right]\left[-i\sin(gt)a + b\cos(gt)\right]\rho(t)\right) \tag{4.64}$$

$$= \sin^2(gt)\langle a^\dagger a \rangle(t) + \cos^2(gt)\langle b^\dagger b \rangle(t) - 2\sin(gt)\cos(gt)\,\mathrm{Im}\left(\langle ab^\dagger \rangle(t)\right). \tag{4.65}$$

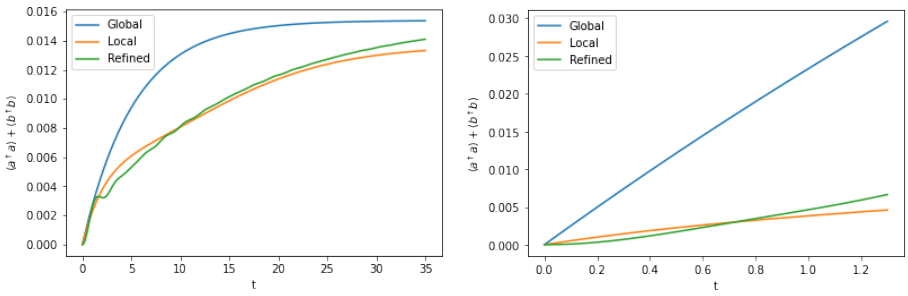
If we sum up these two expectation values, we obtain

$$\langle a^\dagger a \rangle_I(t) + \langle b^\dagger b \rangle_I(t) = \langle a^\dagger a \rangle(t) + \langle b^\dagger b \rangle(t). \tag{4.66}$$

Therefore, our figure of merit will be this sum of expectation values.[5]

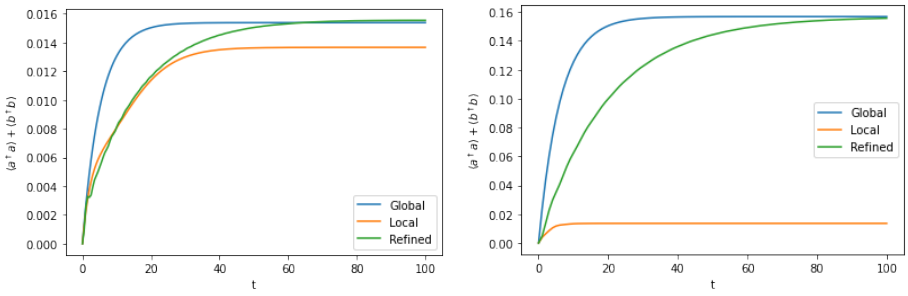
Before presenting the results, we would like to make some comments. For our numerical calculations, we consider the spectral density of the bath to be Ohmic, $J(\nu) = \alpha\nu$. Thus,

[5] As mentioned before, it is easy to see that for the local and global case $\langle a^\dagger a \rangle_I(t) = \langle a^\dagger a \rangle(t)$ and the same for b, because the only difference when moving to the interaction picture is only a phase.



(a) g=0.1ω_0 (b) g=0.6ω_0

Figure 4.1: Plot of $\langle a^\dagger a\rangle(t) + \langle b^\dagger b\rangle(t)$ for local, global, and refined approaches and for short times. For the plot $F = 0.001\omega_0$, $T = 0.2$, $J(\omega) = \alpha\omega$, and $\omega_0 = 1$. For the plot in the left $\alpha = \frac{0.2}{\pi}$, and for the right $\alpha = \frac{0.4}{\pi}$.



(a) g=0.1ω_0 (b) g=0.6ω_0

Figure 4.2: Plot of $\langle a^\dagger a\rangle(t) + \langle b^\dagger b\rangle(t)$ for local, global, and refined approaches and for short times. For the plot $F = 0.001\omega_0$, $T = 0.2$, $J(\omega) = \alpha\omega$, and $\omega_0 = 1$. For the plot in the left $\alpha = \frac{0.2}{\pi}$, and for the right $\alpha = \frac{0.4}{\pi}$.

γ_1 generally diverges because of the term without n_ν. To cure this, we make use of the regularization techniques exposed in [WMHA21], in particular the type ($\star\star$) referred there. For our specific case, we have

$$\int_0^\infty J(\nu)t^2 \operatorname{sinc}^2\left(\frac{\Omega-\nu}{2}t\right) \to 2tJ(\Omega). \tag{4.67}$$

In addition, we would like to remind the reader that we considered the Lamb shift to be zero for practical reasons. Thus, as in the GKLS equation (both local and global), the only divergent term is the Lamb shift, we do not need to put any cut-off term in the spectral density.

Before talking about our numerical results, we would like to argue that the local approach for long times gives unphysical results. To do so, we resort to the analytical derivations presented in [AFM+18]. For temperature $T = 0$, and starting from the ground state, one has that due to the specific characteristics of the model (see [AFM+18] for more details) the energy of the battery E_B is simply given by $E_B(t) = \omega_0|\langle b(t)\rangle|^2$ where one can analytically compute $b(t)$ and get

$$\langle b(t)\rangle = -\frac{F}{g}\left(1 - e^{-\frac{\gamma t}{4}}\left(\cosh(\varepsilon\tau/4) + \frac{\gamma}{\varepsilon}\sinh(\varepsilon\tau/4)\right)\right) \tag{4.68}$$

with $\varepsilon \equiv \sqrt{\gamma^2 - (4g)^2}$. If one takes the limit of $t \to \infty$, one will get $E_B(t\to\infty) = \omega_0(F/g)^2$ which is divergent if g goes to zero. This result contradicts what one would naturally

expect, namely, the energy of the battery going to zero. To cure this, one may use the global approach, perform the same limit and see whether the energy goes to zero. Indeed, this is the case. For global, we have

$$\langle b(t)\rangle = -\frac{2F\left(-i\gamma_+ + 4g\left(-e^{-\frac{\gamma_- t}{4}+igt} - e^{-\frac{1}{4}t(\gamma_+ +4ig)} + 2\right) + i\left(\gamma_- + \gamma_-\left(-e^{-\frac{1}{4}t(\gamma_+ +4ig)}\right) + \gamma_+ e^{-\frac{\gamma_- t}{4}+igt}\right)\right)}{(4g + i\gamma_-)(4g - i\gamma_+)}, \tag{4.69}$$

and taking the limit when g goes to zero we get

$$E_b(t) = \omega_0|\langle b(t)\rangle|^2 = 4\omega_0\left|\frac{F\left(i\left(-e^{-\frac{1}{4}(t\gamma_+)}\gamma_- + \gamma_- + e^{-\frac{1}{4}(t\gamma_-)}\gamma_+\right) - i\gamma_+\right)}{\gamma_-\gamma_+}\right|^2, \tag{4.70}$$

which is indeed zero for all times because $\gamma_+ = \gamma_-$ for $g = 0$. As one will see from our plots, the local approach is not accurate for times bigger than $1/(2g)$ (as expected.) [DTA+18]

We now present our numerical results in two different regimes: long times and short times. In Fig. (4.2) the results for the first scheme are plotted. We can see that regardless of g, the local approach is not good for long times. However, as one decreases g, the local approach gets more similar to the refined and global steady result. The reason is that if we decrease the interaction strength between the subsystems, we almost end up having just one subsystem interacting with the bath and disconnected from the other subsystem.

On the other hand, the global approach gives always the same result in the steady limit as the refined weak coupling, as expected [Riv17, WMHA21]. Furthermore, we can see that in all cases the Markovian dynamics thermalize faster than non-Markovian ones (refined.) Additionally, in Fig. (4.1) we can see the results for the short time scale. We see that especially for small g refined and local approach agree and the plots look very similar to the ones obtained in [WMHA21] for the qutrit case. Finally, for times comparable to $1/(2g)$ both local and global are not accurate to describe the dynamics. The reason is that these times correspond to a transient regime in which non-Markovian effects arise, as one can also notice in subsection (2.1.2).

To conclude, we would like to mention that one could improve the results by diagonalizing the whole Hamiltonian –including the field term–. In that case, the field will appear in the dissipator and the dynamics will be more precise and valid for all values of F. Plus, one has to keep in mind that we are comparing the results with the refined weak coupling equation, which is indeed more precise than both the local and global approach but it is still non-exact.

4.2 Markovian-vacuum approximation

We now present another non-Markovian approximation first stated in [ARAH22]. We call it Markovian-vacuum approximation and the reason for that will be noticed later. The approximation assumes that the long-time behavior of the excited population of the atom decays exponentially. To mathematically express it, we first need to introduce our model.

The setting is a continuous mode quantum laser interacting with an atom[6]. The total Hamiltonian reads

$$H = H_0 + H_I, \tag{4.71}$$
$$H_0 = H_A + H_F, \tag{4.72}$$

where

$$H_A \equiv \omega_0|1\rangle\langle 1|, \tag{4.73}$$
$$H_F \equiv \sum_\lambda \int d^3\vec{k}\,\omega_{\vec{k}\lambda} a^\dagger_{\vec{k}\lambda} a_{\vec{k}\lambda}, \tag{4.74}$$

[6]We will consider the atom to behave as a two-level system.

are the free Hamiltonians of the atom and the field, respectively. The interaction between them is given by

$$H_I = \sum_\lambda \int d^3\vec{k}\,[f(\omega_{\vec{k}\lambda})\sigma^+ a_{\vec{k}\lambda} + f^*(\omega_{\vec{k}\lambda})\sigma^- a^\dagger_{\vec{k}\lambda}], \tag{4.75}$$

where $a_{\vec{k}\lambda}$ is the usual annihilation bosonic operator of mode($\vec{k}$,λ), $\lambda \pm 1$ is the polarization, $\vec{k}$ is the continuous wave vector, and σ^+ (σ^-) is the raising (lowering) operator for the atom. Finally,

$$f(\omega_{\vec{k}\lambda}) = i\sqrt{\frac{\omega_{\vec{k}\lambda}}{2(2\pi)^3\varepsilon_0}}\ \vec{e}_{\vec{k}\lambda}\cdot\vec{D} \tag{4.76}$$

is the coupling constant [MW95], $\vec{e}_{\vec{k}\lambda}$ is the unit vector of the electric field and $\vec{D}$ is the atomic dipole moment vector.

When expanding the dynamics in the Dyson series, infinities (or terms that depend on the cut-off) will appear from the commutation relations. Thus, we would re-normalize the Hamiltonian in a way that all of these divergent terms will be encoded in a single parameter (Lamb Shift $\delta\omega$) whose value can be computed using quantum electrodynamics. Even though the physical meaning of using it is not clear at the moment, it serves as a tool to solve the dynamics of the system in the coherent basis of the laser field.

Thus, we rewrite the Hamiltonian as the sum of two non-Hermitian parts[7] $H = H_{0_r} + H_{I_r}$ where

$$H_{0_r} = H_{A_r} + H_F = \Omega|1\rangle\langle 1| + \int dk\,\omega_k a^\dagger_k a_k \tag{4.77}$$

and

$$H_{I_r} = \int dk\,[f(\omega_k)\sigma^+ a_k + f^*(\omega_k)\sigma^- a^\dagger_k] + ib|1\rangle\langle 1|, \tag{4.78}$$

where $b = i\delta\omega + \gamma$, $\Omega = \omega_A - i\gamma$, and $\omega_A = \omega_0 + \delta\omega$, where as usual, γ is the decay rate. If we now move to the interaction picture with respect to the free Hamiltonian H_{0_r}, we get

$$\tilde{H}_{I_r}(t) = e^{iH_{0_r}t} H_{I_r} e^{-iH_{0_r}t} \tag{4.79}$$

$$= \int dk[f(\omega_k,t)\sigma^+ a_k + f'(\omega_k,t)\sigma^- a^\dagger_k] + ib|1\rangle\langle 1|, \tag{4.80}$$

where we defined

$$f(\omega,t) = f(\omega)e^{-i(\omega-\omega_A+i\gamma)t}, \tag{4.81}$$

$$f'(\omega,t) = f^*(\omega)e^{i(\omega-\omega_A+i\gamma)t}. \tag{4.82}$$

If we choose to define

$$A(t) \equiv \int dk f(\omega_k,t)a_k, \tag{4.83}$$

$$A'(t) \equiv \int dk f'(\omega_k,t)a^\dagger_k, \tag{4.84}$$

we end up with

$$\tilde{H}_{I_r}(t) = \sigma^+ A(t) + \sigma^- A'(t) + ib|1\rangle\langle 1|. \tag{4.85}$$

[7] For simplicity, we have denoted $\int d^3\vec{k}$ as $\int dk$ and we have dropped the λ subscript.

These newly defined operators fulfill the following commutation relations

$$[A(t_i), A'(t_j)] = \left[\int dk\ f(\omega_k, t_i)a_k, \int dk'\ f'(\omega_{k'}, t_j)a^\dagger_{k'}\right] \tag{4.86}$$

$$= \int dk \int dk'\ f(\omega_k, t_i)f'(\omega_{k'}, t_j)[a_k, a^\dagger_{k'}] \tag{4.87}$$

$$= \int dk \int dk' f(\omega_k, t_i)f'(\omega_{k'}, t_j)\delta(\omega_k - \omega_{k'}) \tag{4.88}$$

$$= \int dk\ e^{i(\omega_A - i\gamma)(t_i - t_j)}e^{-i\omega_k(t_i - t_j)}|f(\omega_k)|^2 \tag{4.89}$$

$$= e^{i(\omega_A - i\gamma)(t_i - t_j)} \int dk\ e^{-i\omega_k(t_i - t_j)}|f(\omega_k)|^2 \tag{4.90}$$

$$= F^r(t_i - t_j), \tag{4.91}$$

where $F^r(t) \equiv e^{i(\omega_A - i\gamma)t} \int dk\, e^{-i\omega_k t}|f(\omega_k)|^2$.

We see in the next section, concretely in the Friedrichs-Lee model [Lee54, Fri48, Lon16], that the Markovian-vacuum approximation –namely, that the excited population of the atom decays exponentially for long times– can be cast into

$$F^r(t) \approx b\delta(t), \qquad t > 0, \tag{4.92}$$

in a distributional sense. Specifically, one only performs the approximation inside integrals.

4.2.1 Friedrichs-Lee model

To justify our approximation we consider the Friedrichs-Lee model [Lee54, Fri48, Lon16]. We first consider the model without the re-normalization to make the reader familiar with the kind of calculations we will later apply to the re-normalized one, and from there, we will justify Eq. (4.92).

If one considers the field to be initially in the ground state, the dynamics given by the total system Hamiltonian will leave invariant the space given by the span of the vectors: $|e\rangle \equiv |1\rangle \otimes |\{0\}\rangle$, $|f\rangle \equiv \int dk|0\rangle \otimes f(\omega_k)|\{1_k\}\rangle$ where $|1\rangle$ ($|0\rangle$) denotes the excited (ground) state of the two-level system and $|\{0\}\rangle$ ($|\{1_k\}\rangle$) the vacuum state of the field (the state that has one photon in the k-th mode with an arbitrary weight $f(\omega_k)$). Hence the interaction Hamiltonian, originally given in Eq. (4.75), now reads

$$H_I = |e\rangle\langle f| + |f\rangle\langle e|, \quad |f\rangle = \int dk\ f(\omega_k)|0\rangle|\{1_k\}\rangle, \tag{4.93}$$

where $\{\omega_k\}$ specifies the frequencies corresponding to each excited mode of the electrical field.

As mentioned before, we apply the approximation

$$\langle e|e^{-iHt}|e\rangle \simeq e^{(-i\omega_A - \gamma)t}, \tag{4.94}$$

which means that the survival amplitude (for long times) decays exponentially. H is the total Hamiltonian. If we move to the interaction picture $U_I(t) = e^{iH_0 t}e^{-iHt}$ the evolution fulfills

$$U_I(t) = \mathbb{I} - i\int_0^t e^{iH_0 s}(|e\rangle\langle f| + |f\rangle\langle e|)e^{-iH_0 s}U_I(s)ds. \tag{4.95}$$

where H and H_0 are given in Eqs. (4.71) and (4.72), respectively. We can define the matrix elements as

$$K(t) = \langle e|U_I(t)|e\rangle, \qquad M(t) = \langle f_t|U_I(t)|e\rangle \tag{4.96}$$

and the vector

$$|f_t\rangle = \int dk e^{i\omega_k t} f(\omega_k)|0\rangle|\{1_k\}\rangle. \tag{4.97}$$

Inserting Eq. (4.95) into Eq. (4.96) one obtains

$$\begin{aligned} K(t) &= 1 - i\int_0^t e^{i\omega_0 s} M(s)\, ds, \\ M(t) &= -i\int_0^t e^{-i\omega_0 s} F(t-s) K(s)\, ds, \end{aligned} \tag{4.98}$$

where we define $F(t) \equiv \int dk\, e^{-i\omega_k t}|f(\omega_k)|^2$. Now we can use the Laplace transform

$$\mathcal{F}(z) = \int_0^\infty e^{-zt} F(t)\, dt \tag{4.99}$$

and its properties to transform Eq. (4.98) into

$$\mathcal{K}(z) = \frac{1}{z} - i\frac{1}{z}\mathcal{M}(z - i\omega_0), \quad \mathcal{M}(z) = -i\mathcal{F}(z)\mathcal{K}(z + i\omega_0). \tag{4.100}$$

Finally, we can solve for $\mathcal{K}(z)$ and get

$$\mathcal{K}(z) = \frac{1}{z + \mathcal{F}(z - i\omega_0)}. \tag{4.101}$$

4.2.2 Dissipative re-normalization scheme in Friedrichs-Lee model

Now we move to the (non-unitary) re-normalized interaction picture $U_{I_r}(t) \equiv e^{iH_{0_r}t}e^{-iHt}$. In this picture, the evolution reads

$$U_{I_r}(t) = \mathbb{I} - i\int_0^t ds\; e^{iH_{0_r}s}\big[|e\rangle\langle f| + |f\rangle\langle e| + ib|1\rangle\langle 1|\big]e^{-iH_{0_r}s}U_{I_r}(s), \tag{4.102}$$

where H_{0_r} is previously defined in Eqs. (4.77) and H is the total Hamiltonian as usual. The survival amplitude can be expressed in terms of our new picture as

$$\langle e|e^{-iHt}|e\rangle = e^{(-i\omega_A - \gamma)t}\langle e|U_{I_r}(t)|e\rangle. \tag{4.103}$$

In analogy with what we did in the section before, we define

$$K^r(t) = \langle e|U_{I_r}(t)|e\rangle, \quad M^r(t) = \langle f_t|U_{I_r}(t)|e\rangle, \tag{4.104}$$

where $|f_t\rangle$ is defined in Eq. (4.97).

Hence

$$K^r(t) = \langle e|U_{I_r}(t)|e\rangle = \langle e|\mathbb{I} - i\int_0^t ds\; e^{iH_{0_r}s}\big[|e\rangle\langle f| + |f\rangle\langle e| + ib|1\rangle\langle 1|\big]e^{-iH_{0_r}s}U_{I_r}(s)|e\rangle \tag{4.105}$$

$$= 1 - i\int_0^t e^{i\Omega s}M^r(s)\, ds + i(\delta\omega - i\gamma)\int_0^t K^r(s)\, ds \tag{4.106}$$

Analogously, one obtains

$$M^r(t) = -i\int_0^t e^{-i\Omega s}F(t-s)K^r(s)\, ds. \tag{4.107}$$

We now apply the Laplace transform and get

$$\begin{aligned} \mathcal{K}^r(z) &= \tfrac{1}{z} - i\tfrac{1}{z}\mathcal{M}^r(z - i\Omega) + i(\delta\omega - i\gamma)\tfrac{1}{z}\mathcal{K}^r(z), \\ \mathcal{M}^r(z) &= -i\mathcal{F}(z)\mathcal{K}^r(z + i\Omega), \end{aligned} \tag{4.108}$$

and we finally obtain

$$\mathcal{K}^r(z) = \frac{1}{z + \mathcal{F}(z - i\omega_A - \gamma) - i\delta\omega - \gamma}. \tag{4.109}$$

Therefore, the desired probability can be re-expressed as

$$\langle e|e^{-iHt}|e\rangle = e^{(-i\omega_A-\gamma)t}K^r(t), \tag{4.110}$$

where $K^r(t)$ is obtained by inverting the Laplace transform of Eq. (4.109). From this, we are now ready to justify our approximation.

4.2.3 Justification of the approximation

Looking at Eq. (4.110), we see that our approximation translates to $K^r(t) \simeq 1$, for long times t. We can relate this with its Laplace transform using the Tauberian theorem

$$\mathcal{Y}(z) \simeq z^{-n} \text{ as } z \to 0 \iff Y(t) \simeq \frac{n}{\Gamma(n+1)} t^{(n-1)} \tag{4.111}$$

as $t \to \infty$, where $\Gamma(x)$ is the Gamma function. Setting $n = 1$ we observe that $K^r(t) \simeq 1$ for long times if and only if $\mathcal{K}^r(z) \simeq 1/z$ for small values of z. Making the substitution in Eq. (4.109) we have that

$$\mathcal{F}(z - i\omega_A - \gamma) \simeq \gamma + i\delta\omega \tag{4.112}$$

or consequently

$$\mathcal{F}^r(z) \simeq b. \tag{4.113}$$

Thus, if we take the inverse Laplace transform of Eq. (4.113), our approximation in the time domain becomes

$$F^r(t) \approx b\delta(t), \quad t > 0. \tag{4.114}$$

And for negative times

$$F^r(t) \approx b^*\delta(t), \quad t < 0. \tag{4.115}$$

The proof goes as follows. From the definition of $F^r(t)$ we have

$$F^r(t) = e^{\gamma t}h(t) \approx b\delta(t), \tag{4.116}$$

in which

$$h(t) \equiv \int dk\, e^{-i(\omega_k - \omega_A)t}|f(\omega_k)|^2.$$

Then if $t < 0$ we get

$$F^r(t) = F^r(-u) = e^{-\gamma u}h^*(u) = e^{-2\gamma u}\left(e^{\gamma u}h(u)\right)^* \tag{4.117}$$

$$\approx e^{-2\gamma u}b^*\delta(u) = e^{2\gamma t}b^*\delta(-t) = e^{2\gamma t}b^*\delta(t) \tag{4.118}$$

$$= b^*\delta(t), \tag{4.119}$$

where we dropped $e^{2\gamma t}$ in the last equality because inside the integrals this term will be one.

One can compute explicitly γ and $\delta\omega$. To do so, we compute the Laplace transform of $F^r(t)$

$$\mathcal{F}^r(z) = \int_0^\infty dt e^{-(z_r-\gamma)t}e^{i(\omega_A-\omega-z_i)t}\int d\omega 4\pi\omega^2|f(\omega)|^2, \tag{4.120}$$

where we used the dispersion relation $\omega = kc$, and set c=1. Furthermore, $z_r \equiv \text{Re}(z)$, $z_i \equiv \text{Im}(z)$. To ensure the convergence of the integral when $t \to \infty$ is needed that $z_r - \gamma > 0$. In that case

$$\mathcal{F}^r(z) = \int d\omega \frac{4\pi\omega^2}{z + i(\omega - \omega_A) - \gamma}|f(\omega)|^2. \tag{4.121}$$

Expanding for z small, and consequently γ will be small, we have

$$\frac{1}{z - i\omega_A - \gamma + i\omega} = \frac{z_r - \gamma + i(\omega_A - \omega - z_i)}{|z_r - \gamma|^2 + |\omega_A - \omega - z_i|^2} = \frac{z_r - \gamma}{|z_r - \gamma|^2 + |\omega_A - \omega - z_i|^2} + i\frac{\omega_A - \omega - z_i}{|z_r - \gamma|^2 + |\omega_A - \omega - z_i|^2} \tag{4.122}$$

$$\approx \pi\delta(\omega_A - \omega) + i\mathcal{P}\left(\frac{1}{\omega_A - \omega}\right). \tag{4.123}$$

Now computing the integral we have

$$\mathcal{F}^r(z) \approx 4\pi^2\omega_A^2|f(\omega_A)|^2 + i\mathcal{P}\int \frac{4\pi\omega^2}{\omega_A - \omega}|f(\omega)|^2 d\omega, \tag{4.124}$$

and if we use the approximation from Eq. (4.113) we have

$$\gamma + i\delta\omega + O(z) \approx 4\pi^2\omega_A^2|f(\omega_A)|^2 + i\mathcal{P}\int \frac{4\pi\omega^2}{\omega_A - \omega}|f(\omega)|^2 d\omega, \tag{4.125}$$

and hence

$$\gamma \approx 4\pi^2\omega_A^2|f(\omega_A)|^2, \qquad \delta\omega \approx \mathcal{P}\int \frac{4\pi\omega^2}{\omega_A - \omega}|f(\omega)|^2 d\omega. \tag{4.126}$$

4.2.4 Results

We now extend our approximation to all time values, not just for long times as we used in the derivation. Therefore, using it, the S-matrix elements $S_{I_r,ij}(t,0) \equiv \langle i|U_{I_r}(t,0)|j\rangle$, will be fully determined by the normal ordered terms, the decay rate and the Lamb shift, which facilitates the calculations a lot.

To see this result we first do the Dyson series for $U_{I_r}(t)$ (in the interaction picture with respect to H_{0_r}) and get

$$U_{I_r}(t,0) = \mathbb{I} - i\int_0^t dt_1 \tilde{H}_{I_r}(t_1) + (-i)^2\int_0^t dt_1\int_0^{t_1} dt_2 \tilde{H}_{I_r}(t_1)\tilde{H}_{I_r}(t_2) + \dots \tag{4.127}$$

If we apply now our approximation, the result will be greatly simplified. It is given by the next theorem:

Theorem 4.1. *The evolution of S-propagator elements $S_{I_r,ij}(t,0) \equiv \langle i|U_{I_r}(t,0)|j\rangle$ of the whole system is given by:*

$$S_{I_r,11}(t,0) \simeq \mathbb{I}_F + \sum_{n=1}(-i)^{2n}\int_0^t dt_1 \dots \int_0^{t_{2n-1}} dt_{2n} A'(t_2)\dots A'(t_{2n})A(t_1)\dots A(t_{2n-1}), \tag{4.128}$$

$$S_{I_r,00}(t,0) \simeq \mathbb{I}_F + \sum_{n=1}(-i)^{2n}\int_0^t dt_1 \dots \int_0^{t_{2n-1}} dt_{2n} A'(t_1)\dots A'(t_{2n-1})A(t_2)\dots A(t_{2n}), \tag{4.129}$$

$$S_{I_r,01}(t,0) \simeq \sum_{n=1}(-i)^{2n-1}\int_0^t dt_1 \dots \int_0^{t_{2n-2}} dt_{2n-1} A'(t_1)\dots A'(t_{2n-1})A(t_2)\dots A(t_{2n-2}), \tag{4.130}$$

$$S_{I_r,10}(t,0) \simeq \sum_{n=1}(-i)^{2n-1}\int_0^t dt_1 \dots \int_0^{t_{2n-2}} dt_{2n-1} A'(t_2)\dots A'(t_{2n-2})A(t_1)\dots A(t_{2n-1}), \tag{4.131}$$

where $\mathbb{I}_F$ is the identity matrix in the field space.

We do not prove the theorem here (see [ARAH22] for the whole proof.) However, we apply it to different cases.

First, let us simplify the usual differential equation fulfilled by the time-operator

$$\frac{d}{dt}U_{I_r}(t) = -i\tilde{H}_{I_r}(t)U_{I_r}(t). \tag{4.132}$$

Thanks to our theorem, one can obtain the following equation

$$\frac{d}{dt}S_{I_r}(t) = -i\left(\sigma^+ S_{I_r}(t)A(t) + \sigma^- A'(t)S_{I_r}(t)\right), \quad S_I(0) = \mathbb{I}. \tag{4.133}$$

A convenient representation of the previous differential equation is given in the coherent basis of the field. The basis is spanned by coherent states of the form $|\{\alpha\}\rangle \equiv |\alpha_1, \alpha_2, \ldots, \alpha_n\rangle$. Projecting Eq. (4.133) to this new basis, we easily obtain

$$\frac{d}{dt}S^{\beta\alpha}_{I_r}(t) = -i\Big(A_\alpha(t)\sigma^+ + A'_\beta(t)\sigma^-\Big)S^{\beta\alpha}_{I_r}(t), \quad S^{\beta\alpha}_{I_r}(0) = \langle\{\beta\}|\{\alpha\}\rangle \tag{4.134}$$

where

$$A_\alpha(t) \equiv e^{i\Omega t}f_\alpha(t), \qquad A'_\beta(t) \equiv e^{-i\Omega t}f^*_\beta(t), \tag{4.135}$$

and

$$f_\alpha(t) = \int dk\ f(\omega_k)\alpha(\omega_k)e^{-i\omega_k t}. \tag{4.136}$$

Moving now to the Schrödinger picture and defining

$$U^{\beta\alpha}(t) \equiv \frac{1}{\mathcal{N}_{\beta\alpha}}e^{t(-i\omega_A-\gamma)|1\rangle\langle 1|}S^{\beta\alpha}_{I_r}(t), \tag{4.137}$$

where $\mathcal{N}_{\beta\alpha} \equiv \langle\{\beta\}|\{\alpha\}\rangle$. This new propagator is normalized ($U^{\beta\alpha}(0) = \mathbb{I}$) and satisfies

$$\frac{d}{dt}U^{\beta\alpha}(t) = -i\Big[(\omega_A - i\gamma)|1\rangle\langle 1| + f_\alpha(t)\sigma^+ + f^*_\beta(t)\sigma^-\Big]U^{\beta\alpha}(t). \tag{4.138}$$

Furthermore, we can define the parameter $\xi = \beta - \alpha$ and change the propagator accordingly to $U^{\alpha\beta}(t) \equiv U^\xi_\alpha(t)$. For this new propagator, the evolution reads

$$\frac{d}{dt}U^\xi_\alpha(t) = -i\Big[(\omega_A - i\gamma)|1\rangle\langle 1| + f_\alpha(t)\sigma^+ + f^*_\alpha(t)\sigma^- + f^*_\xi(t)\sigma^-\Big]U^\xi_\alpha(t) = -i\Big[H_{A_r} + H_\alpha(t) + f^*_\xi(t)\sigma^-\Big]U^\xi_\alpha(t). \tag{4.139}$$

where

$$H_{A_r} \equiv (\omega_A - i\gamma)|1\rangle\langle 1|, \tag{4.140}$$

$$H_\alpha(t) \equiv f_\alpha(t)\sigma^+ + f^*_\alpha(t)\sigma^-. \tag{4.141}$$

If we move to the interaction picture (non-unitary) with respect to $H_{A_r} + H_\alpha(t)$, we obtain

$$\tilde{U}^\xi_\alpha = \mathcal{T}e^{i\int_0^t dt'(H_{A_r} + H_\alpha(t'))}\mathcal{T}e^{-i\int_0^t dt'(H_{A_r} + H_\alpha(t') + f^*_\xi(t')\sigma^-)}. \tag{4.142}$$

So $\tilde{U}^\xi_\alpha$ fulfills

$$\frac{d}{dt}\tilde{U}^\xi_\alpha(t) = -if^*_\xi(t)\tilde{\sigma}^-(t)\tilde{U}^\xi_\alpha(t) \tag{4.143}$$

with

$$\tilde{\sigma}^-(t) = \mathcal{T}e^{i\int_0^t dt'(H_{A_r} + H_\alpha(t'))t'}\sigma^-\mathcal{T}e^{-i\int_0^t dt'(H_{A_r} + H_\alpha(t'))t'}. \tag{4.144}$$

Vacuum state of the field

We start with the easiest case in which the initial state field is the vacuum ($\alpha = 0$.) In that case one readily obtains

$$\tilde{U}^{\xi}(t) = e^{-ih_{\xi}(t)\sigma^{-}} = \mathbb{I} - ih_{\xi}(t)\sigma^{-}, \tag{4.145}$$

where

$$h_{\xi}(t) = \int_0^t dt_1 f_{\xi}^*(t_1) e^{-i\omega_A t_1 - \gamma t_1}. \tag{4.146}$$

To get the reduced evolution of the state of the atom, we need to trace out the field

$$\tilde{\rho}_A(t) = tr_F\{\tilde{\rho}_{AF}\} = \int \mathcal{D}\beta \ \langle\{\beta\}|\tilde{\rho}_{AF}(t)|\{\beta\}\rangle = \int \mathcal{D}\beta \ \langle\{\beta\}|\tilde{U}(t)\tilde{\rho}_{AF}(0)\tilde{U}^{\dagger}(t)|\{\beta\}\rangle \tag{4.147}$$

$$= \int \mathcal{D}\beta \ \langle\{\beta\}|\tilde{U}(t)\tilde{\rho}_A(0)\otimes|\{\alpha\}\rangle_F\langle\{\alpha\}|\tilde{U}^{\dagger}(t)|\{\beta\}\rangle = \int \mathcal{D}\beta \ |\mathcal{N}_{\beta\alpha}|^2\tilde{U}^{\alpha\beta}(t)\tilde{\rho}_A(0)(\tilde{U}^{\alpha\beta}(t))^{\dagger} \tag{4.148}$$

$$= \int \mathcal{D}\xi \, e^{-\|\xi\|^2}\tilde{U}^{\xi}(t)\rho_A(0)\big(\tilde{U}^{\xi}(t)\big)^{\dagger} = \int \mathcal{D}\xi \, e^{-\|\xi\|^2}\left(\mathbb{I} - ih_{\xi}(t)\sigma^{-}\right)\rho_A(0)\Big(\mathbb{I} + ih_{\xi}^*(t)\sigma^{+}\Big) \tag{4.149}$$

$$= \int \mathcal{D}\xi \, e^{-\|\xi\|^2}\Big(\rho_A(0) + ih_{\xi}^*(t)\rho_A(0)\sigma^{+} - ih_{\xi}(t)\sigma^{-}\rho_A(0) + |h_{\xi}(t)|^2\sigma^{-}\rho_A(0)\sigma^{+}\Big) \tag{4.150}$$

$$= \int \mathcal{D}\xi \, e^{-\|\xi\|^2}(\rho_A(0) + |h_{\xi}(t)|^2\sigma^{-}\rho_A(0)\sigma^{+}) = \rho_A(0) + \chi(t)\sigma^{-}\rho_A(0)\sigma^{+} \tag{4.151}$$

$$= e^{\tilde{\Gamma}(t)}[\rho_A(0)], \tag{4.152}$$

where during the calculation we used $\alpha = 0$ and we defined the superoperator $\tilde{\Gamma}(t)$ as

$$\tilde{\Gamma}(t) \equiv \chi(t)\sigma^{-}(\cdot)\ \sigma^{+}, \tag{4.153}$$

and

$$\chi(t) \equiv \int \mathcal{D}\xi \, e^{-\|\xi\|^2}|h_{\xi}(t)|^2. \tag{4.154}$$

Moreover, we have considered that for Gaussian complex random noise, the first moments are zero, i.e.

$$\langle h_{\xi}(t)\rangle = \int \mathcal{D}\xi \, e^{-\|\xi\|^2}h_{\xi}(t) = 0. \tag{4.155}$$

$\chi(t)$ is given by

$$\chi(t) = \int \mathcal{D}\xi \, e^{-\|\xi\|^2}\int_0^t dt_1 \int_0^t ds_1 \ f_{\xi}(t_1)f_{\xi}^*(s_1)e^{-i\omega_A(t_1-s_1)-\gamma(t_1+s_1)} \tag{4.156}$$

$$= \int_0^t dt_1 \int_0^t ds_1 \int dk \ e^{-\gamma(t_1+s_1)}e^{-i\omega_k(t_1-s_1)}e^{-i\omega_A(t_1-s_1)}|f(\omega_k)|^2 \tag{4.157}$$

$$= \int_0^t dt_1 \int_0^t ds_1 \ e^{-2\gamma t_1}e^{-2i\omega_A(t_1-s_1)}F^r(t_1-s_1), \tag{4.158}$$

where $F^r(t)$ is defined as usual. We can simplify the $\chi(t)$ expression if we use our approxi-

mation in the time domain. Thus

$$\chi(t) = \int_0^t dt_1 \int_0^t ds_1 \; e^{-2\gamma t_1} e^{-2i\omega_A(t_1-s_1)} F^r(t_1-s_1) \tag{4.159}$$

$$= \underbrace{\int_0^t dt_1 \int_0^{t_1} ds_1 \; e^{-2\gamma t_1} e^{-2i\omega_A(t_1-s_1)} F^r(t_1-s_1)}_{t_1>s_1} + \underbrace{\int_0^t ds_1 \int_0^{s_1} dt_1 \; e^{-2\gamma t_1} e^{-2i\omega_A(t_1-s_1)} F^r(t_1-s_1)}_{t_1<s_1} \tag{4.160}$$

$$\approx \int_0^t dt_1 \int_0^{t_1} ds_1 \; e^{-2\gamma t_1} e^{-2i\omega_A(t_1-s_1)} b\delta(t_1-s_1) + \int_0^t ds_1 \int_0^{s_1} dt_1 \; e^{-2\gamma t_1} e^{-2i\omega_A(t_1-s_1)} b^*\delta(t_1-s_1) \tag{4.161}$$

$$= 2\gamma \int_0^t e^{-2\gamma t_1} dt_1 \; = 1 - e^{-2\gamma t}, \tag{4.162}$$

where we separated the integral in two different regimes, one with the argument of F^r being positive and the other being negative. We also used that $b + b^* = 2\gamma$.

The equation for $\tilde{\rho}_A(t)$ reads

$$\tilde{\rho}_A(t) = \rho_A(0) + \chi(t)\sigma^- \rho_A(0)\sigma^+ = \rho_A(0) + \left(1 - e^{-2\gamma t}\right)\sigma^- \rho_A(0)\sigma^+. \tag{4.163}$$

Thus the master equation in the interaction picture is given by

$$\frac{d}{dt}\tilde{\rho}_A(t) = \frac{d}{dt} e^{\tilde{\Gamma}(t)}[\rho_A(0)] = \int_0^1 ds e^{s\tilde{\Gamma}(t)} \frac{d}{dt}\left(\tilde{\Gamma}(t)\right) e^{(1-s)\tilde{\Gamma}(t)}[\rho_A(0)] = \frac{d}{dt}\left(\tilde{\Gamma}(t)\right)\left[e^{\tilde{\Gamma}(t)}[\rho_A(0)]\right] \tag{4.164}$$

$$= 2\gamma e^{-2\gamma t}\sigma^- \tilde{\rho}_A(t)\sigma^+ = \tilde{\Lambda}[\tilde{\rho}_A(t)], \tag{4.165}$$

where we used the formula for the derivative of an exponential of a matrix [Sni64, Wil67]

$$\frac{d}{dt} e^{A(t)} = \int_0^1 ds e^{sA(t)} \left[\frac{dA(t)}{dt}\right] e^{(1-s)A(t)} ds, \tag{4.166}$$

and defined

$$\tilde{\Lambda}[\cdot] = 2\gamma e^{-2\gamma t}\sigma^-(\cdot)\sigma^+. \tag{4.167}$$

Moving back to Shcrödinger picture we get

$$\frac{d}{dt}\rho_A(t) = \frac{d}{dt}\left(e^{-iH_{A_r}t}\tilde{\rho}_A(t)e^{iH_{A_r}^\dagger t}\right) \tag{4.168}$$

$$= -i[H_A, e^{-iH_{A_r}t}\tilde{\rho}_A(t)e^{iH_{A_r}^\dagger t}] - \gamma\{|1\rangle\langle 1|, e^{-iH_{A_r}t}\tilde{\rho}_A(t)e^{iH_{A_r}^\dagger t}\} + e^{-iH_{A_r}t}\frac{d}{dt}\tilde{\rho}_A(t)e^{iH_{A_r}^\dagger t} \tag{4.169}$$

$$= -i[H_A, \rho_A(t)] - \gamma\{|1\rangle\langle 1|, \rho_A(t)\} + 2\gamma\sigma^-\rho_A(t)\sigma^+, \tag{4.170}$$

where we used $e^{-iH_{A_r}t}\sigma^- = \sigma^-$ and $\sigma^+ e^{iH_{A_r}t} = \sigma^+$ as well as $e^{-iH_{A_r}t}\sigma^+ = e^{\omega_A t+\gamma t}\sigma^+$ and $\sigma^- e^{-iH_{A_r}t} = \sigma^- e^{-\omega_A t+\gamma t}$. We also defined $H_A \equiv \omega_A|1\rangle\langle 1|$. To conclude, we see that the evolution is given by the GKLS master equation. This is why we named the approximation Markovian-vacuum.

Coherent state of the field

Here we compute the case in which the field is in a coherent state. Before any calculation, let us redefine $\gamma \to \frac{\gamma}{2}$ and thus $b + b^* = \gamma$.

The evolution now reads

$$\frac{d}{dt}U_\alpha^\xi(t) = -i\Big[\omega_A P_1 + f_\alpha(t)\sigma^+ + f_\alpha^*(t)\sigma^-\Big]U_\alpha^\xi(t) - \Big[\frac{\gamma}{2}P_1 + if_\xi^*(t)\sigma^-\Big]U_\alpha^\xi(t), \tag{4.171}$$

where $P_1 \equiv |1\rangle\langle 1|$. If we define the unitary interaction picture with respect to $H_\alpha(t) \equiv \omega_A P_1 + f_\alpha(t)\sigma^+ + f_\alpha^*(t)\sigma^-$, the unitary operator will be

$$U_\alpha(t) = \mathcal{T} e^{-i\int_0^t dt' H_\alpha(t')}, \tag{4.172}$$

and the evolution reads

$$\frac{d}{dt}\left(U_\alpha(t)U_\alpha^\xi(t)U_\alpha^\dagger(t)\right) = U_\alpha(t)\left(-\Big[\frac{\gamma}{2}P_1 + if_\xi^*(t)\sigma^-\Big]U_\alpha^\xi(t)\right)U_\alpha^\dagger(t), \tag{4.173}$$

enabling us to calculate the Dyson expansion for $U_\alpha^\xi(t)$ as

$$U_\alpha^\xi(t) = U_\alpha(t,0)\Big[\mathbb{I} - \int_0^t ds_1\left(\frac{\gamma}{2}\tilde{P}_1(s_1) + if_\xi^*(s_1)\tilde{\sigma}^-(s_1)\right) \tag{4.174}$$

$$+ \int_0^t ds_1 \int_0^{s_1} ds_2 \left(\frac{\gamma}{2}\tilde{P}_1(s_1) + if_\xi^*(s_1)\tilde{\sigma}^-(s_1)\right)\left(\frac{\gamma}{2}\tilde{P}_1(s_2) + if_\xi^*(s_2)\tilde{\sigma}^-(s_2)\right)\Big] + \mathcal{O}(\gamma^3), \tag{4.175}$$

where $\tilde{X} \equiv U_\alpha^\dagger(s_1)XU_\alpha(s_1)$.

With this expansion, we are ready to calculate $\rho_A(t)$ up to the first order in γ. Then we have

$$\rho_A(t) = \Lambda(t)\rho_A(0) = \int \mathcal{D}\xi\, e^{-\|\xi\|^2} U_\alpha^\xi(t)\rho_A(0)\big(U_\alpha^\xi(t)\big)^\dagger \tag{4.176}$$

$$= \int \mathcal{D}\xi\, e^{-\|\xi\|^2} U_\alpha(t,0)\Big[\mathbb{I} - \int_0^t ds_1\Big(\frac{\gamma}{2}\tilde{P}_1(s_1) + if_\xi^*(s_1)\tilde{\sigma}^-(s_1)\Big)\Big]\rho_A(0) \tag{4.177}$$

$$\times \Big[\mathbb{I} - \int_0^t ds_2\Big(\frac{\gamma}{2}\tilde{P}_1(s_2) - if_\xi(s_2)\tilde{\sigma}^+(s_2)\Big)\Big]U_\alpha^\dagger(t,0) \tag{4.178}$$

$$= U_\alpha(t,0)\Big[\rho_A(0) - \int_0^t ds_1 \frac{\gamma}{2}\left(\tilde{P}_1(s_1)\rho_A(0) + \rho_A(0)\tilde{P}_1(s_1)\right) \tag{4.179}$$

$$+ \int \mathcal{D}\xi\, e^{-\|\xi\|^2}\int_0^t ds_1 \int_0^t ds_2 f_\xi^*(s_1)f_\xi(s_2)\tilde{\sigma}^-(s_1)\rho_A(0)\tilde{\sigma}^+(s_2)\Big]U_\alpha^\dagger(t,0) \tag{4.180}$$

$$= U_\alpha(t,0)\Big[\rho_A(0) - \frac{\gamma}{2}\int_0^t ds_1\Big(\tilde{P}_1(s_1)\rho_A(0) + \rho_A(0)\tilde{P}_1(s_1)\Big) \tag{4.181}$$

$$+ \int_0^t ds_1 \int_0^t ds_2\; e^{\gamma(s_1-s_2)}e^{-i\omega_A(s_1-s_2)}F^r(s_1-s_2)\tilde{\sigma}^-(s_1)\rho_A(0)\tilde{\sigma}^+(s_2)\Big]U_\alpha^\dagger(t,0) \tag{4.182}$$

$$\approx U_\alpha(t,0)\Big[\rho_A(0) - \frac{\gamma}{2}\int_0^t ds_1\left(\tilde{P}_1(s_1)\rho_A(0) + \rho_A(0)\tilde{P}_1(s_1)\right) \tag{4.183}$$

$$+ \int_0^t ds_1 \int_0^{s_1} ds_2\; \gamma e^{\gamma(s_1-s_2)}e^{-i\omega_A(s_1-s_2)}\delta(s_1-s_2)\tilde{\sigma}^-(s_1)\rho_A(0)\tilde{\sigma}^+(s_2)\Big]U_\alpha^\dagger(t,0) \tag{4.184}$$

$$= U_\alpha(t,0)\Big[\rho_A(0) - \frac{\gamma}{2}\int_0^t ds_1\left(\tilde{P}_1(s_1)\rho_A(0) + \rho_A(0)\tilde{P}_1(s_1)\right) + \gamma\int_0^t ds_1\; \tilde{\sigma}^-(s_1)\rho_A(0)\tilde{\sigma}^+(s_1)\Big]U_\alpha^\dagger(t,0), \tag{4.185}$$

where again we have made use of our approximation. One could expand up to higher orders

in γ and get the solution analogously. We state the result up to the second order here

$$\rho_A(t) = \Lambda(t)\rho_A(0) \approx U_\alpha(t,0)\Big[\rho_A(0) - \int_0^t ds_1 \frac{\gamma}{2}\left(\tilde{P}_1(s_1)\rho_A(0) + \rho_A(0)\tilde{P}_1(s_1)\right) \tag{4.186}$$

$$+ \gamma\int_0^t ds_1\ e^{-\gamma s_1}\tilde{\sigma}^-(s_1)\rho_A(0)\tilde{\sigma}^+(s_1) + \frac{\gamma^2}{4}\int_0^t ds_1\int_0^t ds_1'\tilde{P}_1(s_1)\rho_A(0)\tilde{P}_1(s_1') \tag{4.187}$$

$$- \frac{\gamma^2}{2}\int_0^t ds_1'\int_0^{s_1'} ds_2'\Big(\tilde{\sigma}^-(s_2')\rho_A(0)\tilde{\sigma}^+(s_2')\tilde{P}_1(s_1') + \tilde{P}_1(s_1')\tilde{\sigma}^-(s_2')\rho_A(0)\tilde{\sigma}^+(s_2')\Big) \tag{4.188}$$

$$- \frac{\gamma^2}{2}\int_0^t ds_1\int_0^{s_1} ds_2'\ \Big(\tilde{\sigma}^-(s_1)\rho_A(0)\tilde{P}_1(s_2')\tilde{\sigma}^+(s_1) + \tilde{\sigma}^-(s_1)\tilde{P}_1(s_2')\rho_A(0)\tilde{\sigma}^+(s_1)\Big) \tag{4.189}$$

$$+ \frac{\gamma^2}{4}\int_0^t ds_1\int_0^t ds_1'\Big(\rho_A(0)\tilde{P}_1(s_1')\tilde{P}_1(s_1) + \tilde{P}_1(s_1)\tilde{P}_1(s_1')\rho_A(0)\Big) \tag{4.190}$$

$$+ \gamma^2\int_0^t ds_1\int_0^{s_1} ds_1'\ \tilde{\sigma}^-(s_1)\tilde{\sigma}^-(s_1')\rho_A(0)\tilde{\sigma}^+(s_1)\tilde{\sigma}^+(s_1')\Big]U_\alpha^\dagger(t,0). \tag{4.191}$$

If one moves to the interaction picture with respect to H_α one can see that the evolution that one gets is the same as the one given by $\mathcal{T}e^{\tilde{\Lambda}(t)}$ (expanding it to the second order in γ)[8] where

$$\tilde{\Lambda}(t) = -\frac{\gamma}{2}\int_0^t ds_1\{\tilde{P}_1(s_1),(\cdot)\} + \gamma\int_0^t ds_1\ \tilde{\sigma}^-(s_1)(\cdot)\tilde{\sigma}^+(s_1). \tag{4.192}$$

This generator is of GKLS form for any given t, due to the positivity of γ, and thus the map ensures that the dynamics are CP. Hence, as we already know that the most general solution for a Liouvillian equation is of the form

$$\rho(t) = \mathcal{T}\exp\left[\int_0^t ds\mathcal{L}(s)\right]\rho\left(t_0\right), \tag{4.193}$$

where we set the origin of time at zero, this implies that in our case we have

$$\tilde{\mathcal{L}}(t) = -\frac{\gamma}{2}\{\tilde{P}_1(t),(\cdot)\} + \gamma\tilde{\sigma}^-(t)(\cdot)\tilde{\sigma}^+(t). \tag{4.194}$$

Finally, our master equation reads

$$\frac{d\tilde{\rho}(t)}{dt} = \tilde{\mathcal{L}}(t)\tilde{\rho}(t) = -\frac{\gamma}{2}\{\tilde{P}_1(t),\tilde{\rho}(t)\} + \gamma\tilde{\sigma}^-(t)\tilde{\rho}(t)\tilde{\sigma}^+(t), \tag{4.195}$$

and in the Schrödinger picture

$$\frac{d\rho(t)}{dt} = -i\left[H_\alpha(t),\rho(t)\right] - \frac{\gamma}{2}\{P_1,\rho(t)\} + \gamma\sigma^-\rho(t)\sigma^+. \tag{4.196}$$

The only difference this equation has with respect to the Markovian master equation is the time dependence in the Hamiltonian. Therefore, the dynamics are not Markovian even though they are still CP, so they are more accurate.

[8] As pointed out in our paper [ARAH22], that the evolution is given by this expression is a conjecture. We were only able to prove it up to the second order in γ. However, we strongly believe that it holds for all orders.

Chapter 5

Exact dynamics

Throughout this thesis, it has become apparent that computing the exact dynamics of an Open Quantum System is generally very demanding. Even in one of the simplest cases that one can think of, namely, the Spin-boson model [LCD+87, RH12], there is no exact solution known. However, there still exist some systems which allow for semi-analytical[1] solutions. An example of this is the resonant level model. In this chapter, we first introduce and solve the model and then we use the results from quantum estimation theory to infer and estimate the temperature of the system[2]. While doing so, we benchmark the exact result with those obtained in the weak coupling limit (those given by the GKLS master equation.)

5.1 Resonant level model

The resonant level model [Sch14] consists of a fermionic system (e.g. a quantum dot) interacting with a fermionic bath via linear interaction. The Hamiltonian reads

$$H = \varepsilon d^\dagger d + \sum_q \omega_q b_q^\dagger b_q + \sum_q (t_q b_q^\dagger d + t_q^* d^\dagger b_q), \tag{5.1}$$

where b_q and d annihilate a fermion in the qth mode of the bath and the system, respectively, and ε and ω_q are the gap energies of our system and the qth mode of the bath. Since they are fermions, they obey the fermionic anticommutation relations, i.e. $\{d, d^\dagger\} = \mathbb{I}$, $\{b_q, b_k^\dagger\} = \mathbb{I}\delta_{qk}$, and $\{b_q, b_k\} = \{a, b_q^\dagger\} = \{d, d\} = 0$. Moreover, the coupling strength between the dot and the bath is given by t_q which relates to the spectral density of the bath $\Gamma(\omega)$[3] as follows

$$\Gamma(\omega) = 2\pi \sum_q |t_q|^2 \delta(\omega - \omega_q), \tag{5.2}$$

where we consider that the spectral density is modeled by a Lorentzian distribution

$$\Gamma(\omega) = \frac{\Gamma \delta^2}{\omega^2 + \delta^2}. \tag{5.3}$$

As our last assumption, we use the wideband limit that corresponds to the limit case in which the width of the Lorentzian goes to infinite, making the frequency-dependent density become constant i.e. $\lim_{\delta \to \infty} \Gamma(\omega) \to \Gamma$.

We would like to write the density matrix of the system/dot in the number basis and as it is a fermion, and the eigenvalues of the number operator $N = d^\dagger d$ are either 0 or 1,

[1] Here by semi-analytical solutions we mean that one can arrive at an analytical formula to compute the dynamics but must resort to numerical methods to calculate it.

[2] This is generally called quantum thermometry. See [MSC19] for an extensive review of the field.

[3] We would like to note that we changed the notation from the other chapters, in which the spectral density of the bath was given by $J(\omega)$ because $\Gamma(\omega)$ is the common notation in the literature of resonant level models.

the basis is $\{|0\rangle\langle 0|, |1\rangle\langle 1|\}$. Furthermore, the fermionic superselection rules [FLB13] do not allow for superposition states as $|\psi\rangle = a|0\rangle + b|1\rangle$. This simplifies the problem at hand because the density matrix of the dot at any time t of the evolution, in the aforementioned basis reads

$$\rho(t) = \begin{pmatrix} 1 - p_1(t) & 0 \\ 0 & p_1(t) \end{pmatrix}, \tag{5.4}$$

and an easy calculation shows that $\langle d^\dagger d\rangle(t) = \mathrm{Tr}(d^\dagger d\rho(t)) = p_1(t)$. Thus, just knowing $\langle d^\dagger d\rangle(t)$ is enough to get the whole dynamics of the system. The last thing that is worth mentioning is that since we are considering both the bath and the system, they both form a closed system and hence the evolution is given by a unitary transformation. Then, if one moves to the Heisenberg picture –the time evolution is no longer in the states but in the operators, as opposed to the Schrödinger one– $d^\dagger d(t) = d^\dagger(t)d(t)$ which is not mainly the case when dealing with open systems.

We now resort to Heisenberg equations to get the evolution of the operators. In our case, we get the following system of equations

$$i\dot{d}(t) = \varepsilon d(t) + \sum_q t_q b_q(t), \tag{5.5}$$

$$i\dot{b}_q(t) = \omega_q b_q(t) + t_q^* d(t) \tag{5.6}$$

where $\dot{A}(t)$ corresponds to the time derivative with respect to the operator A. One can readily solve the system of equations by introducing the ansatz $v_q(t) = e^{i\omega_q t} b_q(t)$ and injecting it into (5.6). Then, we can get the solution for this new variable $v_q(t)$ as

$$v_q(t) = -it_q^* \int_0^t ds e^{i\omega_q s} d(s) + v_q(0). \tag{5.7}$$

Now we can move back to the bath operators $b_q(t)$ and we get

$$b_q(t) = -it_q^* \int_0^t ds e^{i\omega_q (s-t)} d(s) + e^{-i\omega_q t} b_q(0), \tag{5.8}$$

where of course we used the fact that $b_q(0) = v_q(0)$ which is given by the definition of $v_q(t)$. Finally, we inject $b_q(t)$ into (5.5) and this gives us

$$\dot{d}(t) = -i\varepsilon d(t) - i\xi(t) - \int_0^t \chi(s-t) d(s) ds, \tag{5.9}$$

where we defined $\xi(t) = \sum_q t_q e^{-i\omega_q t} b_q(0)$ and $\chi(t) = \sum_q |t_q|^2 e^{i\omega_q t}$. The last term on the right-hand side can be simplified by using

$$\int_0^t \sum_q |t_q|^2 e^{i\omega_q (s-t)} d(s) = \int_{-\infty}^{\infty} d\omega \delta(\omega - \omega_q) \frac{2\pi}{2\pi} \int_0^t ds \sum_q |t_q|^2 e^{i\omega(s-t)} d(s) \tag{5.10}$$

$$= \frac{1}{2\pi} \int_0^t ds \int_{-\infty}^{\infty} d\omega \Gamma(\omega) e^{i\omega(s-t)} d(s) \tag{5.11}$$

$$\approx \frac{1}{2\pi} \int_0^t ds \int_{-\infty}^{\infty} d\omega \Gamma e^{i\omega(s-t)} d(s) = \Gamma \int_0^t ds \delta(s-t) d(s) = \frac{\Gamma}{2} d(t), \tag{5.12}$$

where we used (5.2) to go from the first to the second line and the wideband limit for the approximation. The final factor 1/2 appears because of the normalization of the Delta function.

We can now rewrite (5.9) as

$$\dot{d}(t) = -i\varepsilon d(t) - i\xi(t) - \frac{\Gamma}{2}d(t) = -i\left(\varepsilon - i\frac{\Gamma}{2}\right)d(t) - i\xi(t), \tag{5.13}$$

and then solve it in an analogous form as (5.7), i.e. defining another variable. To avoid repetition we just state the result:

$$d(t) = e^{-i(\varepsilon - i\frac{\Gamma}{2})t}d(0) - i\int_0^t ds e^{i(\varepsilon - i\frac{\Gamma}{2})(s-t)}\xi(s), \tag{5.14}$$

with $\xi(s)$ defined as before. Instead of proceeding as we did, we could have solved the system of equations using Laplace transformations [Sch14]. We chose this method because of its simplicity.

As we are interested in the state of the system $\rho(t)$ we need to compute the expectation values from (5.14). As usual in the literature, we would consider that the initial state is a product state (see maybe some references about not having this) and that the bath starts in thermal equilibrium at some inverse temperature β which means that its reduced state is a Gibbs state $\tau_B(\beta) = e^{-\beta(H_B - \mu N)}/Z$ with the Hamiltonian of the bath being $H_B = \sum_q \omega_q b_q^\dagger b_q$, Z the so-called partition function that accounts for the normalization, and μ the chemical potential. Hence, the initial state of the whole closed system (dot + bath) is

$$\rho(0) = \rho_S(0)\tau_B(\beta). \tag{5.15}$$

With this choice of the initial state, we now calculate $\langle d^\dagger d(t)\rangle$. Noting the fermionic nature of both the bath and the dot, we have that $\langle d^\dagger\rangle = \langle d\rangle = \langle b_q\rangle = \langle b_q^\dagger\rangle = 0$ for all q, and as the bath begins in a thermal state $\langle b_q^\dagger b_{q'}(0)\rangle = \delta_{q,q'}f_\beta(\varepsilon_q)$ where $f_\beta(\omega_q) = \frac{1}{1+e^{\beta(\omega_q - \mu)}}$ is the Fermi distribution. Thus,

$$p_1(t) = \langle d^\dagger d(t)\rangle = e^{-\Gamma t}\langle d^\dagger d(0)\rangle + \int_0^t ds\int_0^t ds' e^{\frac{\Gamma}{2}(s-t+s'-t)}e^{-i\varepsilon(s'-s)}\langle\xi^*(s')\xi(s)\rangle \tag{5.16}$$

$$= e^{-\Gamma t}p_1(0) + \int_0^t ds\int_0^t ds' e^{\frac{\Gamma}{2}(s-t+s'-t)}e^{-i\varepsilon(s'-s)}\sum_q |t_q|^2 e^{-i\omega_q(s-s')}f_\beta(\omega_q) \tag{5.17}$$

$$\approx e^{-\Gamma t}p_1(0) + \frac{\Gamma}{2\pi}e^{-\Gamma t}\int_{-\infty}^{\infty}d\omega\int_0^t ds\int_0^t ds' e^{\frac{\Gamma}{2}(s+s')}e^{-i(\varepsilon-\omega)(s'-s)}f_\beta(\omega) \tag{5.18}$$

$$= e^{-\Gamma t}p_1(0) + \frac{2}{\pi}\int_{-\infty}^{\infty}d\omega\Gamma f_\beta(\omega)\frac{1 - 2e^{-\Gamma t/2}\cos[(\omega-\varepsilon)t] + e^{-\Gamma t}}{\Gamma^2 + 4(\omega-\varepsilon)^2}, \tag{5.19}$$

where we defined $p_1(0) \equiv \langle d^\dagger d(0)\rangle$.

Even though (5.19) cannot be solved analytically in general, one can get numerical results. Before moving to the next subsection, we will plot $p_1(t)$ and compare it with the Markovian case and the refined weak coupling case.

For the Markovian case, $p_1(t)$ will simply be given by the Markovian master equation of one fermion interacting with a fermionic bath. It reads [Pot19]

$$\partial_t p_1 = -\gamma\left[1 - f_\beta(\varepsilon)\right]p_1 + \gamma f_\beta(\varepsilon)p_0 = -\gamma\left[p_1 - f_\beta(\varepsilon)\right], \tag{5.20}$$

where γ is the decaying rate and its solution is

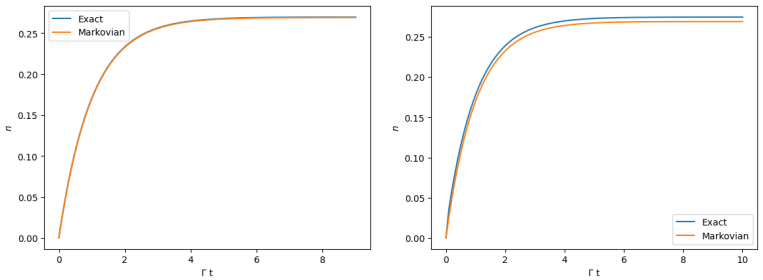
$$p_1(t) = p_1(0)e^{-\gamma t} + f_\beta(\varepsilon)\left(1 - e^{-\gamma t}\right). \tag{5.21}$$

As we used the wide-band limit, this means that $\gamma = 2\pi\Gamma(\varepsilon) \approx 2\pi\frac{\Gamma}{2\pi} = \Gamma$.[4]

[4] 2π appears in the denominator because when computing the Markovian master equation they defined the spectral density as $\Gamma(\omega) = \sum_q |t_q|^2\delta(\omega - \omega_q)$ [Pot19].

We do not compute the refined weak coupling approach in this case. The reason is that not only it is more involving to calculate because the interaction part of the Hamiltonian does not have a tensor structure –as we are dealing with fermions–, but also because the results for the Markovian case are good to differentiate the steady state properties when applying and not applying approximations.[5]

In Fig. (5.1), we can see that the steady state population in the Markovian case does not depend on the coupling between the bath, as previously pointed out in chapter (2), and it only corresponds to the Gibbs state on our subsystem for a given temperature. This is indeed problematic as in reality the steady state depends on Γ (see the exact dynamics in Fig. (5.1).)



(a) Γ=0.01

(b) Γ=0.1

(c) Γ=0.5

Figure 5.1: Plot of the occupation number $n \equiv p_1(t)$ as a function of time for different coupling strengths of the bath. We set $\varepsilon = 1$, $\mu = 0$ and $\beta = 1$ for all of them.

Nevertheless, if one restricts oneself to the weak coupling limit ($\Gamma << \varepsilon$) not only the steady state matches but also the transient dynamics do. It is easy to understand why the reduced Gibbs state is now the correct steady state. In full generality, the steady state of our subsystem is the so-called mean force Gibbs state [TMCA22] and corresponds to

$$\tau_{MF} = \mathrm{Tr}_B(\tau_{SB}) \tag{5.22}$$

where

$$\tau_{SB} \equiv \frac{e^{-\beta H_{tot}}}{Z_{SB}} \tag{5.23}$$

is the Gibbs state for the whole system including the bath, $Z_{SB} = \mathrm{Tr}_{SB}(e^{-\beta H_{tot}})$ is the total partition function, and $H_{tot} = H_S + H_B + H_{SB}$. In the weak coupling limit, as the interaction between the system and the reservoir is weak, one can approximate the mean force Gibbs state by

$$\tau_{MF} \approx \mathrm{Tr}_B\left(\frac{e^{-\beta(H_S+H_B)}}{Z_{SB}}\right) = \frac{e^{-\beta H_S}}{\mathrm{Tr}(e^{-\beta H_S})}, \tag{5.24}$$

[5] It is good to remind the reader that the refined weak coupling approach has the same steady state as the global GKLS master equation.

which is indeed the reduced Gibbs state of the subsystem and corresponds to the steady state given by the GKLS equation.

In the next subsection, we will focus on the precision of measuring the temperature of the system, and for that matter, Quantum Fisher Information will be introduced.

5.1.1 Quantum estimation bounds

In layman's terms, the so-called *classical* Fisher Information (FI) [LMV+17] is a quantity that tells us the amount of information a random variable X, that can be computed in an experiment, carries about some parameter θ that one would like to estimate. In other words, the bigger FI is, the more precision about θ one can get when measuring X. If one then defines $p(x|\theta)$ as the probability of getting an outcome $x \in X$ conditioned on θ, the FI captures the effect of changing infinitesimally θ on $p(x|\theta)$, i.e.

$$\mathcal{F}_c(\theta) := \left\langle \left(\partial_\theta \log p(x|\theta)\right)^2 \right\rangle_x = \sum_x \frac{\left(\partial_\theta p(x|\theta)\right)^2}{p(x|\theta)}, \tag{5.25}$$

where $\langle\cdot\rangle_x$ denotes the expectation value for all the outcomes $x \in X$.

In quantum physics, the probabilities of obtaining some outcome are represented by positive operator-valued measure (POVM) measurements [Hel69, NC02, Wil13]. For our case in hand, we focus on measurements made of a discrete amount of semi-definite positive operators $\mathbf{\Pi} = \{\Pi_l\}$ which can be called POVM-elements. Therefore, following Born's rule [Bor55, Max26] the probability of measuring an outcome l is given by $p_l(\theta) = \mathrm{Tr}(\Pi_l \rho(\theta))$ where $\rho(\theta)$ is the state of our system and that we assume depends on θ in some way. Since we are dealing with probabilities $\sum_l p_l(\theta) = 1$, which translates to operators as $\sum_l \Pi_l = \mathbb{I}$.

Generally, one is interested in sampling n times independently (in other words, n measurements) though. In that case, $\mathbf{x} = (x_1, x_2, \cdots, x_n)$, the total probability factorizes $p(x) = \Pi_{i=1}^n p(x_i)$ as the total Fisher $\mathcal{F}_{c,t}(\theta) = n\mathcal{F}_c(\theta)$. Hence, one could build an estimator $\vartheta(\mathbf{x})$ for the parameter θ. For our results, we will restrict the set of estimators to the subset of unbiased ones, $\langle\vartheta(\mathbf{x})\rangle_{\mathbf{x}} = \theta$. Then we can quantify how the uncertainties when measuring Π affect the statistics through the mean-squared error

$$\delta^2\left(\mathbf{\Pi}; \vartheta(\mathbf{x})\right) = \left\langle \left(\vartheta(\mathbf{x}) - \langle\vartheta(\mathbf{x})\rangle_{\mathbf{x}}\right)^2 \right\rangle_{\mathbf{x}} = \left\langle \left(\vartheta(\mathbf{x}) - \theta\right)^2 \right\rangle_{\mathbf{x}} = \left(\Delta\vartheta(\mathbf{\Pi})\right)^2, \tag{5.26}$$

where of course the results depend on the measurement $\mathbf{\Pi}$.

Importantly, there exists a lower bound on the estimation error that one can obtain when performing n measurements. It is called the Cramér-Rao bound and it holds for any unbiased estimator [GG99, Fri00, Cra16]. It reads

$$\Delta\vartheta(\mathbf{x})(\mathbf{\Pi}) \geq \frac{1}{\sqrt{n\mathcal{F}_c(\mathbf{\Pi}, \theta)}}, \tag{5.27}$$

and in general can be only saturated when $n \to \infty$ (see [MSC19] for more details.) Hence, if we get a smaller error than the bound, we can be sure that there is some quantum-enhanced estimation [CEB+05, BC94, GLM04, GLM11, TA14]. This enhancement is possible thanks to quantum entanglement [HHHH09, HLK+12, Tót12, SML+14].

Since we are interested in thermometry, from now on we will write the temperature T as the parameter to estimate. Let us now introduce a definition that will become meaningful later: the symmetric logarithmic derivative (SLD). The SLD L_T is defined as

$$\frac{\partial\rho_T}{\partial T} = \frac{L_T\rho_T + \rho_T L_T}{2}. \tag{5.28}$$

One should note that as ρ and its derivate are hermitian operators, this implies that L has to be self-adjoint.

Let us note that $\partial_T p(x|\theta) = \mathrm{Tr}(\partial_T \Pi_x \rho_T) = \mathrm{Re}[\mathrm{Tr}(\rho_T \Pi_x L_T)]$ where we used the fact that L is a hermitian operator. Using this at Eq. (5.25) we find

$$\mathcal{F}_c(T) = \sum_x \frac{\left(\partial_T p(x|T)\right)^2}{p(x|T)} = \sum_x \frac{\left(\mathrm{Re}[\mathrm{Tr}(\rho_T \Pi_x L_T)]\right)^2}{\mathrm{Tr}(\rho_T \Pi_x)} \overset{(1)}{\leq} \sum_x \left| \frac{\mathrm{Tr}(\rho_T \Pi_x L_T)}{\sqrt{\mathrm{Tr}(\rho_T \Pi_x)}} \right|^2 \tag{5.29}$$

$$= \sum_x \left| \mathrm{Tr}\left[\frac{\sqrt{\rho_T}\sqrt{\Pi_x}}{\sqrt{\mathrm{Tr}(\rho_T \Pi_x)}} \sqrt{\Pi_x} L_T \sqrt{\rho_T} \right) \right|^2 \overset{(2)}{\leq} \sum_x \mathrm{Tr}\left(\Pi_x L_T \rho_T L_T\right) = \mathrm{Tr}(\rho_T L_T^2). \tag{5.30}$$

A few comments are in order. The inequality (1) can be saturated if $\mathrm{Tr}(\rho_T \Pi_x L_T)$ is real. For (2) we used Cauchy-Schwarz inequality $|\mathrm{Tr}(A^\dagger B)|^2 \leq \mathrm{Tr}(A^\dagger A)\,\mathrm{Tr}(B^\dagger B)$ which holds for every matrix A and B. Finally, for the last equality, we used the normalization constraint, $\sum_x \Pi_x = \mathbb{I}$.

This upper bound to $\mathcal{F}_c(T)$ does not depend on the measurement performed. Therefore, one can define the *quantum* Fisher Information(QFI) as $\mathcal{F}(T) = \max_\Pi \mathcal{F}_c(T)$ where the maximization is over all possible measurements. The optimal measurement –in the sense that gives the best estimation of T– corresponds to projective measurements onto the eigenbasis of L_T [BC94, TA14]. Unfortunately, this is not always feasible in experiments.

Finally, before moving to the results for the thermometry in the resonant level model, let us state the quantum Cramér-Rao bound

$$\Delta\mathcal{T}(\mathbf{x})(\mathbf{\Pi}) \geq \frac{1}{\sqrt{n\mathcal{F}_c(\mathbf{\Pi}, T)}} \geq \frac{1}{\sqrt{n\mathcal{F}(T)}}, \tag{5.31}$$

where $\mathcal{T}$ is the unbiased estimator of the temperature T.

5.1.2 Thermometry in the resonant level model

In the resonant level model, the QFI is given by measuring on the number basis. Indeed, L_T is given by (5.28), so for the model (we omit the label t for the time)

$$\frac{\partial}{\partial T}\rho(T) = \begin{pmatrix} -\dot{p}_1(T) & 0 \\ 0 & \dot{p}_1(T) \end{pmatrix} = \frac{1}{2}\left(L_T \begin{pmatrix} 1-p_1(T) & 0 \\ 0 & p_1(T) \end{pmatrix} + \begin{pmatrix} 1-p_1(T) & 0 \\ 0 & p_1(T) \end{pmatrix} L_T \right), \tag{5.32}$$

where $\frac{\partial p_1}{\partial T} \equiv \dot{p}_1$. Then the expression of L_T that fulfills (5.32) is

$$L_T = \begin{pmatrix} -\frac{\dot{p}_1(T)}{(1-p_1(T)} & 0 \\ 0 & \frac{\dot{p}_1(T)}{p_1(T)} \end{pmatrix} \tag{5.33}$$

and the QFI is

$$\mathcal{F}(T) = \mathrm{Tr}(\rho L_T^2) = \frac{\dot{p}_1^2(T)}{(1-p_1(T))p_1(T)} \tag{5.34}$$

which exactly corresponds to the FI (see Eq. (5.25))

$$\mathcal{F}_c(T) = \frac{\dot{p}_1^2(T)}{p_1(T)} + = \frac{(-\dot{p}_1(T))^2}{(1-p_1(T))} = \frac{\dot{p}_1^2(T)}{(1-p_1(T))p_1(T)}. \tag{5.35}$$

Now we will move to our results obtained performing numerical integration.

Numerical results

In this subsection, we deal with the dynamics of the system through numerical integration of the following[6]

$$p_1(t) = e^{-\Gamma t} p_1(0) + \frac{2}{\pi}\int_{-\infty}^{\infty} d\omega \Gamma f_\beta(\omega) \frac{1 - 2e^{-\Gamma t/2}\cos[(\omega-\varepsilon)t] + e^{-\Gamma t}}{\Gamma^2 + 4(\omega-\varepsilon)^2}, \tag{5.36}$$

and

$$\dot{p}_1(t) = \frac{\Gamma\beta}{2\pi}\int_{-\infty}^{\infty} d\omega \frac{(\omega-\mu)e^{-\Gamma t}\text{sech}^2\left(\frac{1}{2}\beta(\mu-\omega)\right)\left(-2e^{\frac{\Gamma t}{2}}\cos(t(\omega-\varepsilon)) + e^{\Gamma t} + 1\right)}{\Gamma^2 + 4(\omega-\varepsilon)^2}, \tag{5.37}$$

where even though we are getting the derivative with respect to the temperature T, we leave everything as a function of β.

We focused on two quantities: accumulated QFI ($\mathcal{F}_t(T) = \frac{\mathcal{F}(T)}{t}$), and the squared relative error $\frac{\Delta T}{T}$. The former is motivated as follows. Suppose we prepare a state ρ (we call it the probe) which interacts with some bath at temperature T and we let the system evolve for some fixed time t. After the evolution, we measure the probe to estimate the temperature of the system. We reset the system and repeat this procedure $M = \frac{\tau}{t}$ times. We also consider that the time that it takes to prepare the initial probe is not comparable to the duration of the evolution. Then, one can think of using the accumulated QFI (or rate of QFI) as a figure of merit [SPL22, MMRK22].

Regarding the relative error, from Eq. (5.27) we know that (for just one sampling, i.e. $n = 1$)

$$\frac{\Delta T}{T} \geq \frac{1}{\sqrt{\mathcal{F}(T)T^2}}. \tag{5.38}$$

Therefore, we plot $\frac{1}{\mathcal{F}T^2}$ and consider that it is proportional to $\left(\frac{\Delta T}{T}\right)^2$.

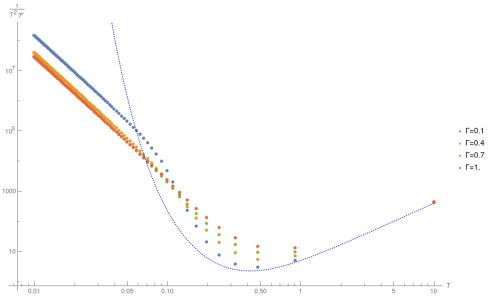
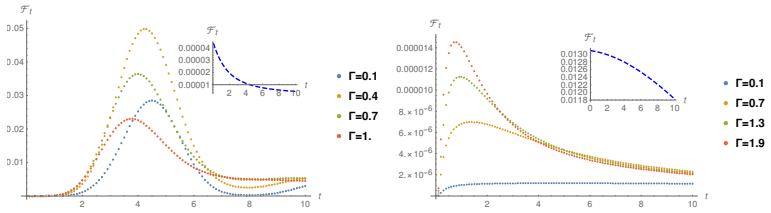


Figure 5.2: Plot of $\frac{1}{\mathcal{F}T^2} \propto (\frac{\Delta T}{T})^2$ (which is the relative error when estimating the temperature T), as a function of T for the steady state. The dashed line corresponds to the Markovian master Equation ($\gamma = 0.1$).

We benchmark our exact results with the Markovian master equation for one fermion introduced in Eq. (5.20). In Fig. (5.2), $\frac{1}{\mathcal{F}T^2}$ the relative error is plotted for the steady state limit, and we can see that as we increase the temperature, the exact results (independently of the coupling Γ) match better with the Markovian approximation. On the other hand, for small temperatures $T << \varepsilon = 1$, the exact results differ from the Markovian ones. This deviation depends on the coupling Γ, albeit in a non-trivial way. If we keep decreasing the

[6] Even though the probability $p_1(t)$ depends on the temperature T, we do not write the dependence explicitly for ease of notation.



(a) T=0.1 (b) T=10

Figure 5.3: Plot of Quantum Fisher Information over time vs time for different Γs. The inset plot corresponds to the case of the Markovian master Equation (with the decaying rate being $\gamma = 0.1$). We set $\varepsilon = 1$, $\mu = 0$, and we start from the ground state of the dot.

temperature, regardless of Γ, the exact results tend to zero Fisher Information (or in other words, infinite error) polynomially and the Markovian ones exponentially.[7]

In addition, in Fig. (5.3) we see $\mathcal{F}_t(T)$ as a function of time t for the exact dynamics for different coupling strengths Γ. We can notice that, especially for $T = 0.1$, in the exact dynamics we get a clear advantage if we wait before performing a measurement. This waiting time depends on the strength of the coupling. On the contrary, in the Markovian regime (inset plots), the accumulated Fisher information monotonically decreases when t increases. Thus, the dynamics of the evolution (in the exact case) help us to get better precision when estimating the temperature of the system, while it is not the case in the Markovian results.

[7] We defer the readers to [RPHP10, GH82, Car99] for a discussion of the validity of Markovian approximation for low temperatures.

Chapter 6

Conclusions

As seen throughout this work, it is difficult to calculate the dynamics of open quantum systems. Thus, it is vitally important to know when one can use a given approximation or another. In this thesis, we focused on three different approaches to dealing with open quantum systems (from the least approximations used to the most): the exact treatment, the refined weak coupling (and in parallel long-times approximation), and the Markovian.

The latter has turned out to be very versatile and easy to apply to different settings, especially the local approach. In particular, in that regime, it has been easy to implement techniques from control theory, and also to add an ancillary system (catalyst), to boost the charging process of a battery. Moreover, in the fermionic system, it has shown good agreement when compared with the exact dynamics for weak coupling with the reservoir.

On the contrary, the second approach (refined weak coupling) is not that easy to be computed in general. However, we have been able to calculate its dynamics and compare it with the global and the local approach –for the battery setting–. For the battery setting, we have seen that it interpolates between the local (for short times) and the global (for long times.) [WMHA21] Hence, it is indeed useful to use the refined weak coupling, especially when one deals with systems made of interacting subsystems that may or may not be connected to different baths. On the contrary, the refined weak coupling approach may not be that interesting when working with single systems as it describes the same steady dynamics as the GKLS master equation.

We are aware that there exist far more approximations that we have not exposed here but the goal of this thesis was never about being an exhaustive list with all the approximations and their pros and cons. The main objective was to take some of the approaches and study them in different scenarios and for different tasks. In addition, we wanted to show the reader the richness and the extension of this field and that all did not end with using the GKLS equation.

We would like to finish enumerating some open problems and improvements that one may try to pursue. From the results presented in chapter 3, more specifically, the ones related to quantum control, one could try to improve them and adapt Krotov's method to use it for the refined weak coupling dynamics. To apply Krotov's algorithm one needs a differential equation. However, for the refined weak coupling evolution, one obtains directly the dynamics. So, it may be cumbersome to get them in terms of a differential equation. One may need to resort to the techniques used in [Riv17]. Certainly, another venue of interest will be to study more complex quadratic systems, such as two batteries (oscillators) interacting with each other.

The results presented in chapter 4 (non-Markovian chapter) for the battery setting could be improved if one came up with a way of diagonalizing the Hamiltonian containing the field term instead of considering it as a perturbation (for global and refined.) This should be doable using the Floquet theory [RH12, San17]. In this way, the field would also appear in the dissipator and the dynamics will be more accurate. Regarding the results for the

Markovian-vacuum approximation, one could try to extend our results to a d-level atom. In addition, the re-normalization scheme that we explained here may be useful to deal with cut-off terms and any kind of divergences that populate open quantum dynamics.

Finally, from the last chapter, one could use the fact that quadratic fermionic systems can be analytically solved and study more difficult systems like the one presented in [MP18]. Doing that, one could again do some benchmarking and probe the quality of the Markovian approximation there. Furthermore, making use of the Jordan-Wigner transformation, one could translate the fermionic systems to spins and again compare the different approaches there. In this case, as spins will have a tensor product structure, one could also compute the refined weak coupling dynamics.

Bibliography

[ABLZ12] Tameem Albash, Sergio Boixo, Daniel A Lidar, and Paolo Zanardi. Quantum adiabatic markovian master equations. *New Journal of Physics*, 14(12):123016, 2012.

[ABN04] A. E Allahverdyan, R Balian, and Th. M Nieuwenhuizen. Maximal work extraction from finite quantum systems. *Europhysics Letters (EPL)*, 67(4):565–571, aug 2004. doi:10.1209/epl/i2004-10101-2.

[AF13] Robert Alicki and Mark Fannes. Entanglement boost for extractable work from ensembles of quantum batteries. *Phys. Rev. E*, 87:042123, Apr 2013. URL: https://link.aps.org/doi/10.1103/PhysRevE.87.042123, doi:10.1103/PhysRevE.87.042123.

[AFH09] Robert Alicki, Mark Fannes, and Michal Horodecki. On thermalization in kitaev's 2d model. *Journal of Physics A: Mathematical and Theoretical*, 42(6):065303, 2009.

[AFM+18] Gian Marcello Andolina, Donato Farina, Andrea Mari, Vittorio Pellegrini, Vittorio Giovannetti, and Marco Polini. Charger-mediated energy transfer in exactly solvable models for quantum batteries. *Phys. Rev. B*, 98:205423, Nov 2018. URL: https://link.aps.org/doi/10.1103/PhysRevB.98.205423, doi:10.1103/PhysRevB.98.205423.

[AKM+19a] Gian Marcello Andolina, Maximilian Keck, Andrea Mari, Michele Campisi, Vittorio Giovannetti, and Marco Polini. Extractable work, the role of correlations, and asymptotic freedom in quantum batteries. *Phys. Rev. Lett.*, 122:047702, Feb 2019. URL: https://link.aps.org/doi/10.1103/PhysRevLett.122.047702, doi:10.1103/PhysRevLett.122.047702.

[AKM+19b] Gian Marcello Andolina, Maximilian Keck, Andrea Mari, Vittorio Giovannetti, and Marco Polini. Quantum versus classical many-body batteries. *Physical Review B*, 99(20):205437, 2019.

[AL07] Robert Alicki and Karl Lendi. *Quantum dynamical semigroups and applications*, volume 717. Springer, 2007.

[AL18] Tameem Albash and Daniel A Lidar. Adiabatic quantum computation. *Reviews of Modern Physics*, 90(1):015002, 2018.

[Ali89] Robert Alicki. Master equations for a damped nonlinear oscillator and the validity of the markovian approximation. *Physical Review A*, 40(7):4077, 1989.

[ARAH22] Borhan Ahmadi, Ricard Ravell Rodríguez, Robert Alicki, and Michał Horodecki. An approximation scheme and non-hermitian re-normalization for description of atom-field system evolution. *arXiv preprint arXiv:2210.10345*, 2022.

[ASFM22] Mohammad B. Arjmandi, Abbas Shokri, Esfandyar Faizi, and Hamidreza Mohammadi. Performance of quantum batteries with correlated and uncorrelated chargers. *Physical Review A*, 106(6), dec 2022. URL: https://doi.org/10.1103%2Fphysreva.106.062609, doi:10.1103/physreva.106.062609.

[BC94] Samuel L Braunstein and Carlton M Caves. Statistical distance and the geometry of quantum states. *Physical Review Letters*, 72(22):3439, 1994.

[BD21] Sourav Bhattacharjee and Amit Dutta. Quantum thermal machines and batteries. *The European Physical Journal B*, 94(12), dec 2021. URL: https://doi.org/10.1140%2Fepjb%2Fs10051-021-00235-3, doi:10.1140/epjb/s10051-021-00235-3.

[BF05] Fabio Benatti and Roberto Floreanini. Open quantum dynamics: complete positivity and entanglement. *International Journal of Modern Physics B*, 19(19):3063–3139, 2005.

[BGGW21] Alexandre Blais, Arne L Grimsmo, SM Girvin, and Andreas Wallraff. Circuit quantum electrodynamics. *Reviews of Modern Physics*, 93(2):025005, 2021.

[BKT97] Allon Bartana, Ronnie Kosloff, and David J Tannor. Laser cooling of internal degrees of freedom. ii. *The Journal of chemical physics*, 106(4):1435–1448, 1997.

[Blo57] Felix Bloch. Generalized theory of relaxation. *Physical Review*, 105(4):1206, 1957.

[Bor55] Max Born. Statistical interpretation of quantum mechanics. *Science*, 122(3172):675–679, 1955.

[BP02] Heinz-Peter Breuer and Francesco Petruccione. *The theory of open quantum systems*. Oxford University Press on Demand, 2002.

[BRH21] Michał Banacki, Ricard Ravell Rodríguez, and Paweł Horodecki. Edge of the set of no-signaling assemblages. *Physical Review A*, 103(5):052434, 2021.

[BVMG15] Felix C Binder, Sai Vinjanampathy, Kavan Modi, and John Goold. Quantacell: powerful charging of quantum batteries. *New Journal of Physics*, 17(7):075015, jul 2015. doi:10.1088/1367-2630/17/7/075015.

[CA21] JD Cresser and J Anders. Weak and ultrastrong coupling limits of the quantum mean force gibbs state. *Physical Review Letters*, 127(25):250601, 2021.

[Car99] Howard Carmichael. *Statistical methods in quantum optics 1: master equations and Fokker-Planck equations*, volume 1. Springer Science & Business Media, 1999.

[CCDWGPH20] Francesco Caravelli, Ghislaine Coulter-De Wit, Luis Pedro García-Pintos, and Alioscia Hamma. Random quantum batteries. *Phys. Rev. Research*, 2:023095, Apr 2020. URL: https://link.aps.org/doi/10.1103/PhysRevResearch.2.023095, doi:10.1103/PhysRevResearch.2.023095.

[CEB+05] Paola Cappellaro, Joseph Emerson, Nicolas Boulant, Chandrasekhar Ramanathan, Seth Lloyd, and David G Cory. Entanglement assisted metrology. *Physical review letters*, 94(2):020502, 2005.

[CLAFLO+23] A Consuelo-Leal, AG Araujo-Ferreira, E Lucas-Oliveira, TJ Bonagamba, and R Auccaise. Nmr relaxation by redfield equation in a spin system i= 7/2. *Journal of Magnetic Resonance*, page 107403, 2023.

[CP17] Dariusz Chruściński and Saverio Pascazio. A brief history of the gkls equation. *arXiv preprint arXiv:1710.05993*, 2017.

[CPB+17] Francesco Campaioli, Felix A. Pollock, Felix C. Binder, Lucas Céleri, John Goold, Sai Vinjanampathy, and Kavan Modi. Enhancing the charging power of quantum batteries. *Phys. Rev. Lett.*, 118:150601, Apr 2017. URL: `https://link.aps.org/doi/10.1103/PhysRevLett.118.150601`, `doi:10.1103/PhysRevLett.118.150601`.

[Cra16] H Cramer. Mathematical methods of statistics (pms-9) volume 9 princeton university press. *Princeton, NJ, USA*, 2016.

[Dav74] E Brian Davies. Markovian master equations. *Communications in mathematical Physics*, 39:91–110, 1974.

[Dav76] E Brian Davies. Markovian master equations. ii. *Mathematische Annalen*, 219:147–158, 1976.

[DCLH+18] Gabriele De Chiara, Gabriel Landi, Adam Hewgill, Brendan Reid, Alessandro Ferraro, Augusto J Roncaglia, and Mauro Antezza. Reconciliation of quantum local master equations with thermodynamics. *New Journal of Physics*, 20(11):113024, 2018.

[DRC17] Christian L Degen, Friedemann Reinhard, and Paola Cappellaro. Quantum sensing. *Reviews of modern physics*, 89(3):035002, 2017.

[DTA+18] Amro Dodin, Timur Tscherbul, Robert Alicki, Amar Vutha, and Paul Brumer. Secular versus nonsecular redfield dynamics and fano coherences in incoherent excitation: An experimental proposal. *Physical Review A*, 97(1):013421, 2018.

[FAM+19] Donato Farina, Gian Marcello Andolina, Andrea Mari, Marco Polini, and Vittorio Giovannetti. Charger-mediated energy transfer for quantum batteries: An open-system approach. *Physical Review B*, 99(3):035421, 2019.

[FC11] Chris H Fleming and Nick I Cummings. Accuracy of perturbative master equations. *Physical Review E*, 83(3):031117, 2011.

[FCA+18a] Dario Ferraro, Michele Campisi, Gian Marcello Andolina, Vittorio Pellegrini, and Marco Polini. High-power collective charging of a solid-state quantum battery. *Physical Review Letters*, 120(11), mar 2018. URL: `https://doi.org/10.1103%2Fphysrevlett.120.117702`, `doi:10.1103/physrevlett.120.117702`.

[FCA+18b] Dario Ferraro, Michele Campisi, Gian Marcello Andolina, Vittorio Pellegrini, and Marco Polini. High-power collective charging of a solid-state quantum battery. *Physical review letters*, 120(11):117702, 2018.

[FLB13] Nicolai Friis, Antony R Lee, and David Edward Bruschi. Fermionic-mode entanglement in quantum information. *Physical Review A*, 87(2):022338, 2013.

[Fri48] K. O. Friedrichs. On the perturbation of continuous spectra. *Communications on Pure and Applied Mathematics*, 1(4):361–406, 1948.

[Fri77] Alberto Frigerio. Quantum dynamical semigroups and approach to equilibrium. *Letters in Mathematical Physics*, 2:79–87, 1977.

[Fri78] Alberto Frigerio. Stationary states of quantum dynamical semigroups. *Communications in Mathematical Physics*, 63(3):269–276, 1978.

[Fri00] B Roy Frieden. Physics from fisher information: a unification, 2000.

[GBGE+19] Michael Goerz, Daniel Basilewitsch, Fernando Gago-Encinas, Matthias G Krauss, Karl P Horn, Daniel M Reich, and Christiane Koch. Krotov: A python implementation of krotov's method for quantum optimal control. *SciPost physics*, 7(6):080, 2019.

[GCCB20] Stefano Gherardini, Francesco Campaioli, Filippo Caruso, and Felix C. Binder. Stabilizing open quantum batteries by sequential measurements. *Phys. Rev. Research*, 2:013095, Jan 2020. URL: https://link.aps.org/doi/10.1103/PhysRevResearch.2.013095, doi:10.1103/PhysRevResearch.2.013095.

[GCN+17] J Onam González, Luis A Correa, Giorgio Nocerino, José P Palao, Daniel Alonso, and Gerardo Adesso. Testing the validity of the 'local'and 'global'gkls master equations on an exactly solvable model. *Open Systems & Information Dynamics*, 24(04):1740010, 2017.

[GG99] Neil A Gershenfeld and Neil Gershenfeld. *The nature of mathematical modeling*. Cambridge university press, 1999.

[GH82] Michel Gross and Serge Haroche. Superradiance: An essay on the theory of collective spontaneous emission. *Physics reports*, 93(5):301–396, 1982.

[GKS76] Vittorio Gorini, Andrzej Kossakowski, and Ennackal Chandy George Sudarshan. Completely positive dynamical semigroups of n-level systems. *Journal of Mathematical Physics*, 17(5):821–825, 1976.

[GLM04] Vittorio Giovannetti, Seth Lloyd, and Lorenzo Maccone. Quantum-enhanced measurements: beating the standard quantum limit. *Science*, 306(5700):1330–1336, 2004.

[GLM11] Vittorio Giovannetti, Seth Lloyd, and Lorenzo Maccone. Advances in quantum metrology. *Nature photonics*, 5(4):222–229, 2011.

[GN99] Pierre Gaspard and Masataka Nagaoka. Slippage of initial conditions for the redfield master equation. *The Journal of chemical physics*, 111(13):5668–5675, 1999.

[Goe19] dec 2019. URL: https://doi.org/10.21468%2Fscipostphys.7.6.080, doi:10.21468/scipostphys.7.6.080.

[GRK14] Michael H Goerz, Daniel M Reich, and Christiane P Koch. Optimal control theory for a unitary operation under dissipative evolution. *New Journal of Physics*, 16(5):055012, 2014.

[GT07] Nicolas Gisin and Rob Thew. Quantum communication. *Nature photonics*, 1(3):165–171, 2007.

[GZZ04] Crispin Gardiner, Peter Zoller, and Peter Zoller. *Quantum noise: a handbook of Markovian and non-Markovian quantum stochastic methods with applications to quantum optics*. Springer Science & Business Media, 2004.

[Hel69] Carl W Helstrom. Quantum detection and estimation theory. *Journal of Statistical Physics*, 1:231–252, 1969.

[HHHH09] Ryszard Horodecki, Paweł Horodecki, Michał Horodecki, and Karol Horodecki. Quantum entanglement. *Reviews of modern physics*, 81(2):865, 2009.

[HLK+12] Philipp Hyllus, Wiesław Laskowski, Roland Krischek, Christian Schwemmer, Witlef Wieczorek, Harald Weinfurter, Luca Pezzé, and Augusto Smerzi. Fisher information and multiparticle entanglement. *Physical Review A*, 85(2):022321, 2012.

[HPLHA13] Karen V. Hovhannisyan, Martí Perarnau-Llobet, Marcus Huber, and Antonio Acín. Entanglement generation is not necessary for optimal work extraction. *Phys. Rev. Lett.*, 111:240401, Dec 2013. URL: `https://link.aps.org/doi/10.1103/PhysRevLett.111.240401`, `doi:10.1103/PhysRevLett.111.240401`.

[HPLM+17] Patrick P Hofer, Martí Perarnau-Llobet, L David M Miranda, Géraldine Haack, Ralph Silva, Jonatan Bohr Brask, and Nicolas Brunner. Markovian master equations for quantum thermal machines: local versus global approach. *New Journal of Physics*, 19(12):123037, 2017.

[JFSR+20] Sergi Julià-Farré, Tymoteusz Salamon, Arnau Riera, Manabendra N Bera, and Maciej Lewenstein. Bounds on the capacity and power of quantum batteries. *Physical Review Research*, 2(2):023113, 2020.

[JIP+15] Jan Jeske, David J Ing, Martin B Plenio, Susana F Huelga, and Jared H Cole. Bloch-redfield equations for modeling light-harvesting complexes. *The Journal of chemical physics*, 142(6):064104, 2015.

[KCK08] Stanislaw Kryszewski and Justyna Czechowska-Kryszk. Master equation-tutorial approach. *arXiv preprint arXiv:0801.1757*, 2008.

[KF83] Vadim F Krotov and IN Feldman. An iterative method for solving optimal-control problems. *Engineering cybernetics*, 21(2):123–130, 1983.

[KK99] AI Konnov and Vadim F Krotov. On global methods of successive improvement of controlled processes. *Automation and Remote Control*, 60(10):1427–1436, 1999.

[Kos72] Andrzej Kossakowski. On quantum statistical mechanics of non-hamiltonian systems. *Reports on Mathematical Physics*, 3(4):247–274, 1972.

[KQC+17] Dvir Kafri, Chris Quintana, Yu Chen, Alireza Shabani, John M Martinis, and Hartmut Neven. Tunable inductive coupling of superconducting qubits in the strongly nonlinear regime. *Physical Review A*, 95(5):052333, 2017.

[kro] Krotov python package. `https://qucontrol.github.io/krotov/v1.2.1/`. Accessed: 2010-09-30.

[Kro88] Vadim F Krotov. A technique of global bounds in optimal control theory. *Control and Cybernetics*, 17(3):2–3, 1988.

[Kro95] Vadim Krotov. *Global methods in optimal control theory*, volume 195. CRC Press, 1995.

[Kub57] Ryogo Kubo. Statistical-mechanical theory of irreversible processes. i. general theory and simple applications to magnetic and conduction problems. *Journal of the Physical Society of Japan*, 12(6):570–586, 1957.

[LBP14] Elsi-Mari Laine, Heinz-Peter Breuer, and Jyrki Piilo. Nonlocal memory effects allow perfect teleportation with mixed states. *Scientific reports*, 4(1):1–5, 2014.

[LBS21a] Patryk Lipka-Bartosik and Paul Skrzypczyk. All states are universal catalysts in quantum thermodynamics. *Physical Review X*, 11(1):011061, 2021.

[LBS21b] Patryk Lipka-Bartosik and Paul Skrzypczyk. Catalytic quantum teleportation. *Physical Review Letters*, 127(8):080502, 2021.

[LCD+87] Anthony J Leggett, SDAFMGA Chakravarty, Alan T Dorsey, Matthew PA Fisher, Anupam Garg, and Wilhelm Zwerger. Dynamics of the dissipative two-state system. *Reviews of Modern Physics*, 59(1):1, 1987.

[Lee54] T. D. Lee. Some special examples in renormalizable field theory. *Phys. Rev.*, 95:1329–1334, Sep 1954.

[Lid19] Daniel A Lidar. Lecture notes on the theory of open quantum systems. *arXiv preprint arXiv:1902.00967*, 2019.

[Lin76] Goran Lindblad. On the generators of quantum dynamical semigroups. *Communications in Mathematical Physics*, 48:119–130, 1976.

[LK14] Amikam Levy and Ronnie Kosloff. The local approach to quantum transport may violate the second law of thermodynamics. *Europhysics Letters*, 107(2):20004, 2014.

[LLM+18] Thao P. Le, Jesper Levinsen, Kavan Modi, Meera M. Parish, and Felix A. Pollock. Spin-chain model of a many-body quantum battery. *Phys. Rev. A*, 97:022106, Feb 2018. URL: `https://link.aps.org/doi/10.1103/PhysRevA.97.022106`, `doi:10.1103/PhysRevA.97.022106`.

[Llo00] Seth Lloyd. Coherent quantum feedback. *Phys. Rev. A*, 62:022108, Jul 2000. URL: `https://link.aps.org/doi/10.1103/PhysRevA.62.022108`, `doi:10.1103/PhysRevA.62.022108`.

[LMV+17] Alexander Ly, Maarten Marsman, Josine Verhagen, Raoul PPP Grasman, and Eric-Jan Wagenmakers. A tutorial on fisher information. *Journal of Mathematical Psychology*, 80:40–55, 2017.

[Lon16] Davide Lonigro. *Quantum decay and Friedrichs-Lee model*. PhD thesis, University of Bari, 2016.

[LP00] R Loudon and Francesco Petruccione. *The Quantum Theory of Light*. Oxford University Press, 2000.

[ŁWS+22] Marcin Łobejko, Marek Winczewski, Gerardo Suárez, Robert Alicki, and Michał Horodecki. Towards reconciliation of completely positive open system dynamics with the equilibration postulate. *arXiv preprint arXiv:2204.00643*, 2022.

[MABL13] Christian Majenz, Tameem Albash, Heinz-Peter Breuer, and Daniel A Lidar. Coarse graining can beat the rotating-wave approximation in quantum markovian master equations. *Physical Review A*, 88(1):012103, 2013.

[Man20] Daniel Manzano. A short introduction to the lindblad master equation. *Aip Advances*, 10(2):025106, 2020.

[mar]

[Max26] Born Max. Zur quantenmechanik der sto vorg nge. *Zeitschrift f r Physik*, 37(12):863–867, 1926.

[Mer07] N David Mermin. *Quantum computer science: an introduction*. Cambridge University Press, 2007.

[MGP21] Mark T. Mitchison, John Goold, and Javier Prior. Charging a quantum battery with linear feedback control. *Quantum*, 5:500, jul 2021. URL: `https://doi.org/10.22331%2Fq-2021-07-13-500`, `doi:10.22331/q-2021-07-13-500`.

[Mit19] Mark T. Mitchison. Quantum thermal absorption machines: refrigerators, engines and clocks. *Contemporary Physics*, 60(2):164–187, 2019. `arXiv:https://doi.org/10.1080/00107514.2019.1631555`, `doi:10.1080/00107514.2019.1631555`.

[MMRK22] Safoura S Mirkhalaf, Mohammad Mehboudi, and Saleh Rahimi-Keshari. Operational significance of nonclassicality in nonequilibrium gaussian quantum thermometry. *arXiv preprint arXiv:2207.10742*, 2022.

[MP18] Mark T Mitchison and Martin B Plenio. Non-additive dissipation in open quantum networks out of equilibrium. *New Journal of Physics*, 20(3):033005, 2018.

[MS59] Paul C Martin and Julian Schwinger. Theory of many-particle systems. i. *Physical Review*, 115(6):1342, 1959.

[MSC19] Mohammad Mehboudi, Anna Sanpera, and Luis A Correa. Thermometry in the quantum regime: recent theoretical progress. *Journal of Physics A: Mathematical and Theoretical*, 52(30):303001, 2019.

[MW95] Leonard Mandel and Emil Wolf. *Optical coherence and quantum optics*. Cambridge university press, 1995.

[NB22] Carlos Navarrete-Benlloch. Introduction to quantum optics. *arXiv preprint arXiv:2203.13206*, 2022.

[NC02] Michael A Nielsen and Isaac Chuang. Quantum computation and quantum information, 2002.

[Nor97] James R Norris. Markov chains. cambridge series in statistical and probabilistic mathematics. *Cambridge: Cambridge Univ. Press. Reprint of*, 1997.

[PGM+20] Archak Purkayastha, Giacomo Guarnieri, Mark T Mitchison, Radim Filip, and John Goold. Tunable phonon-induced steady-state coherence in a double-quantum-dot charge qubit. *npj Quantum Information*, 6(1):27, 2020.

[Pot19] Patrick P Potts. Introduction to quantum thermodynamics (lecture notes). *arXiv preprint arXiv:1906.07439*, 2019.

[QM20] James Q. Quach and William J. Munro. Using dark states to charge and stabilize open quantum batteries. *Phys. Rev. Applied*, 14:024092, Aug 2020. URL: `https://link.aps.org/doi/10.1103/PhysRevApplied.14.024092`, `doi:10.1103/PhysRevApplied.14.024092`.

[RAS+22] RR Rodriguez, B Ahmadi, G Suarez, P Mazurek, S Barzanjeh, and P Horodecki. Optimal quantum control of charging quantum batteries. *arXiv preprint arXiv:2207.00094*, 2022.

[RBRRH22] Ravishankar Ramanathan, Michał Banacki, Ricard Ravell Rodríguez, and Paweł Horodecki. Single trusted qubit is necessary and sufficient for quantum realization of extremal no-signaling correlations. *npj Quantum Information*, 8(1):119, 2022.

[Red57] Alfred G Redfield. On the theory of relaxation processes. *IBM Journal of Research and Development*, 1(1):19–31, 1957.

[RH12] Angel Rivas and Susana F Huelga. *Open quantum systems*, volume 10. Springer, 2012.

[RHP14] Ángel Rivas, Susana F Huelga, and Martin B Plenio. Quantum non-markovianity: characterization, quantification and detection. *Reports on Progress in Physics*, 77(9):094001, 2014.

[Riv17] Ángel Rivas. Refined weak-coupling limit: Coherence, entanglement, and non-markovianity. *Physical Review A*, 95(4):042104, 2017.

[RKK15] Daniel M Reich, Nadav Katz, and Christiane P Koch. Exploiting non-markovianity for quantum control. *Scientific reports*, 5(1):1–7, 2015.

[RMPLH] Ricard Ravell Rodríguez, Mohammed Mehboudi, Martí Perarnau-Llobet, and Michał Horodecki. *In preparation.*

[RNK12] Daniel M Reich, Mamadou Ndong, and Christiane P Koch. Monotonically convergent optimization in quantum control using krotov's method. *The Journal of chemical physics*, 136(10):104103, 2012.

[RPHP10] Angel Rivas, A Douglas K Plato, Susana F Huelga, and Martin B Plenio. Markovian master equations: a critical study. *New Journal of Physics*, 12(11):113032, 2010.

[RRAM+22] Ricard Ravell Rodriguez, Borhan Ahmadi, Pawel Mazurek, Shabir Barzanjeh, Robert Alicki, and Pawel Horodecki. Catalysis in charging quantum batteries. *arXiv e-prints*, pages arXiv–2205, 2022.

[RS+75] Michael Reed, Barry Simon, et al. *Methods of Modern Mathematical Physics II*, volume 2. Academic Press, San Diego, 1975.

[RS+80] Michael Reed, Barry Simon, et al. *Methods of Modern Mathematical Physics I: Functional analysis*, volume 1. Academic Press, San Diego, 1980.

[RSH] Ricard Ravell Rodríguez, Gerardo Suárez, and Michał Horodecki. *In preparation.*

[SAC21] Stefano Scali, Janet Anders, and Luis A Correa. Local master equations bypass the secular approximation. *Quantum*, 5:451, 2021.

[Sak06] Jun John Sakurai. *Advanced quantum mechanics*. Pearson Education India, 2006.

[San17] Giuseppe E Santoro. Introduction to floquet, 2017.

[SB08] Gernot Schaller and Tobias Brandes. Preservation of positivity by dynamical coarse graining. *Physical Review A*, 78(2):022106, 2008.

[SÇCZ19] Alan C Santos, Barış Çakmak, Steve Campbell, and Nikolaj T Zinner. Stable adiabatic quantum batteries. *Physical Review E*, 100(3):032107, 2019.

[Sch14] Gernot Schaller. *Open quantum systems far from equilibrium*, volume 881. Springer, 2014.

[Ser17] A. Serafini. *Quantum Continuous Variables: A Primer of Theoretical Methods*. CRC Press, Boca Raton, FL, 2017.

[Sha12] Ramamurti Shankar. *Principles of quantum mechanics*. Springer Science & Business Media, 2012.

[SHW] Gerardo Suárez, Michał Horodecki, and Marek Winczewski. *In preparation*.

[SKT93] József Somlói, Vladimir A Kazakov, and David J Tannor. Controlled dissociation of i2 via optical transitions between the x and b electronic states. *Chemical physics*, 172(1):85–98, 1993.

[SML+14] Helmut Strobel, Wolfgang Muessel, Daniel Linnemann, Tilman Zibold, David B Hume, Luca Pezzè, Augusto Smerzi, and Markus K Oberthaler. Fisher information and entanglement of non-gaussian spin states. *Science*, 345(6195):424–427, 2014.

[Sni64] Robert F Snider. Perturbation variation methods for a quantum boltzmann equation. *Journal of Mathematical Physics*, 5(11):1580–1587, 1964.

[SPL22] Pavel Sekatski and Martí Perarnau-Llobet. Optimal nonequilibrium thermometry in Markovian environments. *Quantum*, 6:869, December 2022. doi:10.22331/q-2022-12-07-869.

[Spo77] Herbert Spohn. An algebraic condition for the approach to equilibrium of an open n-level system. *Letters in Mathematical Physics*, 2:33–38, 1977.

[ST02] Shlomo E Sklarz and David J Tannor. Loading a bose-einstein condensate onto an optical lattice: An application of optimal control theory to the nonlinear schrödinger equation. *Physical Review A*, 66(5):053619, 2002.

[TA14] Géza Tóth and Iagoba Apellaniz. Quantum metrology from a quantum information science perspective. *Journal of Physics A: Mathematical and Theoretical*, 47(42):424006, 2014.

[TDKP22] Devashish Tupkary, Abhishek Dhar, Manas Kulkarni, and Archak Purkayastha. Fundamental limitations in lindblad descriptions of systems weakly coupled to baths. *Physical Review A*, 105(3):032208, 2022.

[TKO92] David J Tannor, Vladimir Kazakov, and Vladimir Orlov. Control of photochemical branching: Novel procedures for finding optimal pulses and global upper bounds. *Time-dependent quantum molecular dynamics*, pages 347–360, 1992.

[TMCA22] AS Trushechkin, M Merkli, JD Cresser, and J Anders. Open quantum system dynamics and the mean force gibbs state. *AVS Quantum Science*, 4(1):012301, 2022.

[Tót12] Géza Tóth. Multipartite entanglement and high-precision metrology. *Physical Review A*, 85(2):022322, 2012.

[TR08] David Taj and Fausto Rossi. Completely positive markovian quantum dynamics in the weak-coupling limit. *Physical Review A*, 78(5):052113, 2008.

[Tur07] Sadi Turgut. Catalytic transformations for bipartite pure states. *Journal of Physics A: Mathematical and Theoretical*, 40(40):12185, 2007.

[TWH12] Juzar Thingna, Jian-Sheng Wang, and Peter Hänggi. Generalized gibbs state with modified redfield solution: Exact agreement up to second order. *The Journal of chemical physics*, 136(19):194110, 2012.

[UTC+21] Rishabh Upadhyay, George Thomas, Yu-Cheng Chang, Dmitry S Golubev, Andrew Guthrie, Azat Gubaydullin, Joonas T Peltonen, and Jukka P Pekola. Robust strong-coupling architecture in circuit quantum electrodynamics. *Physical Review Applied*, 16(4):044045, 2021.

[WG07] J Werschnik and E K U Gross. Quantum optimal control theory. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 40(18):R175–R211, sep 2007. doi:10.1088/0953-4075/40/18/r01.

[WH19] Mischa P. Woods and Michał Horodecki. The resource theoretic paradigm of quantum thermodynamics with control, 2019. URL: https://arxiv.org/abs/1912.05562, doi:10.48550/ARXIV.1912.05562.

[Whi08] Robert S Whitney. Staying positive: going beyond lindblad with perturbative master equations. *Journal of Physics A: Mathematical and Theoretical*, 41(17):175304, 2008.

[Whi18] Robert S Whitney. Non-markovian quantum thermodynamics: Laws and fluctuation theorems. *Physical Review B*, 98(8):085415, 2018.

[Wil67] Ralph M Wilcox. Exponential operators and parameter differentiation in quantum physics. *Journal of Mathematical Physics*, 8(4):962–982, 1967.

[Wil13] Mark M Wilde. *Quantum information theory*. Cambridge University Press, 2013.

[WMHA21] Marek Winczewski, Antonio Mandarino, Michał Horodecki, and Robert Alicki. Bypassing the intermediate times dilemma for open quantum system. *arXiv preprint arXiv:2106.05776*, 2021.

[ZDZ22] Fang Zhao, Fu-Quan Dou, and Qing Zhao. Charging performance of the su-schrieffer-heeger quantum battery. *Phys. Rev. Research*, 4:013172, Mar 2022. URL: https://link.aps.org/doi/10.1103/PhysRevResearch.4.013172, doi:10.1103/PhysRevResearch.4.013172.

[ZR98] Wusheng Zhu and Herschel Rabitz. A rapid monotonically convergent iteration algorithm for quantum optimal control over the expectation value of a positive definite operator. *The Journal of Chemical Physics*, 109(2):385–391, 1998. arXiv:https://doi.org/10.1063/1.476575, doi:10.1063/1.476575.