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Electron Conduction through Coupled Quantum Thermocouples

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Abstract

Quantum thermodynamics is an area of research with important practical applications as well as fundamental ones. On the practical side, quantum thermal machines which may extract work from nanoscopic differences in temperature may have an improved efficiency due to quantum effects. A particular example of these machines are thermoelectrics, which are composed of a thermocouple joining two reservoirs of different temperature and chemical potential.

Quantum effects can arise from intrinsic vibrational degrees of freedom found in the molecular junction. Other effects may come from a coupling between thermocouples. The later case is here studied. We will investigate the electronic transport going through two ideal electronic sites coupled with each other.

This will be done by investigating the steady-state effects, and by considering the open quantum dynamics of the electronic sites only.

To do this we derive the effective Markovian equations for the dynamics of the system. We then will access the first cumulants of the probability distribution function of the number of electrons through a thermocouple by establishing a counting process and studying its steady-state dynamics.

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I Introduction

I.1 Motivations

Thermodynamics was — and still is — one of the great achievements of the physical sciences in the 19th century: it abled the harnessing of heat, from which work could be extracted. This science ignited the industrial revolution and thus permitted the scientific revolution of the beginning of the 20th century, with the advent of relativity and quantum mechanics. It cannot be doubted that the history of human progress would have been greatly affected, for the worst, without Carnot, Claudius, and others.

Yet progress is far from over, in both a scientific sense, and a human one: indeed while the macroscopic laws of heat are well known, its nanoscopic counter-parts aren't. Quantum phenomena could enable greatly improved ways to store heat and extract work from it, this would be of great benefit for society, in particular for its poorest members in developing and underdeveloped economies who are in dire need to extract electricity cheaply and effectively.

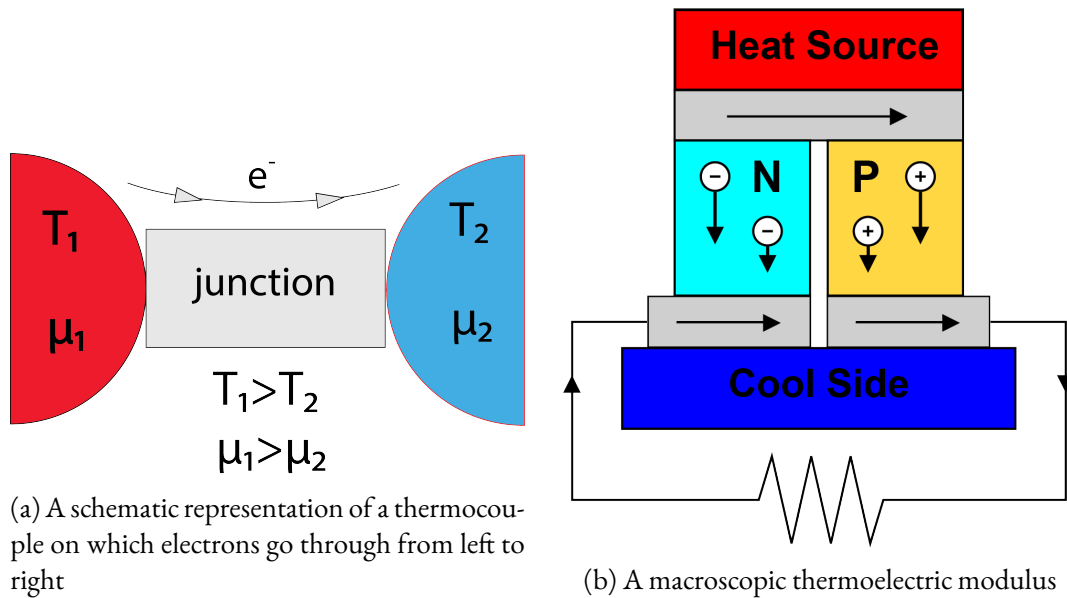
Other applications might be nanoscale local refrigerators, thermal transistors, nanoscale radiation detectors, and thermal logic gates[1]. Nanoscopic refrigerators might also provide an effective way to cool down electrons in solid-state physics[2, 3]. However, there is also interest on the fundamental physics level, since simple quantum machines are prime ground on which the interplay between quantum fluctuations and thermal fluctuations play an important role[4].

We will focus here on quantum thermoelectrics, and the production of current from heat and chemical potential differences.

I.2 Existing litterature

A thermoelectic device is an engine which converts differences of heat into work, or vice-versa. This is done by connecting different reservoirs, at different temperatures and chemical potential together with a thermocouple.

A thermocouple in its simplest form is nothing else than a junction connecting two macroscopic reservoirs having different temperatures and chemical potentials. Then electrons can go from one reservoir to the other through the junction. If the junction is smaller than the electron relaxation length, then quantum effects become important[5], in particular, we can have the entire system be quantum mechanical, including the



reservoirs. A very simple ideal toy model is to take the junction to be a single electronic site, in this case the study is quite simple due to the presence of very few degrees of freedom.

However, real world thermoelectrics have a lot more going on: they have internal degrees of freedom as well as more complicated couplings with the environment. Thus a lot of effort was made to understand these effects on the energy production. As such a few examples are point contact quantum dots[6], metallic wires[7], carbon nanotubes[8], etc.

1.3 Problem studied

It would seldom be the case in practical applications that a single thermoelectric would be placed somewhere and then be used in isolation. On the contrary, there would be quite a large number of them so that the current produced would not be negligible.

We will study two thermoelectrics with a mechanical coupling. We will study if it assists or not the electronic transport.

1.4 Tools used

The main mathematical tools that will be used to study the system are:

1. We will study the open system dynamics of the junctions and the harmonic oscillator. We will thus use the Lindblad quantum master equation which takes dissipation into account.

2. We will assume the harmonic oscillator to have very fast dynamics so that it equilibrates rapidly. We will thus adiabatically eliminate its degrees of freedom.
3. To study the flux of electrons through a junction we will use tools from the thermodynamics of trajectories and large deviation theory to extract the relevant functions describing the number of electrons going through a given junction in a given time interval.

2 Study of the system

2.1 Background Theory

A closed quantum system evolves unitarily according to the following equation:

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] \quad (1)$$

With ρ the density matrix, and H the system's Hamiltonian. If H is of the form $H_0 + H_1 + H_{\text{int}}$, with $H_0 = \epsilon_0 \hat{a}_0^\dagger \hat{a}_0$ the Hamiltonian of a small subsystem, $H_1 = \sum_i \epsilon_{1,i} \hat{a}_{1,i}^\dagger \hat{a}_{1,i}$ is the Hamiltonian of a macroscopic reservoir and $H_{\text{int}} = \sum_i \gamma_i (\hat{a}_0^\dagger \hat{a}_{1,i} + \hat{a}_0 \hat{a}_{1,i}^\dagger)$ the coupling between the reservoir and the small subsystem, we can try to describe the evolution of the subsystem only. To do this we can trace over the bath degrees of freedom, and we obtain the dynamics of an open quantum system. The resulting evolution equation is known as the Lindblad quantum master equation[9, 10]:

$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[H, \rho] + \mathcal{L} \rho \quad (2)$$

where \mathcal{L} is the Lindbladian superoperator, and is of the form

$$\mathcal{L} \bullet = \sum_i \gamma_i \mathcal{D}[\hat{L}_i] \bullet = \sum_i \gamma_i \left(2 \hat{L}_i \bullet \hat{L}_i^\dagger - \{ \hat{L}_i^\dagger \hat{L}_i, \bullet \} \right) \quad (3)$$

where i labels a channel through which our system is in contact with the environment, the \hat{L}_i are known as Lindblad operators, the $\mathcal{D}[\hat{L}_i] \bullet$ are known as dissipators, they describe the effect of dissipation on the system. An important remark is that there is no imaginary unit in front of the Lindbladian superoperator.

Going to the Heisenberg picture, the dissipative time evolution of an operator is given by:

$$\dot{\hat{O}}_H = i[H, \hat{O}] + \mathcal{L}^{(H)} \hat{O}_H \quad (4)$$

$$\mathcal{L}^{(H)} \hat{O}_H = \sum_i \gamma_i \mathcal{D}^{(H)}[\hat{L}_i] \hat{O}_H = \sum_i \gamma_i \left(2\hat{L}_i^\dagger \hat{O}_H \hat{L}_i - \{ \hat{L}_i^\dagger \hat{L}_i, \hat{O}_H \} \right) \quad (5)$$

The Lindbladian has the following important properties:

1. It does not preserve unitarity
2. It is linear
3. It is trace preserving, that is, $\text{Tr} \{ \mathcal{L} \rho \} = 0$ and thus for all t we have: $\text{Tr} \{ \rho(t) \} = 1$
4. It preserves the hermiticity of ρ
5. It is a completely positive mapping, that is, the eigenvalues of ρ do not change of sign

The first three properties can be easily checked, the fourth and fifth must be the case since the eigenvalues of ρ must be real and positive.

2.2 The System Studied

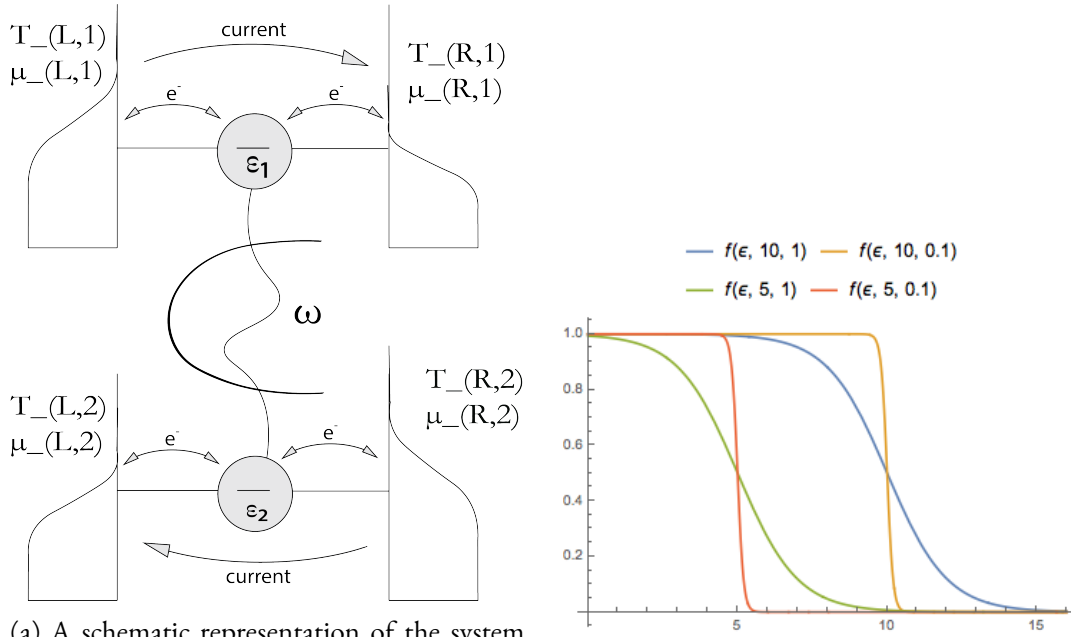
The system consists of two thermoelectrics and an harmonic oscillator coupled to both of them and to a bosonic bath which will take into account the natural dissipation of the oscillator. A thermoelectric consists of a junction, here a single electronic site of energy ϵ_i , joining two macroscopic fermionic baths.

The full Hamiltonian is thus:

$$H_{full} = H_1 + H_2 + H_{\text{H.O.}} + H_{1,2,\text{H.O.}}^c + H_b + H_{\text{H.O.,}b}^c + \sum_{l,s} (H_{l,s} + H_{l,s}^c) \quad (6)$$

where the labels l and s denote the bath (left or right) and the electronic site respectively. And with:

$$H_1 = \epsilon_1 \hat{s}_1^\dagger \hat{s}_1 \quad (7)$$



(a) A schematic representation of the system studied, with the electronic sites of energy ϵ_i and the electronic reservoirs represented by the fermi distribution for different couples $\{T, \mu\}$

(b) the Fermi distribution $f(\epsilon, \mu, T)$ plotted function of the energy ϵ , and with fixed chemical potentials μ , and temperature T

$$H_2 = \epsilon_2 \hat{s}_2^\dagger \hat{s}_2 \quad (8)$$

$$H_{\text{H.O.}} = \omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \quad (9)$$

$$H_{1,2,\text{H.O.}}^c = (\Omega_0 + \Omega_1 \hat{x}) \left(\hat{s}_1^\dagger \hat{s}_1 - \hat{s}_2^\dagger \hat{s}_1 \right) \quad (10)$$

$$H_b = \sum_i \epsilon_i \hat{b}_i^\dagger \hat{b}_i \quad (11)$$

$$H_{\text{H.O.},b}^c = \sqrt{\frac{\gamma}{2}} \sum_i \left(\hat{b}_i^\dagger \hat{a} + \hat{b}_i \hat{a}^\dagger \right) \quad (12)$$

$$H_{l,s} = \sum_i \left(\epsilon_{l,s,i} \hat{c}_{l,s,i}^\dagger \hat{c}_{l,s,i} \right) \quad (13)$$

$$H_{l,s}^c = \Gamma_{l,s} \sum_i \left(\hat{c}_{l,s,i}^\dagger \hat{s} + \hat{c}_{l,s,i} \hat{s}^\dagger \right) \quad (14)$$

H_1 and H_2 are the Hamiltonian of the electronic sites, $H_{\text{H.O.}}$ the Hamiltonian of the Harmonic Oscillator, H_b the Hamiltonian of the bosonic bath, $H_{\text{H.O.},b}^c$ the intercation Hamiltonian between the Harmonic Oscillator and the bath, $\{H_{l,s}\}_{l,s}$ the Hamiltonians for the leads with l labelling the side (Right and Left), and s labelling the site to which it is coupled, and finally $H_{l,s}^c$ the coupling between the leads and the electronic sites.

Of particular interest is the coupling between the harmonic oscillator and the electronic sites, the term $\Omega_0 + \Omega_1 \hat{x}$ is justified by — in the small oscillations regime — being the expansion up to linear order of a

more complicated functional $\Omega[\hat{x}]$. The second term in the hamiltonian corresponds to a phonon-assisted coupling.

We are looking for an evolution equation of the following kind:

$$\dot{\rho} = -i[H_1 + H_2 + H_{\text{H.O.}}, \rho] + \mathcal{L}_b \rho + \sum_{l,s} \mathcal{L}_{l,s} \rho \quad (15)$$

And then we will eliminate the Harmonic Oscillator adiabatically so that we find an equation of the following kind:

$$\dot{\rho} = -i[H_{\text{eff}}, \rho] + \mathcal{L}_{\text{eff}} \rho + \sum_{l,s} \mathcal{L}_{l,s} \rho \quad (16)$$

Since H_{eff} only describes the closed dynamics of the system, and the lead Lindbladians $\{\mathcal{L}_{l,s}\}$ only describe the coupling between the electronic sites and the leads, we expect all the interesting physics included in the coupling $\Omega_1 \hat{x}$ to be encoded in the effective Lindbladian \mathcal{L}_{eff} .

We will now proceed to adiabatically eliminate the harmonic oscillator, to do this we will solve the steady state dynamics of its creation and annihilation operators, then plug this solution into the evolution equation of the electronic sites' creation and annihilation operators. We then can identify the new dynamics with an effective Hamiltonian. To take into account dissipation we will describe the bosonic bath coupled to the harmonic oscillator by a Lindbladian, to which we will also plug the steady state creation and annihilation operators to obtain an effective steady-state Lindbladian.

2.3 Adiabatic Elimination

Let us focus on the harmonic oscillator's contribution to the dynamics of our system. First of all, the bosonic bath contribution may be taken as a Lindbladian, and is of the form^{*}:

$$\mathcal{L}_b \bullet = \gamma \frac{\bar{n}}{2} \mathcal{D}[\hat{a}] \bullet + \gamma \frac{\bar{n} + 1}{2} \mathcal{D}[\hat{a}^\dagger] \bullet \quad (17)$$

Where \bar{n} is the mean number of bosons in the bath.

^{*}See Appendix A for details

If we further take the harmonic oscillator to have a very fast relaxation, we can take it to be in steady-state:

$$0 = \dot{\hat{a}}_{s.s.} = i[H, \hat{a}_{s.s.}] + \mathcal{L}^{(H)} \hat{a}_{s.s.} = -i\omega \hat{a}_{s.s.} - \frac{i\Omega_1}{\sqrt{2}} \left(\hat{s}_1^\dagger \hat{s}_1 - \hat{s}_2^\dagger \hat{s}_2 \right) - \frac{\gamma}{2} \hat{a}_{s.s.} \quad (18)$$

$$(19)$$

We thus find:

$$\hat{a}_{s.s.} = \frac{-i\Omega_1}{\sqrt{2} \left(i\omega + \frac{\gamma}{2} \right)} \left(\hat{s}_1^\dagger \hat{s}_1 - \hat{s}_2^\dagger \hat{s}_2 \right) \quad (20)$$

$$\hat{x}_{s.s.} = \frac{1}{\sqrt{2}} (\hat{a} + \hat{a}^\dagger) = -\frac{\Omega}{\Omega_1} \left(\hat{s}_1^\dagger \hat{s}_1 - \hat{s}_2^\dagger \hat{s}_2 \right) \quad (21)$$

$$\text{With: } \Omega = \frac{\omega\Omega_1^2}{2\omega^2 + \frac{\gamma^2}{2}} \quad (22)$$

Let us look at the evolution equation for \hat{s}_i before taking the harmonic oscillator to be in steady-state:

$$\dot{\hat{s}}_1 = i[H, \hat{s}_1] + \mathcal{L}^{(H)} \hat{s}_1 = -i(\epsilon_1 + \Omega_0 + \Omega_1 \hat{x}) \hat{s}_1 \quad (23)$$

$$\dot{\hat{s}}_2 = i[H, \hat{s}_2] + \mathcal{L}^{(H)} \hat{s}_2 = -i(\epsilon_2 - \Omega_0 - \Omega_1 \hat{x}) \hat{s}_2 \quad (24)$$

Plugging $\hat{x}_{s.s.}$ we find:

$$\dot{\hat{s}}_1 = -i \left(\epsilon_1 + \Omega_0 - \Omega \hat{s}_2^\dagger \hat{s}_2 \right) \hat{s}_1 = i[H_{\text{eff}}, \hat{s}_1] \quad (25)$$

$$\dot{\hat{s}}_2 = -i \left(\epsilon_2 - \Omega_0 - \Omega \hat{s}_1^\dagger \hat{s}_1 \right) \hat{s}_2 = i[H_{\text{eff}}, \hat{s}_2] \quad (26)$$

There is no term in $\hat{s}_i \hat{s}_i$ since the \hat{s}_i are fermionic annihilation operators and vanish when applied to themselves.

We then get an effective Hamiltonian of the form:

$$H_{\text{eff}} = (\epsilon_2 - \Omega_0) \hat{s}_2^\dagger \hat{s}_2 + (\epsilon_1 + \Omega_0) \hat{s}_1^\dagger \hat{s}_1 + \Omega \hat{s}_2^\dagger \hat{s}_2 \hat{s}_1^\dagger \hat{s}_1 \quad (27)$$

This Hamiltonian is diagonal in the Fock basis representation:

$$H_{\text{eff}} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \epsilon_2 - \Omega_0 & 0 & 0 \\ 0 & 0 & \epsilon_1 + \Omega_0 & 0 \\ 0 & 0 & 0 & \epsilon_1 + \epsilon_2 + \Omega \end{pmatrix} \quad (28)$$

We now still must take into account the steady-state dissipation through the Harmonic Oscillator to the bosonic bath, for this we plug $\hat{a}_{s,s}$ and $\hat{a}_{s,s}^\dagger$ into (17), we find the following Lindbladian

$$\mathcal{L}_{\text{eff}} \bullet = \frac{\Gamma}{2} \mathcal{D}[\hat{s}_1^\dagger \hat{s}_1 - \hat{s}_2^\dagger \hat{s}_2] \bullet \quad (29)$$

With $\Gamma = \gamma \left(\bar{n} + \frac{1}{2} \right) \frac{\Omega}{\omega}$.

This effective Lindbladian does not mix diagonal elements of the density matrix, indeed we get:

$$\mathcal{L}_{\text{eff}} \rho = \begin{pmatrix} 0 & -\frac{1}{2}\Gamma\rho_{1,2} & -\frac{1}{2}\Gamma\rho_{1,3} & 0 \\ -\frac{1}{2}\Gamma\rho_{2,1} & 0 & -2\Gamma\rho_{2,3} & -\frac{1}{2}\Gamma\rho_{2,4} \\ -\frac{1}{2}\Gamma\rho_{3,1} & -2\Gamma\rho_{3,2} & 0 & -\frac{1}{2}\Gamma\rho_{3,4} \\ 0 & -\frac{1}{2}\Gamma\rho_{4,2} & -\frac{1}{2}\Gamma\rho_{4,3} & 0 \end{pmatrix} \quad (30)$$

That is, this Lindbladian only makes most off-diagonal elements decay with a timescale inversely proportional to Ω_1^2 .

2.4 Lead Lindbladians

We now turn derive the Lindbladians for the electronic leads:

$$\mathcal{L}_{l,s} \bullet = \Gamma_{l,s}^2 g_{l,s} (f_{l,s} \mathcal{D}[\hat{s}_s^\dagger] \bullet + (1 - f_{l,s}) \mathcal{D}[\hat{s}_s] \bullet) \quad (31)$$

The derivation is analogous to the one for (17) which is found in the appendix, and can also be found in [9, 10].

Here the Lindbladians describe two dissipation channels: one where electrons are coming in the electronic

site, and one where electrons are going out (or alternatively, where holes are coming in), and where $f_{l,s} = f(\epsilon_s \pm \Omega_0 - \mu_{l,s})$ is the Fermi-Dirac distribution, and $g_{l,s}$ is the degeneracy of our lead.

There are two important remarks:

1. Ω does not appear in these Lindbladians, only the shift Ω_0 does
2. the diagonal elements do not vanish, they mix together

2.5 Thermodynamic of Trajectories and Large Deviation Theory

2.5.1 principle

As a system evolves through time, it will visit in a certain order a given number of states, this is a trajectory in the state-space of the system. In some cases, this trajectory is fully deterministic, in the case of open systems, or when a measure occurs in the system, there is an element of randomness introduced, we can then talk not only about the particular realisation of a trajectory, but about all possible trajectories in this space. The idea of thermodynamic of trajectories[11] is to use Large Deviation Theory to study this ensemble of trajectories. This is done by biasing each trajectory by a weight function of a bias parameter s , in practice, this is nothing more than a Laplace Transform on each trajectory. Doing this we can then access the large deviation function $\theta(s)$, which gives us the entire dynamics of the system dynamical phase transitions, marked by non-analyticities in $\theta(s)$, if any.

2.5.2 Counting electrons

We wish to study the flow of electrons through a given site. This can be done by looking at its counting statistics. Where by counting statistics it is meant the knowledge of all cumulants of the probability distribution function of counting a given number of electrons in a given time interval. The relation between the flow of electrons and its counting statistics is straightforward: the first cumulant — the mean — is the current, the second cumulant its variance, and so on.

Let \mathcal{P}^K be a projector onto the subspace where K electrons went through a given channel between a time interval $[0, t]$. Then $p_K = \text{Tr}\{\mathcal{P}^K \rho\}$ is the probability of counting K electrons from 0 to t .

We define the cumulant generating function as the Laplace transform of p_K : $Z(s, t) = \sum_K e^{-sK} p_K = \text{Tr}\{\rho_s\}$ with $\rho_s = \sum_K e^{-sK} \mathcal{P}^K \rho$ the biased density matrix.

We know from Large Deviation Theory that:

$$Z(s, t) \underset{t \gg 1}{\sim} e^{t\theta(s)} \quad (32)$$

And we can access the full counting statistics if we can find $\theta(s)$, since:

$$\kappa_n = (-1)^n \partial_s^n \theta(s) \quad (33)$$

We recall that the two first cumulants are:

$$\kappa_1 = \langle K \rangle \quad (34)$$

$$\kappa_2 = \langle K^2 \rangle - \langle K \rangle^2 \quad (35)$$

2.5.3 Accessing the full counting statistics

The interest of the following method is that we do not need to know the exact probability distribution function: we can directly access the cumulants up to any order.

We know that, in the very big t limit we have:

$$\partial_t \theta = \partial_t \frac{1}{t} \ln Z(s, t) = -\frac{1}{t^2} \ln Z(s, t) + \frac{1}{t} \partial_t \ln Z(s, t) \underset{t \gg 1}{\sim} \frac{1}{t} \partial_t \ln Z(s, t) = \frac{1}{t} \frac{\text{Tr} \{ \dot{\rho}_s \}}{\text{Tr} \{ \rho_s \}} \quad (36)$$

The equation of motion for the biased density is[10]:

$$\dot{\rho}_s = -i[H, \rho_s] + \mathcal{L} \rho_s + \mathcal{L}_s \rho_s \quad (37)$$

$$\mathcal{L}_s \bullet = \sum_j \gamma_j (e^{-s} - 1) \hat{L}_j \bullet \hat{L}_j^\dagger \quad (38)$$

where \mathcal{L}_s is the contribution from counting the electrons leaving a given site, biased by a factor $(e^{-s} - 1)$. The operators \hat{L}_j select the subspace where a counting has occurred, they are usually annihilation and creation operators, or some combination thereof.

where the sum is over the channels where we are counting the electrons, from now on, and for simplicity's sake, we will assume there is only one channel where we are counting the electrons. We thus have:

$$\theta(s) = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t \frac{\text{Tr} \{ \mathcal{L}_s \rho_s \}}{\text{Tr} \{ \rho_s \}} \quad (39)$$

To simplify our notation, and to normalise ρ_s we do the following substitution: $\frac{\rho_s}{\text{Tr} \{ \rho_s \}} \rightarrow \rho_s^*$, and we can thus write:

$$\theta(s) = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t dt' \text{Tr} \{ \mathcal{L}_s \rho_s \} = \gamma_i (e^{-s} - 1) \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t dt' \text{Tr} \{ \hat{L}_i^\dagger \hat{L}_i \rho_s \} \quad (40)$$

From (33) we can write down the first two cumulants[12]:

$$\kappa_1 = \gamma_i \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t dt' \text{Tr} \{ \hat{L}_i^\dagger \hat{L}_i \rho \} \quad (41)$$

$$\kappa_2 = \kappa_1 - 2\gamma_i \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t dt' \text{Tr} \{ \hat{L}_i^\dagger \hat{L}_i \rho' \} \quad (42)$$

Let us investigate the form of $\rho' = \partial_s \rho_s|_{s=0}$.

$$\begin{aligned} \partial_s \rho_s|_{s=0} &= \left. - \frac{\sum_K K e^{-sK} \mathcal{P}^K \rho}{\text{Tr} \left\{ \sum_K e^{-sK} \mathcal{P}^K \rho \right\}} \right|_{s=0} - \left. \frac{\sum_K e^{-sK} \mathcal{P}^K \rho}{\text{Tr} \left\{ \sum_K e^{-sK} \mathcal{P}^K \rho \right\}^2} \text{Tr} \left\{ - \sum_K K e^{-sK} \mathcal{P}^K \rho \right\} \right|_{s=0} \\ &= \frac{- \sum_K K \mathcal{P}^K \rho}{\text{Tr} \left\{ \sum_K \mathcal{P}^K \rho \right\}} - \frac{\sum_K \mathcal{P}^K \rho}{\text{Tr} \left\{ \sum_K \mathcal{P}^K \rho \right\}^2} \text{Tr} \left\{ - \sum_K K \mathcal{P}^K \rho \right\} \end{aligned}$$

Since $\text{Tr} \left\{ \sum_K \mathcal{P}^K \rho \right\}$ is unity we find:

$$\rho' = \sum_K K (p_K - \mathcal{P}^K) \rho \quad (43)$$

*This normalised biased density matrix has the following equation of motion: $\dot{\rho}_s = -i[H, \rho_s] + \mathcal{L} \rho_s + \mathcal{L}_s \rho_s - \rho_s \text{Tr} \{ \mathcal{L}_s \rho_s \}$

Which we can clearly see that has a vanishing trace.

The evolution equation for ρ' is:

$$\dot{\rho}' = -i[H, \rho'] + \mathcal{L} \rho' - \gamma_i \hat{L}_i \rho \hat{L}_i^\dagger + \gamma_i \rho \text{Tr} \left\{ \hat{L}_i^\dagger \hat{L}_i \rho \right\} \quad (44)$$

If the density matrix is in steady-state $\rho = \rho^{\text{s.s.}}$ we get a simple expression for θ and the cumulants:

$$\theta^{\text{s.s.}}(s) = \gamma_i (e^{-s} - 1) \text{Tr} \left\{ \hat{L}_i^\dagger \hat{L}_i \rho^{\text{s.s.}} \right\} \quad (45)$$

$$\kappa_1^{\text{s.s.}} = \gamma_i \text{Tr} \left\{ \hat{L}_i^\dagger \hat{L}_i \rho^{\text{s.s.}} \right\} \quad (46)$$

$$\kappa_2^{\text{s.s.}} = \kappa_1^{\text{s.s.}} - 2\gamma_i \text{Tr} \left\{ \hat{L}_i^\dagger \hat{L}_i \rho^{\text{s.s.}} \right\} \quad (47)$$

To find $\kappa_2^{\text{s.s.}}$ we need to solve the evolution equation for ρ' :

$$0 = -i[H, \rho'^{\text{s.s.}}] + \mathcal{L} \rho'^{\text{s.s.}} - \gamma_i \hat{L}_i \rho^{\text{s.s.}} \hat{L}_i^\dagger + \gamma_i \rho^{\text{s.s.}} \text{Tr} \left\{ \hat{L}_i^\dagger \hat{L}_i \rho^{\text{s.s.}} \right\} \quad (48)$$

2.5.4 First and second cumulants for our system

We want to differentiate electrons coming in from electrons coming out, this is easy to do since their rate γ_i are different. We take the convention of a positive current being a flow from left to right. Let $M_{l,s}$ be a mapping taking this into account:

$$M_{l,s}(\bullet) = \Gamma_{l,s}^2 g_{l,s} (f_{l,s} \text{Tr} \{ \hat{s}_s \hat{s}_s^\dagger \bullet \} - (1 - f_{l,s}) \text{Tr} \{ \hat{s}_s^\dagger \hat{s}_s \bullet \}) \quad (49)$$

We then get:

$$\kappa_{1_s}^{\text{s.s.}} = M_{1,s}(\rho^{\text{s.s.}}) - M_{2,s}(\rho^{\text{s.s.}}) \quad (50)$$

$$\kappa_{2_s}^{\text{s.s.}} = \kappa_{1_s}^{\text{s.s.}} - 2(M_{1,s}(\rho'^{\text{s.s.}}) - M_{2,s}(\rho'^{\text{s.s.}})) \quad (51)$$

where $\kappa_1^{s.s.}$ is the steady-state electron current through site $s \in \{1, 2\}$, while $\kappa_2^{s.s.}$ is the variance of the current. We define the Fano factor as:

$$F = \frac{\kappa_2^{s.s.}}{\kappa_1^{s.s.}} = 1 - 2 \frac{M_{1,s}(\rho'^{s.s.}) - M_{2,s}(\rho'^{s.s.})}{M_{1,s}(\rho^{s.s.}) - M_{2,s}(\rho^{s.s.})} \quad (52)$$

The Fano factor is associated with bunching, that is, the tendency to observe a joint detection of fermions or bosons by two distinct detectors. If $F = 1$ then the probability distribution function is Poissonian, if $F < 1$ then it is sub-Poissonian which is associated with anti-bunching, that is no joint detection, while if $F > 1$ it is super-Poissonian and bunching increases.

Let us compute $M_{l,s}(\rho^{s.s.})$ for $s \in \{1, 2\}$:

$$M_{l,1}(\rho^{s.s.}) = \Gamma_{l,1}^2 g_{l,1} (f_{l,1}(\rho_{1,1}^{s.s.} + \rho_{2,2}^{s.s.}) + (1 - f_{l,1})(\rho_{3,3}^{s.s.} + \rho_{4,4}^{s.s.})) \quad (53)$$

$$M_{l,2}(\rho^{s.s.}) = \Gamma_{l,2}^2 g_{l,2} (f_{l,2}(\rho_{1,1}^{s.s.} + \rho_{3,3}^{s.s.}) + (1 - f_{l,2})(\rho_{2,2}^{s.s.} + \rho_{4,4}^{s.s.})) \quad (54)$$

We can easily access the above two quantities by solving the equation of motion for the steady-state density matrix. We must only concern ourselves with the diagonal elements of ρ' since in $M_{l,s}$, the operators $\hat{s}_s \hat{s}_s^\dagger$ and $\hat{s}_s^\dagger \hat{s}_s$ are themselves diagonal.

2.6 A Few Results

Unfortunately, there is no actual difference with the single uncoupled electronic site case, indeed, the phonon-assisted (Ω_1) coupling only affects the off-diagonal elements of the density matrix, which do not impact the electron transfer. While the normal (Ω_0) only shifts the energy of the electronic sites in different directions: we only get two uncoupled electronic sites with different energy levels.

In the above figure we have plotted the current through sites 1 and 2 as a function of the coupling strength Ω_0 for different values of the temperature and chemical potential of the left and right leads $T_{l,s}$ and $\mu_{l,s}$, and setting $\Gamma_{l,s}$ and $g_{l,s}$ to unity. The different cases are:

- A: The current through the first electronic site, with a higher chemical potential and temperature on the left lead than on the right lead ($\mu_{L,1} = 3.1 > \mu_{R,1} = 2.9$ and $T_{L,1} = 2 > T_{R,1} = 1$)

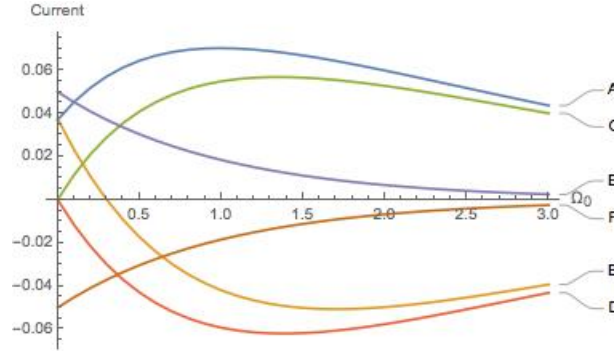


Figure 3: Current in function of the coupling Ω_0

B: Current through the second electronic site with the same configuration as above.

C: As in the case A but without difference in chemical potential

D: As above but in the second site

E: As in the case A but without difference in temperature

F: As above but in the second site

The difference between the first and second electronic site is that the shift in energy occurs with different signs, indeed: $\epsilon_1 \rightarrow \epsilon_1 + \Omega_0$ and $\epsilon_2 \rightarrow \epsilon_2 - \Omega_0$. In the case without temperature difference and without chemical potential difference the current is zero through both sites for all values of the coupling.

In all cases the current tends to zero as Ω_0 goes to ∞ .

3 new proposed model

The results from this section are fresh and the physical interpretation is not completely fleshed out by the time of this report being written.

We propose a second model which may be able to recover interesting phenomena:

Let the coupling between both electronic sites be a little bit different: $H_{1,2,H.O.}^c = (\Omega_0 + \Omega_1 \hat{x}) (\hat{s}_1^\dagger + \hat{s}_1 - \hat{s}_2^\dagger - \hat{s}_2)$.

This gives us a few differences:

$$\hat{a}_{s.s.} = \frac{-i\Omega_1}{\sqrt{2} (i\omega + \frac{\gamma}{2})} (\hat{s}_1^\dagger + \hat{s}_1 - \hat{s}_2^\dagger - \hat{s}_2) \quad (55)$$

$$\hat{x}_{s.s.} = \frac{1}{\sqrt{2}} (\hat{a} + \hat{a}^\dagger) = -\frac{\Omega}{\Omega_1} (\hat{s}_1^\dagger + \hat{s}_1 - \hat{s}_2^\dagger - \hat{s}_2) \quad (56)$$

$$(57)$$

With $\Omega = \frac{\omega\Omega_1^2}{2\omega^2 + \frac{\gamma^2}{2}}$ the same one as in the first model.

For convenience's sake we will write $\hat{s}_i^\dagger + \hat{s}_i = \hat{\xi}_i$, we now write the evolution equation for the \hat{s}_i (for a steady harmonic oscillator):

$$\dot{\hat{s}}_1 = -i\epsilon_1 \hat{s}_1 + i \left(\Omega_0 + \Omega (1 + \hat{\xi}_2) \right) \hat{s}_1^z \quad (58)$$

$$\dot{\hat{s}}_2 = -i\epsilon_2 \hat{s}_2 + i \left(-\Omega_0 + \Omega (1 + \hat{\xi}_1) \right) \hat{s}_2^z \quad (59)$$

With $s^z = [\hat{s}^\dagger, \hat{s}]$ and is such that $s^z|0\rangle = -|0\rangle$ and $s^z|1\rangle = |1\rangle$. The new effective Hamiltonian is:

$$H_{\text{eff}} = \epsilon_1 \hat{s}_1^\dagger \hat{s}_1 + \epsilon_2 \hat{s}_2^\dagger \hat{s}_2 - (\Omega + \Omega_0) \hat{\xi}_1 - (\Omega - \Omega_0) \hat{\xi}_2 - \Omega \hat{\xi}_2 \hat{\xi}_1 \quad (60)$$

This Hamiltonian is not diagonal, indeed:

$$H_{\text{eff}} = \begin{pmatrix} 0 & \Omega_0 - \Omega & -\Omega_0 - \Omega & -\Omega \\ \Omega_0 - \Omega & \epsilon_2 & \Omega_0 - 2\Omega & -\Omega_0 - \Omega \\ -\Omega_0 - \Omega & \Omega_0 - 2\Omega & \epsilon_1 & \Omega_0 - \Omega \\ -\Omega & -\Omega_0 - \Omega & \Omega_0 - \Omega & \epsilon_1 + \epsilon_2 \end{pmatrix} \quad (61)$$

The new Lindbladian for the dissipation of the harmonic oscillator is:

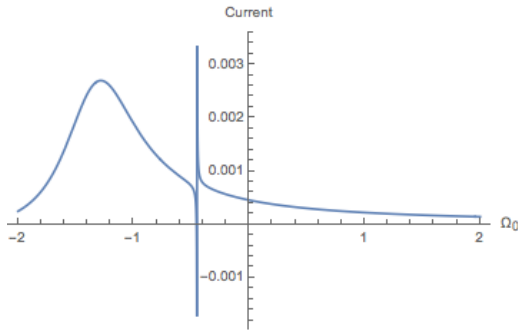
$$\mathcal{L}_{\text{eff}} = \gamma \left(\bar{n} + \frac{1}{2} \right) \frac{\Omega}{\omega} \mathcal{D}[\hat{\xi}_1 - \hat{\xi}_2] \quad (62)$$

In this new model one cannot neglect non diagonal elements of the density matrix since both the commutator $[H, \rho]$ and $\mathcal{L}_{\text{eff}} \rho$ mix the diagonal elements with non diagonal elements: For the commutator the diagonal elements are the imaginary parts of a few off-diagonal elements, while for the lindbladian they are a mix of diagonal elements of the density matrix, and of the real parts of a few off-diagonal elements.

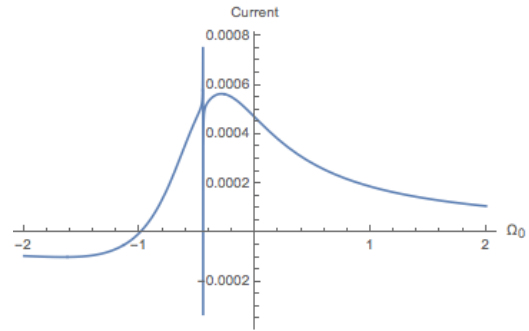
We also remark that for $\Omega_1 = 0$ we have that $\Omega = 0$, and since it is in front of the dissipator, we have no dissipation! thus only the phonon-assisted coupling has dissipative effects.

We expect all interesting effects to be encoded in the effective Lindbladian, since the effects of the commutator alone should not create a current, since it describes the closed dynamics of the system, and the effects of the lindbladian of the lead should just encode the effects of the current through one electronic site, without taking into account the other. Moreover since the current is only concerned with the diagonal elements of the density matrix, the only relevant elements of it are those that contribute to the dissipative (driven by \mathcal{L}_{eff}) evolution of the diagonal elements. These elements are $\{\rho_{1,1}, \rho_{2,2}, \rho_{3,3}, \rho_{4,4}, \rho_{1,4}, \rho_{2,3}, \rho_{3,2}, \rho_{4,1}\}$. To simplify the system we can set up all other elements in the density matrix to be equal to zero.

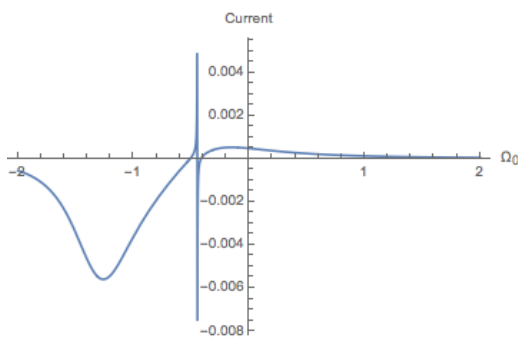
In the same vain, we see that Ω_0 is only in the Hamiltonian, moreover, it is not present in the diagonal elements of it. We can thus set it to zero.



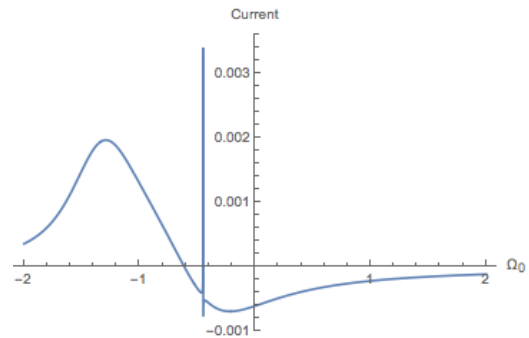
(a) The current on the uppermost electronic site with $\epsilon_1 = \epsilon_2 = 3$, $\mu_{L,1} = 3.1$, $\mu_{R,1} = 2.9$, $\mu_{L,2} = 3.1$, $\mu_{R,2} = 2.9$, $T_{L,1} = 2$, $T_{R,1} = 1$, $T_{L,2} = 2$, $T_{R,2} = 1$



(b) The current on the uppermost electronic site with $\epsilon_1 = \epsilon_2 = 3$, $\mu_{L,1} = 3.1$, $\mu_{R,1} = 2.9$, $\mu_{L,2} = 3.1$, $\mu_{R,2} = 2.9$, $T_{L,1} = 2$, $T_{R,1} = 1$, $T_{L,2} = 1$, $T_{R,2} = 2$



(a) The current on the uppermost electronic site with $\epsilon_1 = 3$, $\epsilon_2 = 2.9$, $\mu_{L,1} = 3.1$, $\mu_{R,1} = 2.9$, $\mu_{L,2} = 3.1$, $\mu_{R,2} = 2.9$, $T_{L,1} = 2$, $T_{R,1} = 1$, $T_{L,2} = 1$, $T_{R,2} = 2$



(b) The current on the uppermost electronic site with $\epsilon_1 = 2.9$, $\epsilon_2 = 3.1$, $\mu_{L,1} = 3.1$, $\mu_{R,1} = 2.9$, $\mu_{L,2} = 3.1$, $\mu_{R,2} = 2.9$, $T_{L,1} = 2$, $T_{R,1} = 1$, $T_{L,2} = 1$, $T_{R,2} = 2$

We can see that the current is significantly altered by the presence of the coupling. The coupling can lead to both a significant improvement of the intensity of the current, or its damping. However, we see that there

is a divergence always at the same intensity of the coupling at around 0.45, this seems to be a problem with the code.

4 Conclusion

4.1 Summary of Internship Achievements

The goal of this internship was to see if quantum effects coming from a mechanical coupling between two thermoelectric devices increased the efficiency of these thermal machines. We showed that the minimal model we first used was not able to recover the interesting physical phenomena after an adiabatic elimination of the Harmonic Oscillator. We find ourselves forced to consider more complicated models.

Is it surprising to have this result? Not that much, indeed, from the start the interaction hamiltonian is $H_{\text{H.O.,1,2}} = (\Omega_0 + \Omega_1 \hat{x}) \cdot (\hat{s}_1^\dagger \hat{s}_1 - \hat{s}_2^\dagger \hat{s}_2)$ is such that the normal (non-phonon assisted) coupling is just a shift in the energies. The adiabatic elimination just deleted the second part of the interaction, which was the interesting one. However, we may have effects on higher order cumulants, or when driving adiabatically the oscillator.

Why do we think the second model resolves this problem? The first effective Lindbladian \mathcal{L}_{eff} does not mix the element of the density matrix, and thus does not really affect it qualitatively. The second model does this, mixing all elements of the density matrix into a huge mess. An important drawback of this model is that the number of electrons is not conserved, that is, electrons can be created or annihilated without them hopping to one of the reservoirs thanks to the term $\hat{s}_1^\dagger + \hat{s}_1 - \hat{s}_2^\dagger - \hat{s}_2$.

A more realistic model would be to couple the Harmonic Oscillator to the leads:

$$\begin{aligned}
 H_{\text{H.O.,1,2,leads}} = & (\Omega_0 + \Omega_1 \hat{x}) \\
 & \cdot \left(\hat{s}_1^\dagger \sum_i (\hat{c}_{\text{L},1,i} + \hat{c}_{\text{R},1,i}) + \hat{s}_1 \sum_i (\hat{c}_{\text{L},1,i}^\dagger + \hat{c}_{\text{R},1,i}^\dagger) \right. \\
 & \left. - \hat{s}_2^\dagger \sum_i (\hat{c}_{\text{L},2,i} + \hat{c}_{\text{R},2,i}) - \hat{s}_2 \sum_i (\hat{c}_{\text{L},2,i}^\dagger + \hat{c}_{\text{R},2,i}^\dagger) \right)
 \end{aligned} \tag{63}$$

So that the electrons are not created out of nowhere, but come from one of the reservoirs and vice versa. This model is more complex since the effect will be found on both \mathcal{L}_{eff} — which will have a dissipator func-

tion of the sum and difference of the $\hat{s}_s^\dagger \hat{c}_{l,s,i}$ and the $\hat{s}_s \hat{c}_{l,s,i}^\dagger$ — and the $\{\mathcal{L}_{l,s}\}$ of the leads in a more complex manner.

4.2 Future Work

The internship work can be readily extended, first of all, we must finish the analysis of the second model more thoroughly, that is, finding its first few cumulants for the electron flux through the sites. Second of all would be to add more electronic sites in series and in parallel to see how they all affect each other. Another extension could be to add more structure to the electronic sites, it might be done by giving them vibrational degrees of freedom, or by taking them to be one dimensional lattices with electrons hopping from left to right on which the coupling with the harmonic oscillator might act. In all of these extensions the density matrix increases dramatically, making the density matrix representation more cumbersome, and thus making progress slower and more computationally intensive. This internship was mostly analytical, future work cannot be expected to be of this kind.

A Derivation of the Lindbladians

The following derivation is mostly borrowed from H. Carmichael's *An Open Systems Approach to Quantum Optics*[9] and C. Gardiner's *Quantum Noise*[10]

A.1 Interaction Picture

Let the Hamiltonian be $\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_{\text{int}}$, where 0 labels the system, and 1 an external bath. One goes to the interaction picture by doing the following transformation on all operators of the systems (including the density matrix and the Hamiltonian): $\hat{O} \rightarrow \tilde{O} = \hat{U}_{0,1}^\dagger \hat{O} \hat{U}_{0,1}$ with $\hat{U}_{0,1} = e^{-i(\hat{H}_0 + \hat{H}_1)t}$. The equation of motion becomes in this picture:

$$\dot{\tilde{\rho}}(t) = -i \left[\tilde{H}_{\text{int}}(t), \tilde{\rho}(t) \right] \quad (64)$$

The solution is, formally:

$$\tilde{\rho}(t) = \rho(0) - i \int_0^t dt' \left[\tilde{H}_{\text{int}}(t'), \tilde{\rho}(t') \right] \quad (65)$$

Inserting it in (64), and then tracing over the bath degrees of freedom we get:

$$\dot{\tilde{\rho}}_0 = - \int_0^t dt' \text{Tr}_1 \left\{ \left[\tilde{H}_{\text{int}}(t), \left[\tilde{H}_{\text{int}}(t'), \tilde{\rho}(t') \right] \right] \right\}$$

With $\partial_t \text{Tr}_1 \{ \tilde{\rho} \} = \dot{\tilde{\rho}}_0$

A.2 Derivation of the Lindbladians

The Born-Markov Approximation states that the evolution only depends on the state of the system at time t , and that the system and the bath are uncorrelated, that is the above equation reads:

$$\dot{\tilde{\rho}}_0 = - \int_0^t dt' \text{Tr}_1 \left\{ \left[\tilde{H}_{\text{int}}(t), \left[\tilde{H}_{\text{int}}(t'), \tilde{\rho}_0(t) \otimes \tilde{\rho}_1(0) \right] \right] \right\} \quad (66)$$

We will write the interaction hamiltonian as: $\tilde{H}_{\text{int}} = \sqrt{\frac{\gamma}{2}} \left(\tilde{s}^\dagger \tilde{b} + \tilde{s} \tilde{b}^\dagger \right)$ with \tilde{s} and \tilde{b} interaction picture operators for the system and the bath respectively. Then expanding equation (66) by plugging the previous expression for \tilde{H}_{int} , and by writing $\text{Tr}_1 \{ \bullet \tilde{\rho}(0) \} = \langle \bullet \rangle_1$ we get:

$$\begin{aligned}
\dot{\rho}_0 = & -\gamma \int_0^t dt' \left\{ (\tilde{s}^\dagger(t)\tilde{s}^\dagger(t')\tilde{\rho}_0(t) - \tilde{s}^\dagger(t')\tilde{\rho}_0(t)\tilde{s}^\dagger(t)) \langle \tilde{b}(t)\tilde{b}(t') \rangle_1 + (\tilde{s}(t)\tilde{s}(t')\tilde{\rho}_0(t) - \tilde{s}(t')\tilde{\rho}_0(t)\tilde{s}(t)) \langle \tilde{b}^\dagger(t)\tilde{b}^\dagger(t') \rangle_1 \right. \\
& + (\tilde{s}(t)\tilde{s}^\dagger(t')\tilde{\rho}_0(t) - \tilde{s}^\dagger(t')\tilde{\rho}_0(t)\tilde{s}(t)) \langle \tilde{b}^\dagger(t)\tilde{b}(t') \rangle_1 + (\tilde{s}^\dagger(t)\tilde{s}(t')\tilde{\rho}_0(t) - \tilde{s}(t')\tilde{\rho}_0(t)\tilde{s}^\dagger(t)) \langle \tilde{b}(t)\tilde{b}^\dagger(t') \rangle_1 \\
& \left. + \text{h.c.} \right\}
\end{aligned} \tag{67}$$

To go further we must look more specifically at the operators \tilde{s} and \tilde{b} . First of all, the \tilde{b} operators are annihilation operators, when taking the trace they destroy a level on the right, while they create one on the left, thus $\langle \tilde{b}(t)\tilde{b}(t') \rangle_1 = \langle \tilde{b}^\dagger(t)\tilde{b}^\dagger(t') \rangle_1 = 0$, from the remaining terms we can already recognise the Lindbladian structure! Let us look at what the interaction picture does to the system and bath operators in the case of the Harmonic oscillator.

$$\tilde{s}(t) = \tilde{a}(t) = e^{iH_0 t} \hat{a} e^{-iH_0 t} = e^{i(\omega \hat{a}^\dagger \hat{a}) t} \hat{a} e^{-i(\omega \hat{a}^\dagger \hat{a}) t} = \hat{a} e^{-i\omega t} \tag{68}$$

$$\tilde{b}(t) = \sum_i \tilde{b}_i(t) = \sum_i e^{i \sum_j \epsilon_j \hat{b}_j^\dagger \hat{b}_j t} \hat{b}_i e^{-i \sum_j \epsilon_j \hat{b}_j^\dagger \hat{b}_j t} = \sum_i \hat{b}_i e^{-i\epsilon_i t} \tag{69}$$

We can thus write:

$$\begin{aligned}
\dot{\rho}_0(t) = & -\gamma \int_0^t dt' \left\{ (\hat{a} \hat{a}^\dagger \tilde{\rho}_0(t) - \hat{a}^\dagger \tilde{\rho}_0(t) \hat{a}) \sum_i e^{i(\epsilon_i - \omega)(t-t')} \bar{n}(\epsilon_i, T) \right. \\
& \left. + (\hat{a}^\dagger \hat{a} \tilde{\rho}_0(t) - \hat{a} \tilde{\rho}_0(t) \hat{a}^\dagger) \sum_i e^{-i(\epsilon_i - \omega)(t-t')} (\bar{n}(\epsilon_i, T) + 1) + \text{h.c.} \right\}
\end{aligned} \tag{70}$$

Assuming* the following we recover the Lindbladian (17):

$$\sum_i e^{i(\epsilon_i - \omega)(t-t')} \sim \int \delta(\epsilon - \omega) \delta(t - t') d\epsilon$$

Indeed we get:

$$\begin{aligned}
\dot{\rho}_0(t) = & \frac{1}{2} \gamma \bar{n}(\omega, T) (2\hat{a} \rho \hat{a}^\dagger - \{\hat{a}^\dagger \hat{a}, \rho\}) \\
& + \frac{1}{2} \gamma (\bar{n}(\omega, T) + 1) (2\hat{a}^\dagger \rho \hat{a} - \{\hat{a} \hat{a}^\dagger, \rho\})
\end{aligned} \tag{71}$$

However, we recover it for $\tilde{\rho}_0$, not for ρ_0 , to truly recover the equation of motion, let us go back to the one for the full system:

$$\dot{\rho} = -i [H_0 + H_1 + H_{\text{int}}, \rho] \tag{72}$$

$$\text{Tr}_1 \dot{\rho} = \dot{\rho}_0 = -i [H_0, \rho_0] - i \text{Tr}_1 \{ [H_{\text{int}}, \rho] \} \tag{73}$$

*The sources cited do not proceed as follow, but argue it differently and more thouroughly.

Where the evolution driven by the bath vanishes due to the Markov Approximation where the bath is in steady state and uncorrelated with the system.

$$-i \text{Tr}_1 \{ [H_{\text{int}}, \rho] \} = -i \text{Tr}_1 \left\{ \hat{U}_{0,1} \hat{U}_{0,1}^\dagger H_{\text{int}} \hat{U}_{0,1} \hat{U}_{0,1}^\dagger \rho \hat{U}_{0,1} \hat{U}_{0,1}^\dagger - \hat{U}_{0,1} \hat{U}_{0,1}^\dagger \rho \hat{U}_{0,1} \hat{U}_{0,1}^\dagger H_{\text{int}} \hat{U}_{0,1} \hat{U}_{0,1}^\dagger \right\} \quad (74)$$

$$-i \text{Tr}_1 \{ [H_{\text{int}}, \rho] \} = \hat{U}_0 \text{Tr}_1 \left\{ -i \left[\tilde{H}_{\text{int}}(t'), \tilde{\rho}(t') \right] \right\} \hat{U}_0^\dagger = \hat{U}_0 \dot{\rho}_0(t) \hat{U}_0^\dagger \quad (75)$$

Plugging the Lindbladian coming from (69) yields a Lindbladian not in the interaction picture, and thus $\dot{\rho}_0 = -i [H_0, \rho_0] + \mathcal{L} \rho_0$, which was the desired result. The exact same procedure is followed to obtain the Lindbladians for the leads, however it is a more tedious one since we have to keep track of each lead, and the Hamiltonians are less straightforward.

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