Work extraction from quantum systems

Andrea Rodriguez Blanco

Supervisor: Alexandra Olaya-Castro

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Abstract

From the first law of thermodynamics, it seems to be well-defined which part of the internal energy is related with work and which one with heat. Being this splitting in the quantum regime not clearly defined yet, it has been proved that we do not need a statistical ensemble of particles to talk about thermodynamical concepts as work or heat. We cannot find any definition without imposing constraints; however, most of those proposed so far are based on time-dependent Hamiltonians or on how the state of my system change when it is kept in contact with a thermal bath. Here we use a local effective measure basis (LEMBAS), where considering a bipartite quantum systems, and just taking into account the effect of one system over the other, we are able to split a local effective energy into work and heat flux, without using drivers or resources.

Contents

1 Introduction

The first question that might arise when one reads the title of the project is: What could be the relationship between the work as a classical thermodynamical concept and quantum physics? From its very beginning, thermodynamics has had an important impact, as we can see with the invention of the steam machine, and it still has a huge applicability nowadays. It was a phenomenological origin but with years it was proved by the hand of scientics as Boltzman, Maxwell or Gibbs that thermodynamical concepts could be explained from a microscopical point of view making use of the statistical classical mechanics.

Since the beginnings of Quantum Physicis in the 20th century it was proved that the use of a quantum statistical point of view was needed to achieve a proper understanding of the thermodynamical concepts emerging from the microscopic world. From then on, there have been several attempts of linking thermodynamics with quantum phenomena. Moreover, both biomolecular motors and micro- and nanodevices are being implemented in the lab nowadays.

Therefore, it is clear that there exits an important motivation in the study of how matter behaves at those scales. Our objective here is twofold: on the one hand, we are interested in how and under what conditions thermodynamical concepts such as work or heat can emerge in the quantum regime. On the other hand, we are interested in how is the transport and dissipation of energy in this regime, so that we can obtain the maximum benefit. This project is organized as follows: in a first part we are comparing some definitions of work that can be found in the literature, and why we choose to follow the definitions given by Mahler et *al.* in [1]. We are going to explain such definitions, and then we will apply them to different quantum systems. Finally, we will discuss the results and suggest open questions.

2 Definitions of work in literature

It is difficult to find a definition of work that could be generalized, however we discover in many papers different descriptions of how to describe thermodynamical concepts when quantum substances are present. The concept of quantum *working substance* is used in [4] as a quantum supply in quantum heat engines (QHE's) in order to produce work through several quantum thermodynamical processes. All processes considered in [4] are quasiestatic processes, that is, the evolution of the system through such thermodynamical cycles is slow enough in order to keep the thermal equilibrium in each step. Under this assumption the energy is conserved in each step and thus from the first law of thermodynamics:

$$dU = đW + đQ \tag{1}$$

where $đW$ and $đQ$ are infinitesimal changes in work and heat respectively, in [4] and in many papers they define a quantum version of this law based on the expected value of the total internal energy:

$$dU = dTr\{\hat{H}\hat{\rho}\} = Tr\{d\hat{H}\hat{\rho} + \hat{H}d\hat{\rho}\} \tag{2}$$

Where $\hat{\rho}$ is the density operator and $\hat{H}$ the Hamiltonian of the system. In this expression we can identify two terms, the former related with a change in the Hamiltonian is identified as work and the latter with a change in the density operator is identified as heat. Since the eigenenergies of the Hamiltonian define our system, as the volume defines the initial state of a gas container, it is reasonable to think that if volume is modified or the eigenergies change, a work should be performed on or by the system.

On the other hand a change in the density operator is related with a change in the entropy, $S = -Tr\{\hat{\rho}ln\hat{\rho}\}$. If we are considering processes slow enough in order to be able to apply the thermodynamic definitions $đQ = TdS$, a relation between entropy and heat should exit closed to the equilibrium.

In [4], quantum Carnot(QCE) and Otto (QOE) engines using quantum substances are implemented and satisfactory definitions of heat absorbed(released) and work(performed), by(on) the system are obtained. Some classical analogies are found such as positive work extraction needs that temperature of the heat bath was bigger than the cold bath or that the efficiency of a quantum Carnot engine is equal to the classical efficiency. However, there exit some interesting features that are noticeable. For instance, the efficiency of a QOE is bigger than its classical counterpart, or there is not a quantum analogue of a classical isoenergetic process, as we can see in the following figure:
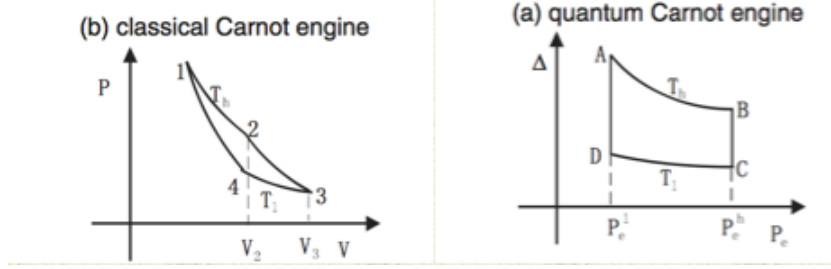
Figure 1: *H.T. Quan, Yu-xi Liu, C.P.Sun, and Franco Nori, Quantum thermodynamic cycles and quantum heat engines.Phys. Rev. E 76. 031105 (2007)*

The image on the left describes a Carnot cycle and the right image a Quantum Carnot cycle. In this last it is plotted the energy gap Δ between the ground and excited state for an atom versus P_e, the probability of finding the electron in the excited state. We can see that for an isothermal process, Δ changes and thus the energy of the system changes. It is the opposite of what we would expect for a classical isoenergetic process.

Another effort to give a definition of work is in the context of *resource theories*. In [5] , using concepts from quantum information, they quantify deterministically the amount of work that we need to create a state, *work formation* and the amount of work that we can extract from a quantum state, *extractable work*, when the system is in contact with a thermal bath. All the states that are not in thermal equilibrium are used as resources to extract work. Ensuring energy conserving through thermal operation they calculate work as the difference between two free energies, redefined in the quantum regime. Such difference is related with the information that we have about the distance to the Gibbs state, that in the thermodynamic limit it turns into the relative entropy.

Following in the context of resource theories, in [6, 7] they use the change in the free energy of a system to determine the work that can be extracted from it, even for just a copy of such a system the change in the free energy is a relevant quantity. The *work storage* system is a *weight* instead of a *wit*, work bit used in [5]. And unlike in the previous case, they focus on a non-deterministic work extraction quantifying the *average* work.

In all the situations described above they need a classical driving or an external source as thermal baths to identify work in the quantum regime. Here we wonder if it could be possible to have fully quantized setups. In particular, we investigate if it is possible and how can work and heat emerge when I leave two quantum systems in contact evolving in time. How the influence of a system influences the evolution of the other? and how such dynamics could have relation with quantum thermodynamical concepts?

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These questions have been already formulated in [8], but whilst they let the composite system evolve between a heat and a cold bath to study the power generation in QHE's, we are interested in autonomous systems without external drivers. Using a local effective basis (LEMBAS), we study how the effect of one subsystem over the other induces an effective evolution. Computing the change in the local effective energy of one subsystem we will identify in it terms related with a change in entropy, and thus related with heat and others that do not , that will contribute to the work.

3 Work and heat using LEMBAS

As we have mentioned above, we want to investigate if we are able to talk about thermodynamics in quantum systems, and namely analyze whether we can define in the same way classical concepts as work or heat. To do that, we follow the method described by Mahler at al. in[1]. In this section we will try to show how these concepts arises studying the local dynamics of a subsystem. We consider a bipartite quantum system described by the following Hamiltonian:

$$\hat{H} = \hat{H}_A + \hat{H}_B + \hat{H}_{AB} \tag{3}$$

Where $\hat{H}_A$ represents the Hamiltonian acting over the Hilbert space of subsystem A, $\mathcal{H}_A$. $\hat{H}_B$ is the Hamiltonian acting over the Hilbert space of system B, $\mathcal{H}_B$ and $\hat{H}_{AB}$ the interaction Hamitonian acting over the tensor product of both subspaces $\mathcal{H}_A \otimes \mathcal{H}_B$. Choosing the measurement basis with respect to the subsystem A, we study the evolution of this system under the coupling with B. Starting with the Liouville Von-Neuman equation for system A:

$$\frac{\partial \hat{\rho}_A}{\partial t} = -i\hbar Tr_B\{[\hat{H}, \hat{\rho}]\} = -i\hbar Tr_B\{[\hat{H}_A + \hat{H}_B + \hat{H}_{AB}, \hat{\rho}]\} \tag{4}$$

Now we suppose that the evolved density matrix of the full system can be written as:

$$\hat{\rho} = \hat{\rho}_A \otimes \hat{\rho}_B + \hat{C}_{AB} \tag{5}$$

Where $\hat{\rho}_A$ is the reduced density matrix of the system A, $\hat{\rho}_B$ the reduced density matrix of system B and $\hat{C}_{AB}$ the correlated terms that can appear after the evolution. As we will study, this additional term depends on the initial state of the subsystems and on the interaction. In general, when we have two coupled systems that evolve together in time, correlations between them appear. Considering some trace theorems and follow all the algebra (see Appendix A), we arrive at:

$$\frac{\partial \hat{\rho}_A}{\partial t} = -i\hbar[\hat{H}_A + \hat{H}_A^{eff}, \hat{\rho}_A] + \mathcal{L}_A^{eff}[\hat{\rho}(t)]] \tag{6}$$

This is not a closed differential equation since we have this additional term $\mathcal{L}_A^{eff}[\hat{\rho}(t)] = -i\hbar Tr_B\{[\hat{H}_{AB}, \hat{C}_{AB}]\}$. Since it depends on the correlations between subsystems $\hat{C}_{AB}$, this is a source of mixedness, and thus, if it is present the purity of the system A is going to change in time. For that reason, this term is usually related with a non-unitary dynamics of subsystem A.

The another term that we can identify is related with the unitary dynamics and is the effective Hamiltonian $\hat{H}_A^{eff} = Tr_B\{\hat{H}_{AB}(\hat{1} \otimes \hat{\rho}_B)\}$. The effective Hamiltonians that are implied in the dynamics of one of the systems, are the expected value of the interaction or in other words, the weight of the interaction in the basis of the other system which is coupled with. Once we know the dynamics of the system we can compute the change in the internal energy, as the change in the expectation value of the energy in the basis of system A:

$$dU = \frac{d}{dt}Tr_A\{\hat{H'}_A\hat{\rho_A}\}dt = Tr\{\dot{\hat{H'}}_A\hat{\rho_A} + \hat{H'}_A\dot{\hat{\rho_A}}\} \tag{7}$$

Where $\hat{H'}_A = \hat{H}_A + \hat{H}_{1,A}^{eff}$. $\hat{H}_{1,A}^{eff}$ is the part of the effective Hamiltonian $\hat{H}_A^{eff}$ that commutes with the free Hamiltonian of the system $\hat{H}_A$.

Following several steps (for derivation, see Appendix A) we can arrive a the following expression for the local effective energy for the subsystem A:

$$dU = Tr_A\{(\dot{\hat{H}}_{1,A}^{eff})\hat{\rho}_A - i[\hat{H'}_A, \hat{H}_{2,A}^{eff}]\hat{\rho}_A + \hat{H'}_A\mathcal{L}_A^{eff}[\hat{\rho}(t)]\}dt \tag{8}$$

Now we can split this expression into two, one the work flux relates with non-entropy changes:

$$\dot{W}_A = Tr_A\{(\dot{\hat{H}}_{1,A}^{eff})\hat{\rho}_A - i[\hat{H'}_A, \hat{H}_{2,A}^{eff}]\hat{\rho}_A\} \tag{9}$$

Where $\hat{H}_{2,A}^{eff}$ is the part of the effective Hamiltonian $\hat{H}_A^{eff}$ that does not commute with $\hat{H}_A$. The other part of the effective energy flow associated with a change in the entropy of the system will be a heat flux:

$$\dot{Q}_A = Tr_A\{\hat{H'}_A\mathcal{L}_A^{eff}[\hat{\rho}(t)]\}dt \tag{10}$$

These are the definitions of work and heat fluxes that we will use to study the energy exchange between different interacting quantum systems.

4 Commuting interactionHamiltonian

4.1 Energy exchange in a closed system

In this section we will study the energy transfer in a closed quantum bipartite system. In particular we investigate the energy exchange between the electronic and vibrational degrees of freedom in a molecule. To do that, we consider a two level system(TLS) coupled linearly with the position of a harmonic oscillator(QHO). The Hamiltonian of the full system is given by:

$$H = \frac{\omega_{TLS}}{2}\hat{\sigma}_z + \omega_{QHO}\hat{a}^\dagger\hat{a} + g\hat{\sigma}_z(\hat{a} + \hat{a}^\dagger) \tag{11}$$

The first term of the right hand side represents the Hamiltonian of the TLS where ω_{TLS} is the difference between the frequencies of the upper and ground states and σ_z is the z-Pauli's matrix.The second term represents the Hamiltonian of the QHO where $\hat{a}^\dagger$ and $\hat{a}$ are the creation and annihilation operators and ω_{QHO} the oscillation frequency of the QHO.In this case we have redefined the zero-energy for the oscillator. The last term represents the coupling between both systems, where g is the strength constant.

An aspect to highlight here is that the TLS and the interacting Hamiltonians commute $[H_{TLS}, H_{int}] = 0$, and thus the population of the TLS remains invariable after the evolution. This is going to be crucial in the study of the evolution and thus of the thermodynamic properties. Another thing to take into account is that we have to distinguish between starting in an initial pure state,tensor product of initial pure states, or in a semi-mixed initial state, tensor product of a pure and a mixed state. In the former, after the evolution it is still possible to factorize the system as a product state, however in the latter since the TLS starts in a mixed state this is not going to be true any more and correlations between them are going to appear in time.We start considering the most general initial state for the TLS:

$$\rho_{TLS}(0) = c \mid e\rangle\langle e \mid + \sqrt{c(1-c)}\big(\mid e\rangle\langle g \mid + \mid e\rangle\langle g \mid\big) + (1-c)\mid g\rangle\langle g \mid \tag{12}$$

Where e and g make reference to the excited and ground state respectively and c is the probability of finding the electron in the excited state. For the oscillator we chose a coherent state, that is the best approximation to a classical wave [12]:

$$\rho_{QHO}(0) = \mid \alpha\rangle\langle \alpha \mid \tag{13}$$

Where $\mid \alpha\rangle = e^{\frac{-|\alpha|^2}{2}}\sum_{n=0}^\infty \frac{\alpha^n}{\sqrt{n!}}\mid n\rangle$, expanding it in the Fock basis $\mid n\rangle$. Now, if he density matrix of the full system at the beginning is given by:

$$\hat{\rho}(0) = \hat{\rho}_{TLS}(0) \otimes \hat{\rho}_{QHO}(0) \tag{14}$$

The evolved state of the full system can be written as:

$$\hat{\rho}(t) = U_I(t)\hat{\rho}_{TLS}(0) \otimes \hat{\rho}_{QHO}(0)U_I^\dagger(t) \tag{15}$$

Where $U_I(t) = e^{\frac{\sigma_z}{2}(\hat{a}^\dagger \alpha(t) - \hat{a}\alpha^*(t))}$ is the evolving operator in the interaction picture and $\alpha(t)$ is given by $\alpha(t) = \frac{2g}{\omega}(1 - e^{i\omega t})$ (for the derivation, see Appendix B). By studying (see Appendix C) the effective dynamics induced by one system over the other, and then based on the definitions of work and heat that Mahler & al. give in [1, 2, 3] we arrive at the following expression for the work flux into the oscillator:

$$\dot{W}_{TLS} = g(2c - 1)\left\{ \sqrt{\frac{2\omega_{QHO}}{m}}\langle \hat{p}\rangle + 2(2c - 1)g\sin(\omega_{QHO}t) \right\} \tag{16}$$

Where $\langle \hat{p} \rangle$ is the expected value of the oscillator momentum. Likewise studying the dynamics of the oscillator, we arrive at:

$$\dot{W}_{QHO} = -\dot{W}_{TLS} \tag{17}$$

We find that the work made by the TLS over the QHO is the same that the performed by the oscillator on the spin. We can see that this is a periodic function in time that depending on the probably c the sign and the amplitude of the work exchange between system will change.

Regarding to the heat, we do not find the same. Firstly, in order to have heat we need that the interaction Hamiltonian does not commutes with the Hamiltonian of the subsystem A in which we are studying the dynamics, $[H'_A, H_{int}] \neq 0$. We can check that under the interaction that we consider here $[H'_{TLS}, H_{int}] = 0$ since both, $H'_{TLS} = H_{TLS} + H^{eff}_{1,TLS}$ and H_{int} are proportional to σ_z, hence there is never a heat flowing into the spin. However, this is different for the oscillator where the commutator does not vanish and hence it is possible a heat flux into the spin. In order to this heat flows, we also need that correlated terms appear during the evolution and this only happens when we start with a semi-mixed state. Then, if the subsystem considered satisfied these two conditions, in our case the oscillator when the TLS starts in a mixed state, the heat flux into the oscillator is:

$$\dot{Q}_{QHO} = -iTr\left\{ [H'_{QHO}, H_{int}]C_{TLS,QHO}] \right\} \tag{18}$$

We arrive at that the purity of the initial state of the spin determines the thermodynamic behavior of our system. In the following table we present how is the energy exchange in this system where $[H_{TLS}, H_{int}] = 0$ based on the purity of the initial state of the TLS $P[\rho_{TLS}(0)]$:

Work flux	Heat flux
Does not depend on $P[\rho_{TLS}(0)]$: $\dot{W}_{QHO} = -\dot{W}_{TLS}$	Does depend on $P[\rho_{TLS}(0)]$: Pure state $\Rightarrow \dot{Q}_{QHO} = 0$ Mixed state $\Rightarrow \dot{Q}_{QHO} \neq 0$

Table 1: Energy exchange in a closed system based on the purity of the initial state of the oscillator $P[\rho_{TLS}(0)]$.

To sum up, what he have found so far is that if we have a pure initial state both systems behave as perfect drivers over each other, exchanging energy as work without any loses. It is not completely true, since due to the interaction there is always a drop in the purity of the oscillator that implies heat loses. However, it is insignificant, and we can neglect it. On the other hand, if we start in a semi-mixed state, the work exchange between them is the same but there is also a heat flux into the oscillator.

In both cases the work flux over the oscillator is based on displacement respect to its equilibrium position in one direction or another depending on the initial state of the TLS. In the case of the spin as the populations do not change in time, it less obvious how the work flux into the TLS modifies it. What really happens is that the effective dynamics induced by the QHO makes the energy gap of the TLS oscillate periodic in time.

Next, we show same graphs for the energy exchange dynamics in this closed system in resonance for different values of the probability c.
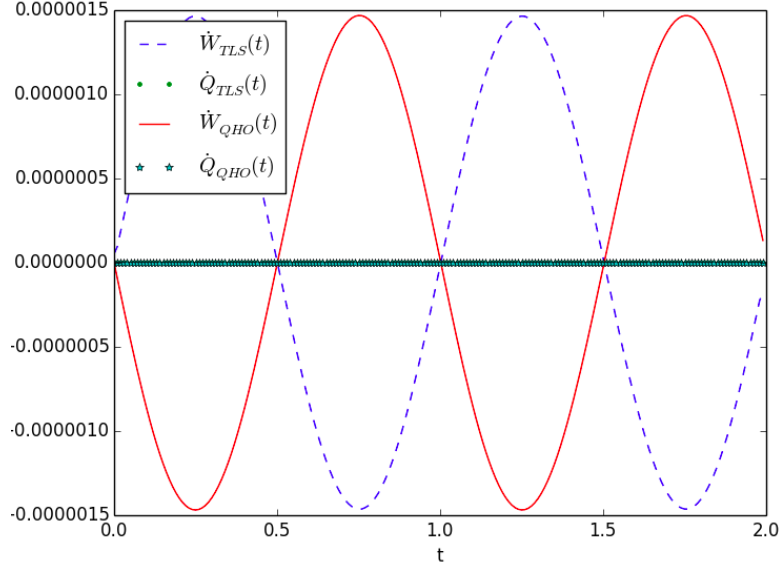
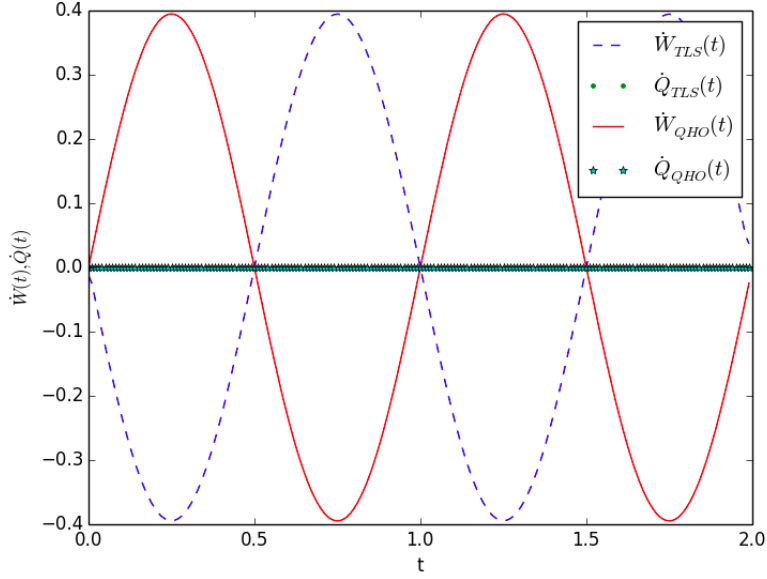Figure 2: Energy exchange.$g = 0.05 \cdot 2\pi, N = 15, \alpha = 0.1 + 0.0j, c = 0$

Figure 3: Energy exchange. $g = 0.05 \cdot 2\pi, N = 15, \alpha = 0.1 + 0.0j, c = 1$

In both cases presented above, we are dealing with a reciprocal energy transfer in form of work. Classically when we have a process where there is no heat present, we talk about an adiabatic thermodynamical process. But this behavior is not satisfied when the TLS starts in a mixed state as we show below:
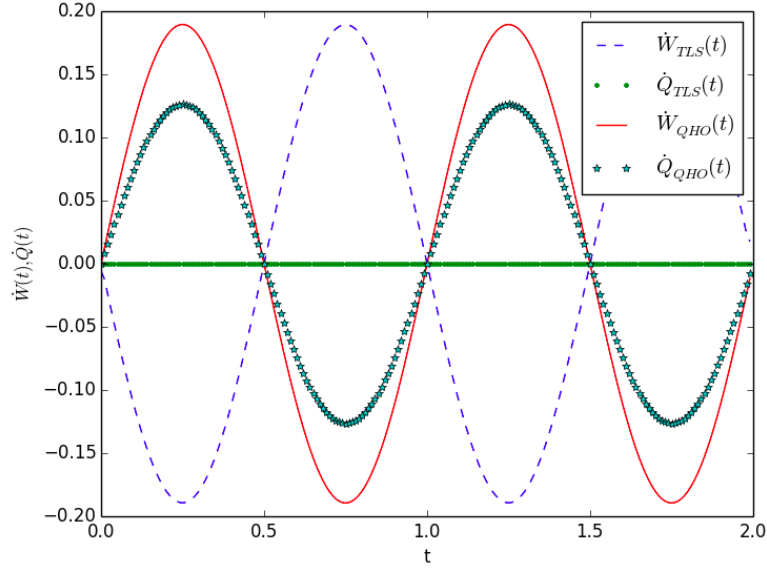
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Figure 4: Energy exchange.$g = 0.05 \cdot 2\pi, N = 15, \alpha = 0.1 + 0.0j, c = 0.8$
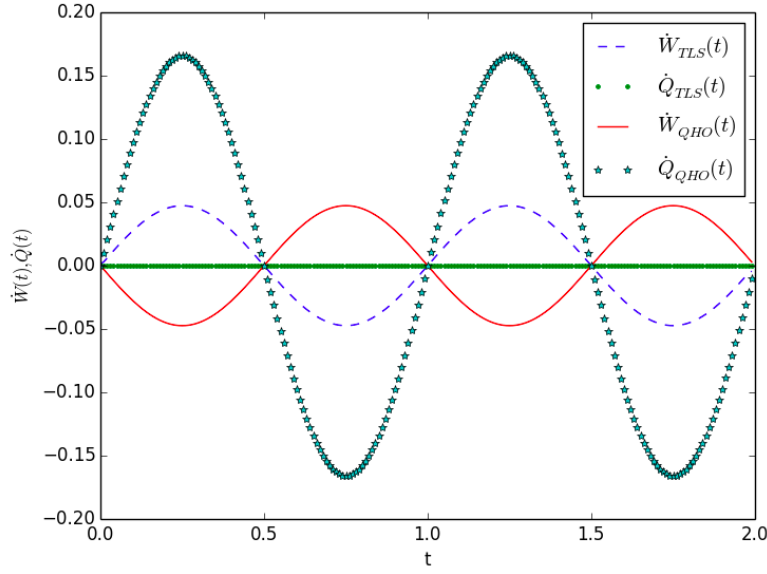
Figure 5: Energy exchange. $g = 0.05 \cdot 2\pi, N = 15, \alpha = 0.1 + 0.0j, c = 0.3$

As we have already mentioned, if the system starts in a mixed state, the heat flux for the TLS continues being zero $\dot{Q}_{TLS} = 0$, due to the interaction commutes with the Hamiltonian of the TLS, and thus the oscillator behaves still as a perfect driver in the sense that all the energy is transferred as work. But, what does happen with the heat flux into the oscillator? We said that

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a change in the purity is related with a change in the entropy. At first sight, if we associate entropy with disorder,we would hope that the entropy modified the dynamics of the oscillator losing such periodic behavior, but this is not what happens. The relation between purity, heat and entropy will be discussed further forward in the text.
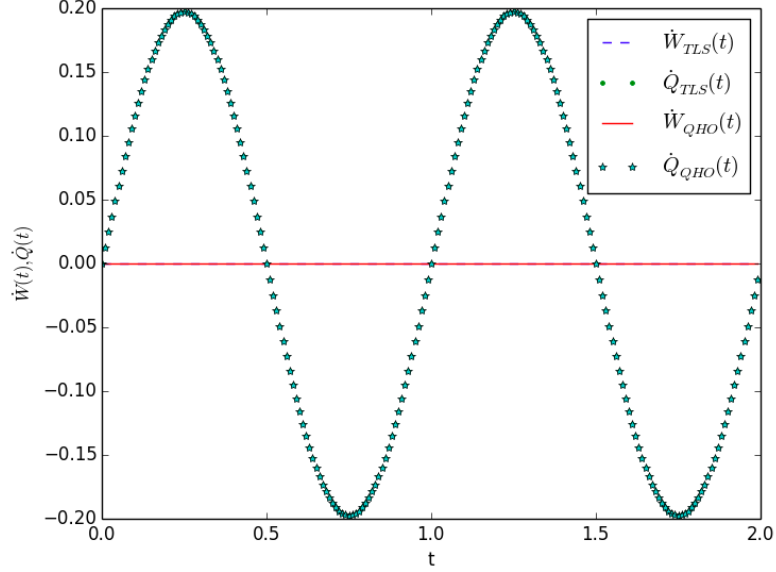
Figure 6: Energy exchange. $g = 0.05 \cdot 2\pi, N = 15, \alpha = 0.1 + 0.0j, c = 0.5$

In this graph we can see that there is only a heat flux into the oscillator. This leads to think if the local effective energy is conserved or not. What we realize is that in general, even in the case of a closed system the local effective energy is not conserved. In the following graph we plot the effective energy for the spin $\dot{U}_{TLS} = Tr_{TLS}\{H'_{TLS}\rho_{TLS}(t)\}$ and for the oscillator $\dot{U}_{QHO} = Tr_{TLS}\{H'_{TLS}\rho_{TLS}(t)\}$ and we see that this is not equal to zero.

Figure 7: Local effective energy. $g = 0.05 \cdot 2\pi, N = 15, \alpha = 0.1 + 0.0j, c = 0.3$

Therefore, although in general this energy is not conserved the total energy must be. This will not be just the sum of the effective local energies, but have to include the energy associated to the interaction.
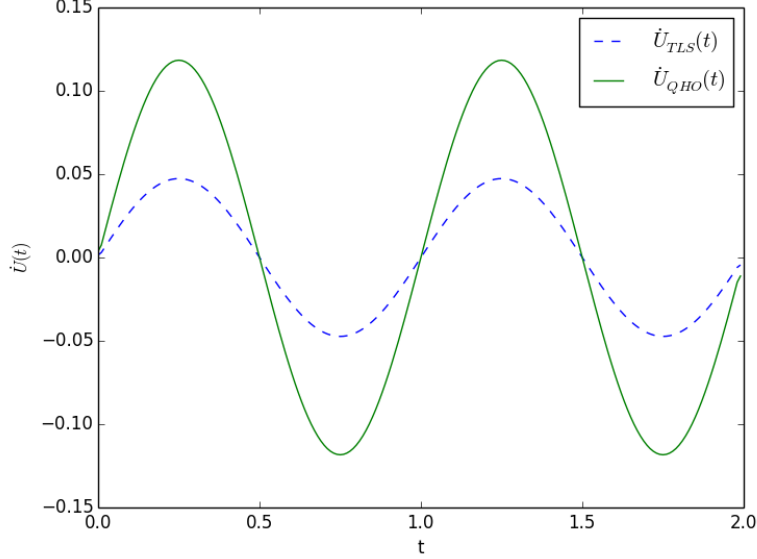
4.2 Purity behavior

When someone is working with classical heat engines or even quantum heat engines(QHE's), the efficiency of the process is given by the ratio between the work performed and the heat absorbed by the working substance. A system is considered to be more efficient as much as heat is transformed into work without loses.

Here we do not address the problem of defining an efficiency between work and heat fluxes for a subsystem, but it is of interest to investigate under what conditions a subsystem loses the ability of acting as a work source. In particular we analyze if the purity of the oscillator plays any role.

Why could the purity be a good candidate?. Since we have a interacting Hamiltonian that commutes with the TLS, independently of the initial state of this, its purity does not change in time, and hence we will never have a heat flux into the spin. However such commutation relation vanishes for the oscillator, and thus it is possible that a heat flows into it. As we have seen above heat appears for semi-mixed initial states, that facilitate the creation of correlations.

Such correlations depend on the mixedness of the composite system. The only possibility so that the full system keeps in a mixture of states during the evolution is that the mixedness of the reduced state of the oscillator changes in time. For this reason we consider that the heat in the system could be related with the purity of the QHO.

We make clear that there exits a relation between the purity of the initial state and the heat flux (Table.1). But what we want to investigate now is if such relation remains when we study the time-evolution of the purity. And this is what we show in the following graphs for different initial states of the spin.
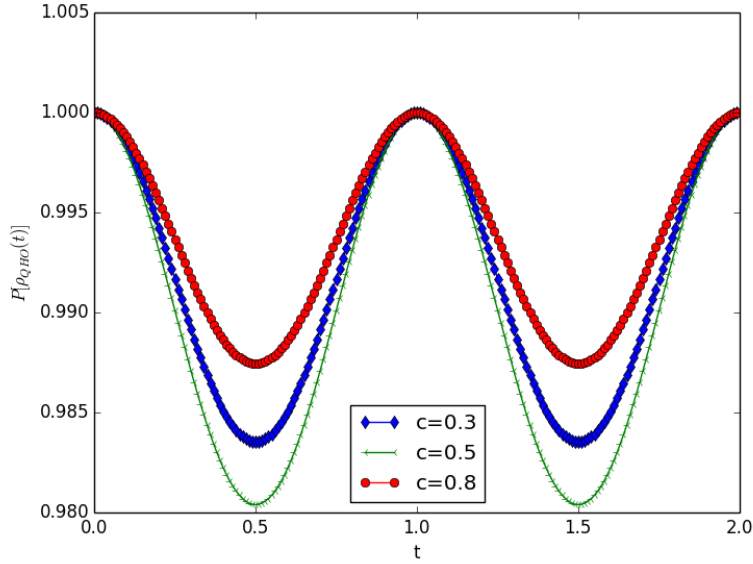

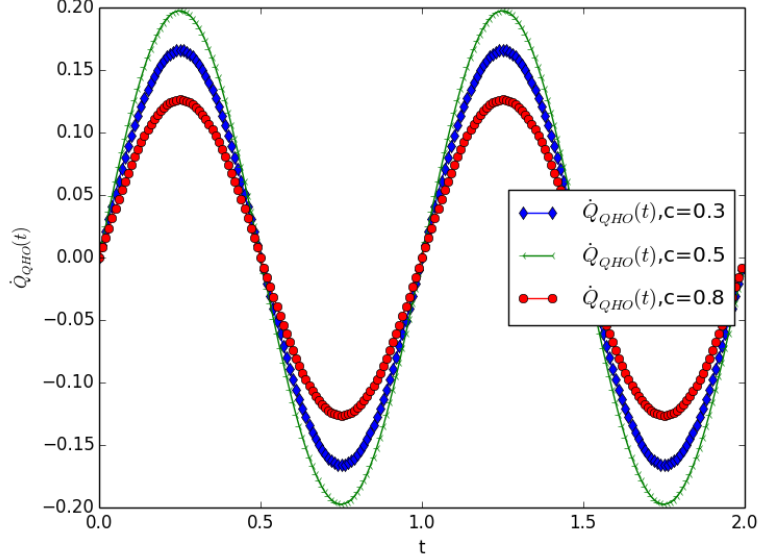Figure 8: Behavior of the purity $P[\rho_{QHO}(t)]$ for different values of c.

Figure 9: Heat flux $\dot{Q}_{QHO}(t)$ for different values of c.

We can observe that for $0 < c < 1$ the purity oscillates periodically in time, at the same frequency that the heat. and for the case of $c = 0.5$, the maximum of mixture, the purity reaches the minimum value.

The first thing that we notice and indicates us that maybe the purity is not a good candidate, appears looking at $c = 0.3$ and $c = 0.8$. In the former the purity decreases less than in the latter and nevertheless the amount of heat is bigger than for $c = 0.8$, therefore *less purity does not imply more heat.*

The only possible relation between the purity and the heat flux in time is given when the purity of the two subsystems evolve in the same way. In this case this is only true for pure states, where they are constant. Hence, with $c = 0$ and $c = 1$ the systems behave as perfect drivers over each other, but since there is no relation between purity and the amount of heat exchange we can not say that as closer as c is of one of these values my system will be acting better as a work source.

4.3 Energy exchange in an open system

Up to here we have studied the dynamic of our system coupled with a harmonic oscillator as closed system. Now we are going to put the system in contact with an environment, this would be a more realistic interpretation of what really happens in nature. In order to solve the evolution of this open quantum system we are going to derive the Master equation in the Lindblad

form making use of the Krauss decomposition.

One thing we have to take into account is that we consider that the environment is only seen by the QHO, and thus the jump operators ,that we define, simply affect the QHO. The interaction with the environment will be represented as a bath of harmonic oscillators described by the following Hamiltonian:

$$H_E = \sum_j \omega_{E,j} b_j^\dagger b_j \tag{19}$$

Where $\omega_{E,j}$ represents the different frequencies of each mode of oscillation and $b_j^\dagger b_j$ are the creation and annihilation operators of the bath respectively. The interaction with the oscillator is given by the following Hamiltonian:

$$H_I = \sum_j (\kappa_j^* a b_j^\dagger + \kappa_j a^\dagger b_j) \tag{20}$$

Where κ_j and κ_j^* are the coupling constants and $a^\dagger, a$ are the creation and annihilation operators of the oscillator. Therefore we can write the full Hamiltonian as:

$$H = \frac{\omega_{TLS}}{2} + \omega_{QHO} \hat{a}^\dagger \hat{a} + g\sigma_z (\hat{a}^\dagger + \hat{a}) + \sum_j \omega_{E,j} b_j^\dagger b_j + \sum_j (\kappa_j^* a b_j^\dagger + \kappa_j a^\dagger b_j) \tag{21}$$

We have already studied the dynamics considering the three first terms on the right hand side of the equation and we have seen that if our system was initially in a product of pure states, the evolution considering the H_{int} let us factorize the system as a tensor product $\rho(t) = \rho_{TLS}(t) \otimes \rho_{QHO}(t)$ without correlated terms. Now, even starting in a pure state this splitting is not going to be possible any more since the QHO is in contact with the bath.

We consider that the bath is only seen by the QHO, but as it is coupled with the spin as well , the dynamics of the TLS is also influenced by the environment. The steps that we follow to study the dynamics and hence the emergence of thermodynamics effects are the following:

- Firstly, we study the dynamics of the QHO under the coupling with the bath without forgetting that it is coupled with the TLS at the same time.

- Then, we study the dynamics of the closed system considered in the previous section, but taking into account the dynamics of the damped harmonic oscillator.

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- Finally, tracing over the system in which we are interested in studying the thermodynamic properties, we calculate the work and heat fluxes as we did in the case of a closed system.

Following the steps enumerate above, we start with the evolution of the QHO in contact with an environment represented by the following master equation:

$$\frac{\partial \rho_{QHO}(t)}{\partial t} = \frac{-i}{\hbar}[\hat{H}_{eff}, \hat{\rho_{QHO}(t)}]^* + \sum_{j=1} L_j \rho_{QHO}(t) \ L_j^\dagger \qquad (22)$$

The asterisk means that $\hat{H}_{eff}$ is non hermitian, but it is not related with the effective Hamiltonian that Mahler et *al* define in [1]. Indeed, it is define as $\hat{H}_{eff} = \hat{H}_{QHO} - \frac{-i\hbar}{2}\sum_{j=1} L_j^\dagger L_j$ where L_j are the jump operators. In this case we define two jump oscillators. One $L_1 = \sqrt{\Gamma}\hat{a}$, lets the harmonic oscillator jump down from upper to down levels where Γ is the rate of decaying and another, $L_2 = \sqrt{\gamma}\hat{a}^\dagger$ lets it jump up with a rate of absorption given by γ. Following all the algebra (see Appendix E), we arrive at the Markovian Master equation for the damped harmonic oscillator:

$$\frac{\partial \rho_{QHO}(t)}{\partial t} = \frac{-i}{\hbar}[H_{QHO}, \hat{\rho}_{QHO}(t)] + \hat{D}(\hat{\rho}_{QHO}(t)) \qquad (23)$$

where $\hat{D}(\hat{\rho}_{QHO}(t))$ is named the dissipator of the oscillator given by:

$$\hat{D}(\hat{\rho}_{QHO}(t)) = \Gamma\hat{a}\hat{\rho}_{QHO}(t)\hat{a}^\dagger + \gamma\hat{a}^\dagger\hat{\rho}_{QHO}(t)\hat{a} - \frac{1}{2}\{\Gamma\hat{a}^\dagger\hat{a} + \gamma\hat{a}\hat{a}^\dagger, \hat{\rho}_{QHO}(t)\} \qquad (24)$$

Computing the populations and coherences we finally arrive at the following expression for the reduced density operator of the oscillator:

$$\rho_{QHO}(t) = P(n)e^{-(n\Gamma+(n+1)\gamma)t} \mid n\rangle\langle n \mid \qquad (25)$$

Where $P(n)$ is the Poissonian distribution that defines the probability of finding n photon in a coherent state, what means that photons in a coherent state behave as a randomly distributed classical particles. In this case such a probability decay exponentially in time. Taking all of this into account we can now study the energy flow for the total system. Writing the master equation of the full evolve state and using the same jumps operator, we arrive at the Markovian Master equation for the full system:

$$\frac{\partial \rho_{TLS}(t)}{\partial t} = \frac{-i}{\hbar}Tr_{QHO}\{[H_{TLS} + H_{QHO} + H_{int}, \hat{\rho}(t)]\} + Tr_{QHO}\{\hat{D}(\hat{\rho}(t))\} \qquad (26)$$

where $\hat{D}(\hat{\rho}(t))$ is the dissipator, but now of the full system:

$$\hat{D}(\hat{\rho}(t)) = \Gamma\hat{a}\hat{\rho}(t)\hat{a}^\dagger + \gamma\hat{a}^\dagger\hat{\rho}(t)\hat{a} - \frac{1}{2}\{\Gamma\hat{a}^\dagger\hat{a} + \gamma\hat{a}\hat{a}^\dagger, \hat{\rho}(t)\} \qquad (27)$$

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Choosing one of the systems as the measurement basis, for example the TLS in an initial pure state and following the same steps that in previous cases (Appendix E) we arrive at the following expression for work flux:

$$\dot{W}_{TLS} = -(P(n))^2 e^{-2(n\Gamma + (n+1)\gamma)t} 2g^2 \sin(\omega t) \qquad (28)$$

And can be proved that for the spin the heat flux is null:

$$\dot{Q}_{TLS} = Tr_{TLS}\left\{\hat{H}'_{TLS}\hat{D}(\rho_{TLS}(t))\right\} = 0 \qquad (29)$$

Where $\hat{H}'_{TLS} = \hat{H}_{TLS} + \hat{H}_{1,TLS}^{eff}$. Doing the same for the oscillator we find:

$$\dot{W}_{QHO} = -\dot{W}_{TLS} \qquad (30)$$

for the work flux and for the heat flux:

$$\dot{Q}_{QHO} = Tr_{QHO}\left\{\hat{H}_{QHO}\hat{D}(\rho_{QHO}(t))\right\} \qquad (31)$$

So far we have what we had for the closed system; the work exchange depends on the purity of the initial state of the TLS and it is reciprocal between subsystems. However, the heat flux never vanishes into the oscillator independently of the initial state of the spin.

The way in which a damped harmonic oscillator changes the dynamics is that we have no longer neither periodic displacements for the QHO nor periodic energy gap oscillations. The coupling of the oscillator with the environment induces a decaying in the amplitude in the dynamics and thus in the work and heat fluxes. In this case, likewise in the closed system the local effective energy is not conserved, but the total energy of the spin, oscillator and bath has to be despite of the dissipation.

If the time t approaches to infinite, the absorption and emission rate would satisfy the detailed balance, and hence the populations of the QHO would reach the thermal equilibrium. This yields to a situation without any decay in the amplitude of the oscillations, as if the initial state of the oscillator were a Gibbs state.

To sum up, in this more realistic interpretation, in spite of the fact that the system is not closed any more, is possible a work exchange between them. The oscillator is still a good driver over the spin, in the sense that there is not heat flux into it, but not perfect since the energy flux decays exponentially in time. However, after a relaxation time if the oscillator reaches such Gibbs state, we will recover a periodic energy exchange without dissipation.

5 Non-commuting interaction Hamiltonian

Up to here we have studied an interacting Hamiltonian that commutes with the Hamiltonian of the TLS. In this section we deal with an interaction that does not. The Hamiltonian that we consider is the well-studied Jaynes-Cummings Hamiltonian that reproduces the interaction between the light an atom in a cavity:

$$H = \frac{\omega_{TLS}}{2}\hat{\sigma}_z + \omega_{QHO}\hat{a}^\dagger\hat{a} + g(\hat{a}\sigma_+ + \hat{a}^\dagger\sigma_-) \tag{32}$$

Where the first two terms are the Hamiltonians of the TLS and the QHO respectively and the last one the intreating Hamiltonian in the rotating wave approximation(RWA). The term $\hat{a}\sigma_+$ describes the process in which an atom is taken from the lower state into the upper and a photon is annihilated, whilst $\hat{a}^\dagger\sigma_-$ describes the opposite process with the creation of a photon; in both cases the energy is conserved.

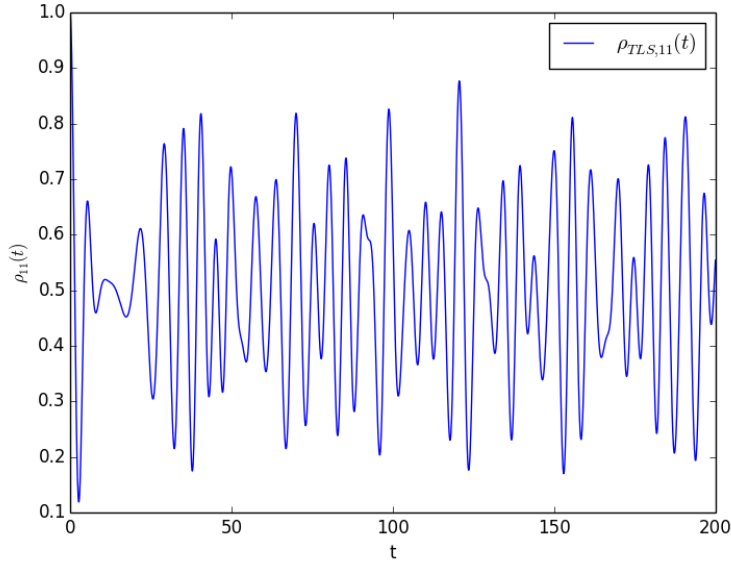Figure 10: Collapse and revival for the population$\rho_{11,TLS}(t)$in resonance for $g = 0.05 \cdot 2\pi, N = 30, \alpha = 3 + 0.0j, c = 1$

In this approximation is possible to diagonalize the Hamiltonian analitically, however here we studied the dynamics and the thermodynamic properties numerically. The numerical results that we show below have been computed using *QuTiP* a Quantum Toolbox in *Python.*(See Appendix F)

5.1 Energy exchange in a closed system

As we did with the first Hamiltonian studied above, here we show several graphs of the work and heat in this system for different values of the probability c.
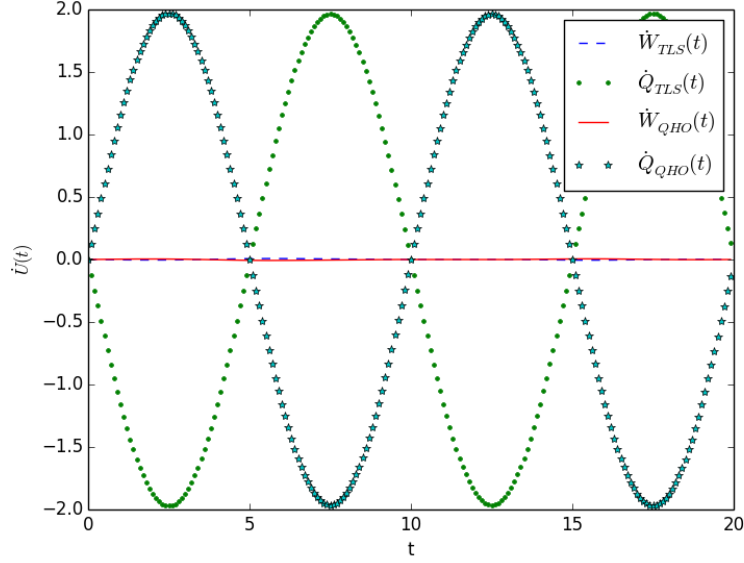
Figure 11: Energy exchange $\dot{U}(t)$ in resonance for c=1.

What we can observe in this figure and if we plotted for the rest of values of c is that the heat flux is the way in which the subsystem exchanges energy throughout the JCH in the RWA. The heat flux oscillates periodically, and as long as we decrease in c, the amplitude of heat exchange decrease as well, as we can see in the following figure:
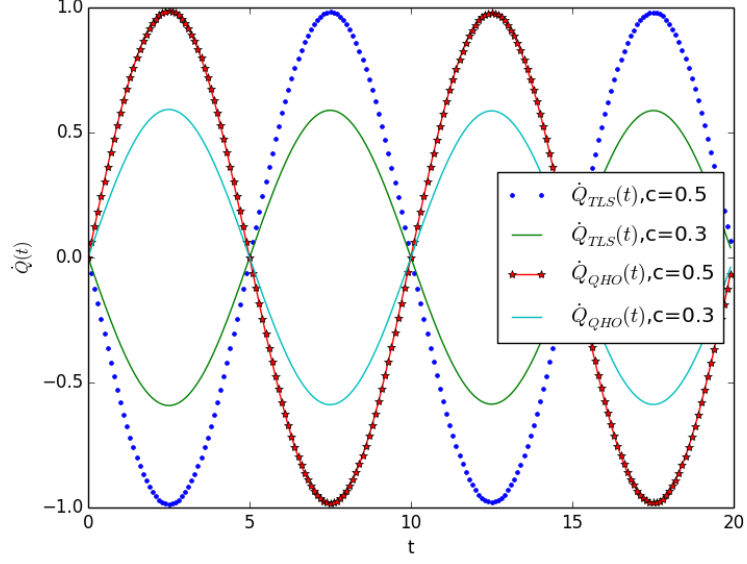
Figure 12: Decreasing of the heat flux $\dot{Q}(t)$ for different values of c.

And finally when the spin is in the ground state, what we obtain is:
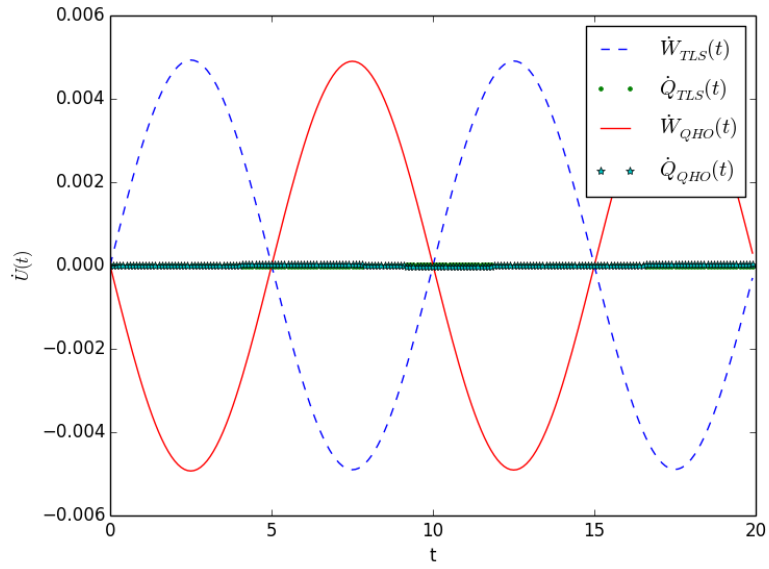
Figure 13: Energy exchange $\dot{U}(t)$ in resonance for c=0.

In this situation the predominant form of exchanging energy is as work,

although is very small. If we amplified the image we could see that there exits a heat flux, although it is very small:
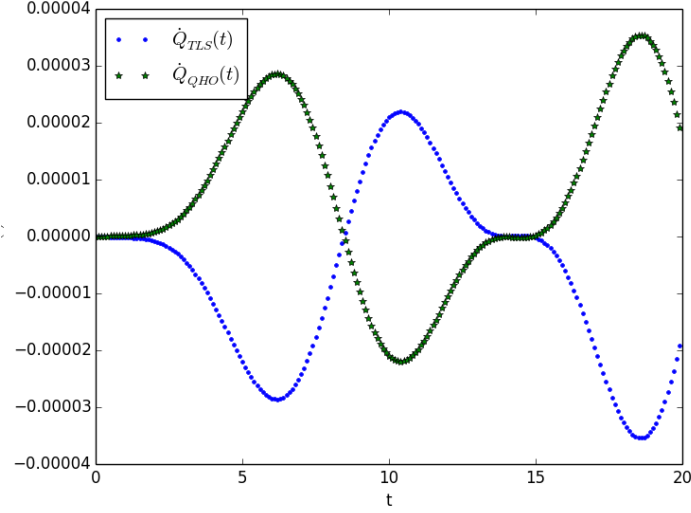
Figure 14: Heat beating pattern for c=0.

This beating pattern is also exhibited by the work during all the time that the heat dominates:
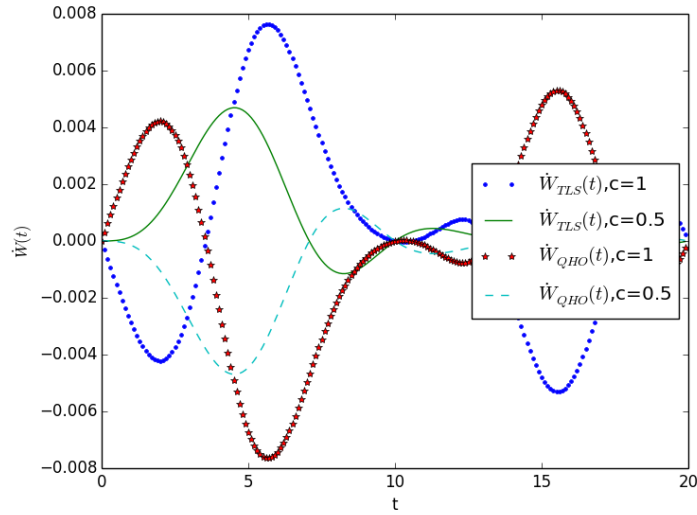
Figure 15: Work beating pattern for different values of c.

What we understand studying these graphs is that if we have a interact-

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ing Hamiltonian that does not commute with none of the Hamiltonians of the system, the predominant way of exchange energy is as heat. One thing that we notice is that under this interaction both are always present. When heat dominates, we have small work fluxes oscillating at different frequencies and if the work dominates there are heat fluxes oscillating with more than one frequency as well.

Likewise in the other studied cases, although the total energy is conserved the local effective energy is not. But in contrast with such previous situations, here the heat is exchanged in a reciprocal way as the work does. Therefore, if we have a resonant cavity and suppressing these beating patterns we could say that if the spin starts in the excited state, they act as a perfect heat sources over each other. The amplitude of the heat fluxes decay as soon as the probability of finding the electron in the ground state increases. When it decays into the state with lower energy, the heat is minimum and it could be possible to talk about a reciprocal work exchange, although the amount is much lower than when they acted as heat sources.

5.2   Purity behavior

We had arrived at the conclusion that the heat did not depend on the purity of the oscillator in the case that the populations of the TLS did not change in time. Just in case that we had pure states $c = 0$ and $c = 1$, where there is only work, the purity and the amount of heat are agreed, but in general they do not.

Here, trying to look for a relation could be more difficult since the purity of both changes in time, as we show in the following graphs:
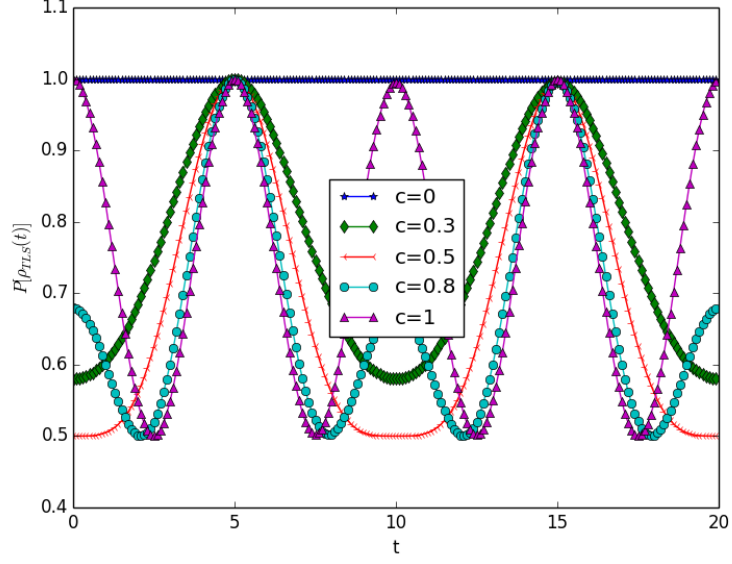
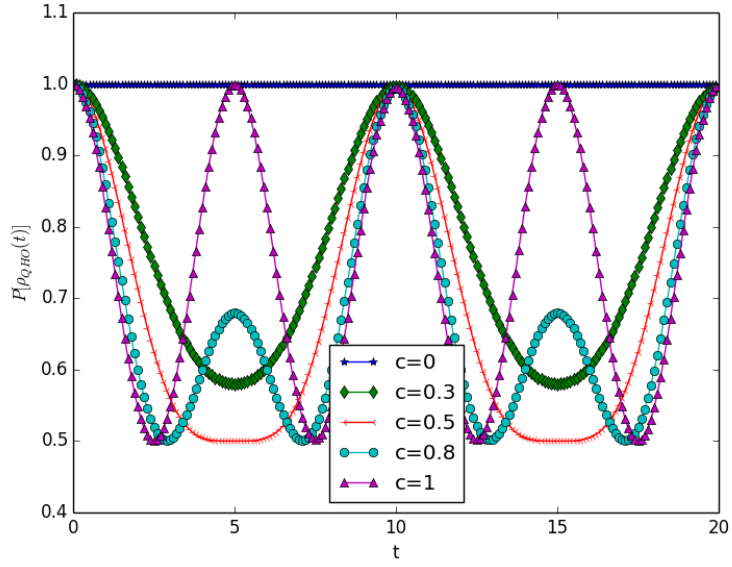Figure 16: Behavior of the purity $P[\rho_{TLS}(t)]$ for different values of c.

Figure 17: Behavior of the purity $P[\rho_{QHO}(t)]$ for different values of c.

We can notice that for $c = 0$, the purity of both remains constant in time and without taking into account the beating patterns there is only work, that is what we would expect. In the case of $c = 1$ the purity changes

in time, but both purities change in the same way, with the same frequency and amplitude. Looking at Fig.11 we see that every semi period the heat is null, and that corresponds with a purity equal to the unity each semi period as well. For the rest values of c the behavior of the two purities is the same with the exception of phase differences, but we cannot relate them with the heat graphs

In the both cases studied, we realized that the purity has different behaviors depending on the interaction and the initial state of my system, and as we have already said in the study of the purity of the closed system, *just in case that the purities of both systems have the same behavior in time, we can know deterministically the conduct of the heat* . If they do not behave in the same way, we can not use the purity as a measure for the capacity of work source.

To sum up, if my system remains always in a pure state, it means in a product of pure states every time, there is only work exchange, or at least the work dominates. In that sense a constant purity has more weight in the emergence of energy exchange as work than a non commuting Hamiltonian that creates correlations. But in the competition between non- commuting Hamiltonian, and commuting- hamiltonian, between work or heat domination, the latter wins.

6   Conclusion and remarks

Comparing our results with those discussed in the literature, we see that we do not need the presence of an external driver or time-dependent Hamiltonians to identify work and heat in the quantum regime, other thing would be if we wanted implement a QHE. We show that choosing two quantum systems and letting them evolve by means of an interaction, the effect of one subsystem over the other is enough to induce time-dependent Hamiltonians in the local dynamics of the other subsystem, and thus work can be present.

What we find is that classical concepts as work and heat can emerge from quantum systems when I consider the local properties of one subsystem, that is, when I measure the basis of the system which we are interested in studying the thermodynamic behavior. These quantities are not symmetrical and they are also state-dependent. However, if my systems are in resonance, independently from the chosen basis, the amount of work exchanged between them is equal and reciprocal. This is fulfilled by closed and open systems, by commuting or non-commuting Hamiltonians.

But if we are looking for a perfect driver, energy exchange without heat

loses, we have to take into account, the state of my system, the interaction, and the surroundings. For example in the first case studied, we have seen that considering a commuting interaction with my system, the QHO was always a perfect driver over the spin, nevertheless the spin only acted as a good driver when it started in a pure state . For semi-mixed states a heat always flows into the QHO, and hence although the local effective energy is conserved, the total energy does not.That extra heat in the system should be related with the linear entropy of the oscillator. An increase in the heat flux, should imply an increase in the linear entropy.

The behavior of purity, entropy and heat is not entirely clear and it needs a deep understanding. The definition of heat given in Eq.(2) does not go far enough out of the equilibrium or when we have to include the interaction with the environment. If at the beginning we said: *a change in the purity is related with a change in the entropy and thus with heat*, now we can affirm that the purity can determine the appearance of heat, but in general it could not be used as indicator of the amount of heat in the system. Although the entropy depends on the purity, it is only true that an amount of entropy is directly related with the amount of heat, not the purity.

The question is that the heat flux into a system takes into account the correlation terms between subsystems whereas the purity of such system does not. For instance, the purity can decrease and it reaches a minimum due to the fact that systems are more correlated. However, the correlation terms Eq.(D.15) can tend to zero since it is more difficult to split the evolve state as tensor product of states and thus the heat tends to zero as well Eq.(A.38). The sign of such correlation affects the heat, but not the purity, and for that reason the definition of heat given in Eq.(2) fails when we consider the effects of one system over the other.

We have also studied the difference between having a non-commuting or a commuting interaction, and we have seen that in general every time that we have an interaction that does not commute with none of the coupled systems, the heat dominates, and it is usually much bigger than the work, independently on the purity. However, in the case of a commuting Hamiltonian, changing the purity, I can do comparable both quantities, or even suppress one of them .

What we can conclude is that, it is possible to find quantum composite systems that behave in the same way that classical drivers. Isolating my system, choosing a proper initial state, and a commuting-interaction, they can act as an autonomous work drivers over each other, and thus we see that thermodynamics is not only linked to macroscopic concepts.

7 Open questions

A further research could be done regarding to the linear entropy. It would be interesting to study the correlations that exist between this and the heat flux, and which physical effects have the entropy in the systems studied. In equilibrium thermodynamics, we know that entropy and heat are linear dependents with temperature. Up to know such relation is not clear in quantum systems, therefore a research in this area could be motivated but at the same time delicate.

Another future research could be studying the coupling considering other quantum systems, as for example two spins. Using different environments and put the full system embedded into it. It would be also fine to see if this model could be generalized for more than one bipartite system.

Finally, we could try to use composite bipartite systems as a *quantum substance* for QHE's to implement quantum thermodynamical cycles and analyze in these cases how is the efficiency of the machine or try to see if the composite system could be use as a *resource* to extract work.

Appendix A

Work and Heat using LEMBAS

We want to investigate if we are able to talk about thermodynamics in quantum systems, and namely analyze whether we can define in the same way classical concepts as work or heat. To do that we follow the method described by Mahler at al. in[**?**], therefore the first step is try to understand how they define these concepts.In order to do this, here we try to arrive at the same expressions. We consider a bipartite quantum system described by the following Hamiltonian:

$$\hat{H} = \hat{H}_A + \hat{H}_B + \hat{H}_{AB} \tag{A.1}$$

Where $\hat{H}_A$ represents the Hamiltonian acting over the subspace A, $\hat{H}_B$ the subsystem acting over the space of the system B and $\hat{H}_{AB}$ the interaction between the two subsystems. We are interesting in knowing the evolution of the system A under the interaction with the system B , thus the evolution of A can be written as:

$$\frac{\partial \hat{\rho}_A}{\partial t} = -i\hbar Tr_B\{[\hat{H}, \hat{\rho}]\} = -i\hbar Tr_B\{[\hat{H}_A + \hat{H}_B + \hat{H}_{AB}, \hat{\rho}]\} \tag{A.2}$$

$$\frac{\partial \hat{\rho}_A}{\partial t} = -i\hbar \left(Tr_B\{[\hat{H}_A, \hat{\rho}]\} + Tr_B\{[\hat{H}_B, \hat{\rho}]\} + Tr_B\{[\hat{H}_{AB}, \hat{\rho}]\} \right) \tag{A.3}$$

For the following property of the trace:

$$Tr_B\{[1 \otimes B; C]\} = 0 \tag{A.4}$$

the term relationed with the trace over B disappears, and thus we have that the trace of a commutator vanishes:

$$\frac{\partial \hat{\rho}_A}{\partial t} = -i\hbar\left(Tr_B\{[\hat{H}_A, \hat{\rho}]\} + Tr_B\{[\hat{H}_{AB}, \hat{\rho}]\}\right) \qquad (A.5)$$

Now we suppose that the evolved density matrix of the full system can be written as:

$$\hat{\rho} = \hat{\rho}_A(t) \otimes \hat{\rho}_B(t) + \hat{C}_{AB}(t) \qquad (A.6)$$

Where $\hat{\rho}_A(t)$ is the reduced density matrix of the system A, $\hat{\rho}_B(t)$ the ones of the system B and $\hat{C}_{AB}(t)$ the correlated term that can appear after the evolution due to the coupling. Here, we supposed that these terms arise and substituting above we arrive at:

$$\frac{\partial \hat{\rho}_A}{\partial t} = -i\hbar\left(Tr_B\{[\hat{H}_A, \hat{\rho}_A(t) \otimes \hat{\rho}_B(t)]\} + Tr_B\{[\hat{H}_A, \hat{C}_{AB}(t)]\right.$$
$$\left. +Tr_B\{[\hat{H}_{AB}, \hat{\rho}_A \otimes \hat{\rho}_B(t)] + Tr_B\{[\hat{H}_{AB}, \hat{C}_{AB}(t)]\}\right) \qquad (A.7)$$

Making use of the invariance of the trace we have :

$$Tr_B\{[\hat{H}_A, \hat{C}_{AB}(t)]\} = \hat{H}_A Tr_B\{\hat{C}_{AB}(t)\} - \hat{H}_A Tr_B\{\hat{C}_{AB}(t)\} = 0 \quad (A.8)$$

Since $Tr_B\{\hat{H}_A \hat{C}_{AB}(t)\} = Tr_B\{\hat{H}_A \hat{C}_{AB}(t)\}$ and $Tr_B\{\hat{C}_{AB}(t)\} = 0$

Taking this into account:

$$\frac{\partial \hat{\rho}_A}{\partial t} = -i\hbar\left(Tr_B\{[\hat{H}_A, \hat{\rho}_A(t) \otimes \hat{\rho}_B(t)]\} + Tr_B\{[\hat{H}_{AB}, \hat{\rho}_A(t) \otimes \hat{\rho}_B(t) + Tr_B\{[\hat{H}_{AB}, \hat{C}_{AB}(t)]\}\right)$$
$$(A.9)$$

Another trace theorem sais:

$$Tr_B\{[\hat{C}, \hat{A} \otimes \hat{B}]\} = [Tr_B\{\hat{C}(\hat{1} \otimes \hat{B})\}, \hat{A}] \qquad (A.10)$$

therefore:

$$Tr_B\{[\hat{H}_{AB}, \hat{\rho}_A(t) \otimes \hat{\rho}_B]\} = [Tr_B\{\hat{H}_{AB}(\hat{1} \otimes \hat{\rho}_B)\}, \hat{\rho}_A] = [\hat{H}_A^{eff}(t), \hat{\rho}_A(t)]$$
$$(A.11)$$

And thus we define the effective Hamiltonian $\hat{H}_A^{eff}(t)$ as:

$$\hat{H}_A^{eff}(t) = Tr_B\{\hat{H}_{AB}(\hat{1} \otimes \hat{\rho}_B(t))\} \qquad (A.12)$$

Here we can see that these effective Hamiltonians that are implied in the evolution of one of the systems, are the expectation value of the interaction in the basis of the other system which is coupled. The first term of the right hand side in Eq.(A.9) also turns into:

$$Tr_B\{[\hat{H}_A, \hat{\rho}_A(t) \otimes \hat{\rho}_B(t)]\} = [Tr_B\{\hat{H}_A(\hat{1} \otimes \hat{\rho}_{B(t)})\}, \hat{\rho}_A] = [\hat{H}_A, \hat{\rho}_A(t)] \quad (A.13)$$

Therefore the evolve density matrix of the system A is

$$\frac{\partial \hat{\rho}_A}{\partial t} = -i\hbar\bigg([\hat{H}_A + \hat{H}_A^{eff}(t), \hat{\rho}_A(t)] + Tr_B\{[\hat{H}_{AB}, \hat{C}_{AB}(t)]\}\bigg) \qquad (A.14)$$

Where we denote $\mathcal{L}_{inc}(\hat{\rho}(t)) = -i\hbar Tr_B\{[\hat{H}_{AB}, \hat{C}_{AB}(t)]\}$ and thus we have:

$$\frac{\partial \hat{\rho}_A}{\partial t} = -i\hbar[\hat{H}_A + \hat{H}_A^{eff}(t), \hat{\rho}_A] + \mathcal{L}_{inc}(\hat{\rho}(t)) \qquad (A.15)$$

As we are interested in obtain the properties of the system A only the part of $\hat{H}_A^{eff}(t)$ that commuteS with $\hat{H}_A$ will affect the evolution.

We can rewrite the effective Hamiltonian making use of the spectral decomposition:

$$\hat{H}_A^{eff} = \sum_{j,k}(\hat{H}_A^{eff})_{jk} \mid j\rangle\langle k \mid \qquad (A.16)$$

The commutation relation will be:

$$[\hat{H}_A, \hat{H}_A^{eff}(t)] = \sum_{j,k}[\hat{H}_A, \mid j\rangle\langle k \mid] = \sum_{j,k}\omega_{jk} \mid j\rangle\langle k \mid \qquad (A.17)$$

Therefore in order to this begins zero its necessary that the energetic differences becomes zero, and that is that the energy levels are the same. Under this consideration we can write that $\hat{H}_{1,A}^{eff}$ will be:

$$\hat{H}_{1,A}^{eff} = \sum_{j,j}(\hat{H}_A^{eff})_{jj} \mid j\rangle\langle j \mid \qquad (A.18)$$

And thus the part that does not commute with $\hat{H}_A$ is:

$$\hat{H}_{2,A}^{eff} = \hat{H}_A^{eff} - \hat{H}_{1,A}^{eff} \qquad (A.19)$$

Therefore is more appropriately to write the Eq.(A.15) as:

$$\frac{\partial \hat{\rho}_A}{\partial t} = -i\hbar[\hat{H}_A + \hat{H}_{1,A}^{eff}, \hat{\rho}_A] + \mathcal{L}_{inc}(\rho(t)) \qquad (A.20)$$

with $\hat{H}'_A$ is:

$$\hat{H}'_A = \hat{H}_A + \hat{H}_{1,A}^{eff} \qquad (A.21)$$

Now the change in the internal energy is given by:

$$dU = \frac{d}{dt}Tr_A\{\hat{H}'_A\hat{\rho}_A\}dt = Tr\{\dot{\hat{H}'_A}\hat{\rho}_A + \hat{H}'_A\dot{\hat{\rho}_A}\}dt \qquad (A.22)$$

Since $\hat{H}_A$ does not depend on time, the first term of the right hand side vanishes:

$$Tr_A\{(\dot{\hat{H}}_A + \dot{\hat{H}}_{1,A}^{eff})\hat{\rho}_A\} = Tr_A\{(\dot{\hat{H}}_{1,A}^{eff})\hat{\rho}_A\} \tag{A.23}$$

In the second part that includes the change in the density operator we include what we obtained in Eq.(A.15):

$$Tr_A\{\hat{H}'_A\dot{\hat{\rho}}_A\} = Tr_A\{-i\hbar\hat{H}'_A[\hat{H}_A + \hat{H}_A^{eff}, \hat{\rho}_A] + \hat{H}'_A\mathcal{L}_{inc}(\rho(t))\} \tag{A.24}$$

By including the following relations $\hat{H}_A = \hat{H}'_A - \hat{H}_{1,A}^{eff}$ and $\hat{H}_A^{eff} = \hat{H}_{1,A}^{eff} + \hat{H}_{2,A}^{eff}$ we can rewrite the commutator as:

$$\hat{H}'_A[\hat{H}'_A + \hat{H}_{2,A}^{eff}, \hat{\rho}_A] = \hat{H}'_A[\hat{H}'_A, \hat{\rho}_A] + \hat{H}'_A[\hat{H}_{2,A}^{eff}, \hat{\rho}_A] \tag{A.25}$$

Taking into account the following relation between commutators:

$$B[A, C] = [A, BC] - [A, B]C \tag{A.26}$$

We finally arrive at:

$$\hat{H}'_A[\hat{H}'_A, \hat{\rho}_A] = [\hat{H}'_A, \hat{H}'_A\hat{\rho}_A] - [\hat{H}'_A, \hat{H}'_A]\hat{\rho}_A \tag{A.27}$$

After tracing over these terms, the first commutator vanishes due to the fact that the trace of a commutator is zero and the second commutator vanishes since operators acting over the same subspace commute, thus:

$$\hat{H}'_A[\hat{H}'_A, \hat{\rho}_A] = 0 \tag{A.28}$$

Doing the same with the second term of Eq.(25):

$$\hat{H}'_A[\hat{H}_{2,A}^{eff}, \hat{\rho}_A] = [\hat{H}_{2,A}^{eff}, \hat{H}'_A\hat{\rho}_A] - [\hat{H}_{2,A}^{eff}, \hat{H}'_A]\hat{\rho}_A \tag{A.29}$$

Where the first term on the right hand side vanishes when we tracing over it and the second remains. Therefore we can write down the change in the internal energy as:

$$dU = \frac{d}{dt}Tr_A\{\hat{H}'_A\hat{\rho}_A\} = Tr_A\{(\dot{\hat{H}}_{1,A}^{eff})\hat{\rho}_A - i[\hat{H}'_A, \hat{H}_{2,A}^{eff}]\hat{\rho}_A + \hat{H}'_A\mathcal{L}_{inc}(\rho(t))\}dt \tag{A.30}$$

By splitting this equation into one part, the work flux relates with a non-entropy change :

$$\dot{W}_A = Tr_A\{(\dot{\hat{H}}_{1,A}^{eff})\hat{\rho}_A - i[\hat{H}'_A, \hat{H}_{2,A}^{eff}]\hat{\rho}_A\} \tag{A.31}$$

And into another one with a change in the entropy of the system, that is a heat flux:

$$\dot{Q}_A = Tr_A\{\hat{H}'_A\mathcal{L}_{inc}(\hat{\rho}(t))\} \tag{A.32}$$

We are going to rewrite this expression in such a way that let us determine faster if there is heat flux or not.

By introducing $\mathcal{L}_{inc}(\hat{\rho}(t)) = -iTr_B\{[\hat{H}_{AB}, \hat{C}_{AB}(t)]\}$ (with $\hbar = 1$),into the formula of the heat:

$$\dot{Q}_A = Tr_A\{\hat{H}'_A - iTr_B\{[\hat{H}_{AB}, \hat{C}_{AB}(t)]\}\} \tag{A.33}$$

Where $\hat{H}'_A = \hat{H}_A + \hat{H}_{1,A}^{eff}$. We can take out the two traces:

$$\dot{Q}_A = -iTr_A Tr_B\{\hat{H}'_A[\hat{H}_{AB}, \hat{C}_{AB}(t)]\} \tag{A.34}$$

The product of the trace acting over two different spaces is equal to the the trace of the tensor product of spaces, and thus $Tr_A \cdot Tr_B = Tr$ acting over $\mathcal{H}_A \otimes \mathcal{H}_B$. Expanding the commutator:

$$\dot{Q}_A = -iTr\{\hat{H}'_A(\hat{H}_{AB}\hat{C}_{AB}(t) - \hat{C}_{AB}(t)\hat{H}_{AB})\} \tag{A.35}$$

Multiplying both terms by $\hat{H}'_A$:

$$\dot{Q}_A = -iTr\{\hat{H}'_A\hat{H}_{AB}\hat{C}_{AB}(t) - \hat{H}'_A\hat{C}_{AB}(t)\hat{H}_{AB})\} \tag{A.36}$$

Using the cyclic property of the trace $Tr\{ABC\} = Tr\{CAB\}$ in the second term:

$$\dot{Q}_A = -iTr\{\hat{H}'_A\hat{H}_{AB}\hat{C}_{AB}(t) - \hat{H}_{AB}\hat{H}'_A\hat{C}_{AB}(t))\} \tag{A.37}$$

Where substituting by the commutator $[\hat{H}'_A, \hat{H}_{AB}] = \hat{H}'_A\hat{H}_{AB}\hat{C}_{AB}(t) - \hat{H}_{AB}\hat{H}'_A$, we finally arrive at:

$$\dot{Q}_A = -iTr\{[\hat{H}'_A(t), \hat{H}_{AB}]\hat{C}_{AB}(t)\} \tag{A.38}$$

We can see directly from here that I need two conditions to have heat flux into the subsystem considered, one that $[\hat{H}'_A(t), \hat{H}_{AB}] \neq 0$ and the other that $\hat{C}_{AB}(t) \neq 0$.

Appendix B

Evolution operator in the interaction picture

In order to calculate the evolving operator we consider that the Hamiltonian that described our system can be write n as: $H = H_o + V$ where $H_o = H_{TLS} + H_{QHO}$ is the free Hamiltonian and $V = H_{int}$ the interaction Hamiltonian. In this picture we know how states evolve according to the interaction Hamiltonian:

$$\frac{d}{dt} \mid \psi(t)_I \rangle = -iV_I(t) \mid \psi(0)_I \rangle \tag{B.1}$$

And thus the solution to this equation is $U_I(t) = \tau e^{-i \int_0^t V_I(s)ds}$ where τ preserves the time ordering if the operators $V_I(t)$ do not commute. In our case $H_o = \frac{\omega_{TLS}}{2}\hat{\sigma}_z + \omega_{QHO}\hat{a}^\dagger \hat{a}$ and $V_I = g\hat{\sigma}_z(\hat{a} + \hat{a}^\dagger)$ and thus what we have to do is calculate the evolution of this operator. As the operators in the interaction pictures evolves according to the free Hamiltonian, we have:

$$V_I(t) = e^{iH_o t}V_I(0)e^{-iH_o t} \tag{B.2}$$

And using the relation:

$$e^B A e^B = A + [B, A] + \frac{1}{2!}[B, [B, A]] + \frac{1}{3!}[B, [B, [B, A]]] + ... \tag{B.3}$$

We calculate $\hat{a}(t)$, and $\hat{a}^\dagger(t)$ as follow:

$$\hat{a}(t) = e^{iH_o}\hat{a}e^{-iH_o} = \hat{a} + i[\hat{a}, H_o] + \frac{1}{2!}i[H_o, i[H_o, \hat{a}]] + ... = \tag{B.4}$$

We can divide the commutator into two commutators:

$$[\hat{a}, H_o] = [\hat{a}, H_{TLS} + H_{QHO}] = [\hat{a}, H_{TLS}] + [\hat{a}, H_{QHO}] = [\hat{a}, H_{QHO}] = \omega_{QHO}[\hat{a}, \hat{a}^\dagger \hat{a}] \tag{B.5}$$

Where the term relationed with H_{TLS} vanishes since it commutes with the annihilation operator of the oscillator.Calculating the another term we arrive at:

$$[\hat{a}^\dagger \hat{a}, \hat{a}] = \hat{a}^\dagger \hat{a}\hat{a} - \hat{a}\hat{a}^\dagger \hat{a} = (\hat{a}^\dagger \hat{a} - \hat{a}\hat{a}^\dagger)\hat{a} = [\hat{a}^\dagger, \hat{a}]\hat{a} = -\hat{a} \qquad (B.6)$$

Can be shown that following with the expansion:

$$\hat{a}(t) = \hat{a}(1 - i\omega_{QHO}t - \omega_{QHO}^2 t^2 - ....) = \hat{a}e^{-i\omega_{QHO}t} \qquad (B.7)$$

Likewise for the creation operator $\hat{a}^\dagger(t) = \hat{a}^\dagger e^{i\omega_{QHO}t}$.Then we can write:

$$V_I(t) = g\sigma_z(\hat{a}e^{-i\omega_{QHO}t} + \hat{a}^\dagger e^{i\omega_{QHO}t}) \qquad (B.8)$$

By doing the time integration of the above expression:

$$U_I(t) = T_\leftarrow \exp\left(-i\int_0^t V_I(s)ds\right) \qquad (B.9)$$

Where $T_\leftarrow$ denotes the chronological time-ordering operator. One important thing to notice here, is that $[V(t), V(t')] = g^2[a^\dagger, a]e^{-i\omega_{QHO}(t'-t)} + g^2[a, a^\dagger]e^{i\omega_{QHO}(t'-t)} = -2ig^2 \sin\omega_{QHO}(t - t') \neq 0$, that is the commutator to the interaction Hamiltonian at two different times is a complex number expression. And thus we can order adjacent $V(t_n)'s$ in the higher order terms just by adding the commutator:

$$U_I(t) = \left(-i\int_0^t V_I(s)ds - 1/2\int_0^t ds\int_0^t ds'[V(s), V(s')]\theta(s - s')\right) \quad (B.10)$$

Where $\theta(t)$ is the step function. Finally we can rewrite this expression as:

$$U_I(t) = \exp\left(-i\int_0^t V_I(t')dt'\right)\exp\left(-i\Phi(t)\right) \qquad (B.11)$$

Therefore, except for time dependent phase factor, the evolution depends only on the operator $V_I(t)$ obtained in Eq(B.8). The phase accumulation can be neglected because it is not going to affect a none of the measurable quantities. Therefore suppressing such phase factor, we have:

$$-i\int_0^t V_I(s)ds = -ig\sigma_z\left(\int_0^t \hat{a}e^{-i\omega_{QHO}s}ds + \int_0^t \hat{a}^\dagger e^{i\omega_{QHO}s}ds\right) \qquad (B.12)$$

$$-i\int_0^t V_I(s)ds = -ig\sigma_z\left(\frac{\hat{a}}{-i\omega_{QHO}}(e^{-i\omega_{QHO}t} + 1) + \frac{\hat{a}^\dagger}{i\omega_{QHO}}(e^{i\omega_{QHO}t} + 1)\right) \tag{B.13}$$

$$- i \int_0^t V_I(s)ds = \frac{g}{\omega_{QHO}} \sigma_z \left(\hat{a}^\dagger (1 - e^{i\omega_{QHO}t}) - \hat{a}(1 - e^{-i\omega_{QHO}t}) \right) \quad (\text{B.14})$$

$$- i \int_0^t V_I(s)ds = \frac{\sigma_z}{2}(\hat{a}^\dagger \alpha(t) - \hat{a}\alpha^*(t)) \quad (\text{B.15})$$

Where $\alpha = \frac{2g}{w_{QHO}}(1 - e^{i\omega_{QHO}t})$

And finally, the evolving operator in the interaction picture is given by:

$$U_I(t) = e^{\frac{\sigma_z}{2}(\hat{a}^\dagger \alpha(t) - \hat{a}\alpha^*(t))} \quad (\text{B.16})$$

Appendix C

Local thermodynamics for the TLS in a closed system

In this section we study the local thermodynamics properties in the spin due to the coupling with the oscillator. We study the heat performed and the heat flux into it choosing as local measurement basis the Hamiltonian of the spin H_{TLS}.

1 Work performed on the spin

To simplify the equations, here we show the method that we follow to arrive at the expression of work flux into the spin considering that it starts in an initial pure state, for example in the excited state $\rho_{TLS}(0) = \mid e \rangle \langle e \mid$ instead of a general mixed state. Using the evolve density operator $U_I(t)$ is easy to check that the evolve density operator for the full system is:

$$\hat{\rho}(t) = \hat{\rho}_{TLS}(t) \otimes \hat{D}(\alpha/2) \rho_{QHO}(0) \hat{D}^\dagger(\alpha/2) \tag{C.1}$$

The reduced density operator for the TLS coincides with initial pure state $\hat{\rho}_{TLS}(t) = \hat{\rho}_{TLS}(0)$ due to that de H_{int} commutes with H_{TLS}.
For the reduced state of the oscillator we have $\rho_{QHO}(t) = \hat{D}(\alpha/2) \rho_{QHO}(0) \hat{D}^\dagger(\alpha/2)$ where $\hat{D}(\alpha/2) = e^{\frac{1}{2}(\alpha \hat{a}^\dagger - \alpha \hat{a})}$ is the displacement operator with the $\alpha(t)$ obtained in Appendix B.
Now basing on the definitions of he work and heat using LEMBAS , for a bipartite system, we start computing the effective Hamiltonian:

$$H_{TLS}^{eff} = Tr_{QHO}\{H_{int}(\mathbb{1} \otimes \rho_{QHO}(t))\} \tag{C.2}$$

Introducing H_{int} and $\rho_{QHO}(t)$ and tracing over the oscillator:

$$H_{TLS}^{eff} = Tr_{QHO}\{H_{int}\hat{D}(\alpha) \mid \alpha_o \rangle \langle \alpha_o \mid \hat{D}^\dagger(\alpha)\} = \sum_n \langle n \mid H_{int}\hat{D}(\alpha) \mid \alpha_o \rangle \langle \alpha_o \mid \hat{D}^\dagger(\alpha) \mid n \rangle \tag{C.3}$$

Then:

$$H_{TLS}^{eff} = \langle \alpha_o \mid \hat{D}^\dagger(\alpha) \Big(\sum_n \mid n \rangle \langle n \mid \Big) H_{int} \hat{D}(\alpha) \mid \alpha_o \rangle \qquad \text{(C.4)}$$

Where we have used $\sum_n \mid n \rangle \langle n \mid = 1$, and thus we arrive at:

$$H_{TLS}^{eff} = \langle \alpha_o \mid \hat{D}^\dagger(\alpha) H_{int} \hat{D}(\alpha) \mid \alpha_o \rangle = g\sigma_z \langle \alpha_o \mid \hat{D}^\dagger(\alpha)(\hat{a} + \hat{a}^\dagger)\hat{D}(\alpha) \mid \alpha_o \rangle \qquad \text{(C.5)}$$

By using the properties of the displacement operator:

$$\hat{D}^\dagger(\alpha/2)\hat{a}\hat{D}(\alpha/2) = \hat{a} + \alpha/2 \qquad \text{(C.6)}$$

$$\hat{D}^\dagger(\alpha/2)\hat{a}^\dagger \hat{D}(\alpha/2) = \hat{a}^\dagger + \alpha^*/2 \qquad \text{(C.7)}$$

We can finally write:

$$H_{TLS}^{eff} = g\sigma_z \left(\langle \alpha_o \mid (\hat{a} + \hat{a}^\dagger) \mid \alpha_o \rangle + \frac{\alpha}{2} + \frac{\alpha^*}{2} \right) \qquad \text{(C.8)}$$

We can identify the expectation value of the position $\langle x \rangle$ of the oscillator, that is $\langle \alpha_o \mid (\hat{a} + \hat{a}^\dagger) \mid \alpha_o \rangle = \sqrt{2m\omega_{QHO}}\langle x \rangle$.

By remembering the expression of $\alpha(t)$:

$$\frac{\alpha(t) + \alpha(t)^*}{2} = \frac{g}{\omega_{QHO}} \left(1 - e^{i\omega_{QHO}t} + 1 - e^{-i\omega_{QHO}t} \right) = \frac{2g}{\omega_{QHO}}(1 - cos(\omega_{QHO}t)) \qquad \text{(C.9)}$$

And thus finally the effective Hamiltonian of the TLS is given by:

$$H_{TLS}^{eff} = \sigma_z \left(g^2 \sqrt{2m\omega_{QHO}}\langle x \rangle + \frac{2g}{\omega_{QHO}}(1 - cos(\omega_{QHO}t)) \right) \qquad \text{(C.10)}$$

Now we need divide H_{TLS}^{eff} in the part that commutes with H_{TLS}^{eft} and in another that does not. The commuting part can be calculated in the following way:

$$H_{TLS,1}^{eff} = \sum_j (H_{TLS}^{eff})_{jj} \mid j \rangle \langle j \mid \qquad \text{(C.11)}$$

Doing that, we just need to compute the expectation value of σ_z in the ground an upper state. With $\langle e \mid \sigma_z \mid e \rangle = 1$ and $\langle g \mid \sigma_z \mid g \rangle = -1$ we write the commuting part as:

$$H_{TLS,1}^{eff} = \left(g\sqrt{2m\omega_{QHO}}\langle x \rangle + \frac{2g^2}{\omega_{QHO}}(1 - cos(\omega_{QHO}t)) \right) \left(\mid e \rangle \langle e \mid - \mid g \rangle \langle g \mid \right) \qquad \text{(C.12)}$$

This correspond to the spectral decomposition of H_{TLS}^{eff}.

Being $\sigma_z = (\ |e\rangle\langle e| - |g\rangle\langle g|\ )$, it is clear that $H_{TLS,1}^{eff} = H_{TLS}^{eff}$ and thus $H_{TLS,2}^{eff} = H_{TLS}^{eff} - H_{TLS,1}^{eff} = 0$

But what we really need in order to compute the work flux is the time derivative of this term:

$$\dot{H_{TLS}^{eff}} = \sigma_z\left(g\sqrt{2m\omega_{QHO}}\langle\dot{x}\rangle + 2g^2 sin(\omega_{QHO}t)\right) \qquad (C.13)$$

As $H_{TLS,2}^{eff} = 0$, the commutator that appears in the second part of the expression of work (A.31) vanishes:

$$[H'_{TLS}, H_{2,TLS}^{eff}] = [H'_{TLS}, 0] = 0 \qquad (C.14)$$

And that the work just depends on $\dot{H_{TLS}^{eff}}$:

$$\dot{W}_{TLS} = Tr_{TLS}\{\dot{H}_{TLS,1}^{eff}\rho_{TLS}\} = g\sqrt{2m\omega_{QHO}}\langle\dot{x}\rangle + 2g^2 sin(\omega_{QHO}t) \quad (C.15)$$

Rewritiong $\langle\dot{x}\rangle = \langle\hat{p}\rangle/m$, the final expression for the work flux into the TLS is:

$$\dot{W}_{TLS} = g\sqrt{\frac{2\omega_{QHO}}{m}}\langle\hat{p}\rangle + 2g^2 sin(\omega_{QHO}t) \qquad (C.16)$$

Where $\langle\hat{p}\rangle$ is the expectation value of the momentum of the spin at time t.

2   Heat flux into the spin

From the equation (A.38) we have for the spin:

$$\dot{Q}_{TLS} = -iTr\{[\hat{H}'_{TLS}(t), \hat{H}_{int}]\hat{C}_{TLS,QHO}(t)\} \qquad (C.17)$$

Where $\hat{H}'_{TLS}(t) = \hat{H}_{TLS} + \hat{H}'^{eft}_{1,TLS}(t)$ and $\hat{C}_{TLS,QHO}(t)$ the correlation terms between the two systems that can appear during the evolution. We can see then that $[\hat{H}_{TLS}, \hat{H}_{int}] = [\hat{H}'^{eff}_{1,TLS}(t), \hat{H}_{int}] = 0$, since the three terms are proportional to σ_z. Therefore, in this case independently of the initial state of the TLS, pure or mixed there is no flux due to the commuting relation. Hence:

$$\dot{Q}_{TLS} = 0 \qquad (C.18)$$

Appendix D

Local thermodynamics for the QHO in a closed system

Now we study the emergence of thermodynamical concepts related with the oscillator choosing as local basis the $\hat{H}_{QHO}$

1 Work performed on the QHO

As we did above, to simplify we consider here two initial pure state as well. The excited state $\rho_{TLS}(0) = \mid e \rangle \langle e \mid$ for the spin and a coherent state $\rho_{QHO}(t) = \mid \alpha_o \rangle \langle \alpha_o \mid$ for the oscillator. Tracing over the spin we start computing the effective Hamiltonian for the QHO:

$$H_{QHO}^{eff} = Tr_{TLS}\{H_{int}(\rho_{TLS}(t) \otimes \mathbb{1})\} \tag{D.1}$$

$$H_{QHO}^{eff} = g(a + a^{\dagger})Tr_{TLS}\{\sigma_z \mid e \rangle \langle e \mid\} = g(a + a^{\dagger}) \tag{D.2}$$

Now, we have to divide this time-independent Hamiltonian into two parts, one that commutes with H_{QHO} and another that does not. By computing the former:

$$H_{QHO,1}^{eff} = \sum_n (H_{QHO}^{eff})_{n,n} \mid n \rangle \langle n \mid = \sum_n \langle n \mid H_{QHO}^{eff} \mid n \rangle \mid n \rangle \langle n \mid \tag{D.3}$$

We arrive at this term vanishes:

$$H_{QHO,1}^{eff} = -(1 - 2c)g \sum_n \langle n \mid (a + a^{\dagger}) \mid n \rangle \mid n \rangle \langle n \mid = 0 \tag{D.4}$$

And, hence:

$$H_{QHO,2}^{eff} = H_{QHO}^{eff} - H_{QHO,1}^{eff} = H_{QHO}^{eff} \tag{D.5}$$

This term is the only that contributes to the work through the commutator $[\hat{H}'_{QHO}, \hat{H}^{eff}_{2,QHO}]$, present in the expression of work flux:

$$\dot{W}_{QHO} = Tr_{QHO}\{-i[\hat{H}'_{QHO}, \hat{H}^{eff}_{2,QHO}]\rho_{QHO}(t)\} \tag{D.6}$$

where $\hat{H}'_{QHO} = \hat{H}_{QHO} + \hat{H}^{eff}_{1,QHO} = \hat{H}_{QHO} = \omega_{QHO}\hat{a}^\dagger\hat{a}$ And thus, the commutator between those Hamiltonian is:

$$[\hat{H}'_{QHO}, \hat{H}^{eff}_{2,QHO}] = g\omega_{QHO}[\hat{a}^\dagger\hat{a}, (\hat{a}^\dagger + \hat{a})] \tag{D.7}$$

This reduces to solve another one $[\hat{a}^\dagger\hat{a}, (\hat{a}^\dagger + \hat{a})]$:

Where taking into account the commutation relation between the annihilation and creation operators we arrive at:

$$[\hat{a}^\dagger\hat{a}, (\hat{a}^\dagger + \hat{a})] = \hat{a}^\dagger[\hat{a}, \hat{a}^\dagger] + [\hat{a}^\dagger, \hat{a}]\hat{a} = \hat{a}^\dagger - \hat{a} \tag{D.8}$$

And thus the expression for the work looks like::

$$\dot{W}_{QHO} = Tr_{QHO}\{-ig\omega_{QHO}(\hat{a}^\dagger - \hat{a})\rho_{QHO}(t)\} \tag{D.9}$$

Where $\rho_{QHO}(t) = \hat{D}(\alpha/2)\rho_{QHO}(0)\hat{D}^\dagger(\alpha/2)$. Introducing this above and tracing over the oscillator we arrive at:

$$\dot{W}_{QHO} = -ig\omega_{QHO}\langle\alpha_o \mid \hat{D}^\dagger(\alpha/2)(\hat{a}^\dagger - \hat{a})\hat{D}(\alpha/2) \mid \alpha_o\rangle \tag{D.10}$$

Using the already known properties of the displacement operator and remembering the expression for α, we can write:

$$\dot{W}_{QHO} = -ig\omega_{QHO}\left(\langle\alpha_o \mid \hat{a}^\dagger - \hat{a} \mid \alpha_o\rangle + \frac{\alpha^*(t)}{2} - \frac{\alpha(t)}{2}\right) \tag{D.11}$$

Taking into account that $\langle\hat{p}\rangle = \frac{\langle\alpha|a-a^\dagger|\alpha\rangle}{2i} = \frac{1}{\sqrt{2m\omega_{QHO}}}\langle\hat{p}\rangle$, where $\langle\hat{p}\rangle$ is the expectation value of the momentum of the oscillator, and thus we can rewrite our expression as: $\langle\alpha \mid a - a^\dagger \mid \alpha\rangle = i\sqrt{\frac{2}{m\omega_{QHO}}}\langle\hat{p}\rangle$. By evaluating:

$$\frac{\alpha^*(t) - \alpha(t)}{2} = \frac{g}{\omega_{QHO}}(1 - e^{-i\omega_{QHO}t} - 1 + e^{i\omega_{QHO}t}) = \frac{g}{\omega_{QHO}}2i\sin(\omega_{QHO}t) \tag{D.12}$$

Introducing all of this in the expression of the work flux, we obtain:

$$\dot{W}_{QHO} = -g\left(i\sqrt{\frac{2\omega_{QHO}}{m}}\langle\hat{p}\rangle + 2g\sin(\omega_{QHO}t)\right) \tag{D.13}$$

We arrive at that the work made by the TLS over the QHO is the same that the QHO does over the TLS changing only the sign. And it is equal to what we would hope to obtain in a classical sense.

2 Heat flux into the QHO

From the Eg.(A.38) we have for the oscillator:

$$\dot{Q}_{QHO} = -iTr\{[\hat{H}'_{QHO}(t), \hat{H}_{int}]\hat{C}_{TLS,QHO}(t)\} \qquad (D.14)$$

Where $\hat{H}'_{QHO}(t) = \hat{H}_{QHO}, since \hat{H}'^{eft}_{1,QHO}(t) = 0$ and $\hat{C}_{TLS,QHO}(t)$ the correlation terms between the two systems that can appear during the evolution. We can see then that $[\hat{H}_{QHO}, \hat{H}_{int}] \neq 0$. Since that term does not vanishes we have to see when $\hat{C}_{TLS,QHO}(t)$ neither if we are looking for the presence of heat. In general, there will be always correlated terms although the full system starts in a pure state due to the coupling, but the purity of the full system remains close to the unity. With this interaction Hamiltonian there are not correlations for pure initial states, but they appear when we have a semi-mixed initial state, that is, a state given by the tensor product of a pure and mixed state.

Under this assumption considering a general mixed initial state for the spin and a coherent state for the oscillator, we study the dynamics in the interaction picture. One we know the dynamics of the full system, and the reduced states for each subsystem after the evolution we can obtain the correlated terms as:

$$\hat{C}_{TLS,QHO}(t) = \hat{\rho}(t) - \hat{\rho}_{TLS}(t) \otimes \hat{\rho}_{QHO}(t) \qquad (D.15)$$

Introducing this in (D.14) and following all the algebra as we did with the work we can arrive at an expression for the heat flux into the oscillator:

$$\dot{Q}_{QHO} = -g\left\{\sqrt{\frac{2\omega_{QHO}}{m}}\langle\hat{p}\rangle + 2(1-2c)g\sin(\omega_{QHO}t)\right\} \qquad (D.16)$$

What we can see is that it is going to oscillate at the same frequency that the work flux.The amount of heat flux is related with the probably c, that is, it depends on the initial state of the spin.

Appendix E

Energy exchange in an open quantum system

1 Master equation damped harmonic oscillator

The evolution of the QHO in contact with an environment modeled by a bath of harmonic oscillators is represented by the following master equation:

$$\frac{\partial \rho_{QHO}(t)}{\partial t} = \frac{-i}{\hbar}[\hat{H}_{eff}, \hat{\rho_{QHO}}(t)]^* + \sum_{j=1} L_j \rho_{QHO}(t) \ L_j^\dagger \qquad \text{(E.1)}$$

The asterisk means that $\hat{H}_{eff}$ is not hermitian, and it is define as $\hat{H}_{eff} = \hat{H}_{QHO} - \frac{-i\hbar}{2}\sum_{j=1} L_j^\dagger L_j$ where L_j are the jump operators.In this case we define two jump oscillators. One $L_1 = \sqrt{\Gamma}\hat{a}$, lets the harmonic oscillator jump down from upper to down levels where Γ indicates the rate of decaying and another, $L_2 = \sqrt{\gamma}\hat{a}^\dagger$ lets it jump up with a rate of absorption given by γ. Then the effective Hamiltonian are:

$$\hat{H}_{eff} = \omega_{QHO}\hat{a}^\dagger\hat{a} - \frac{i\hbar}{2}\Gamma\hat{a}^\dagger\hat{a} - \frac{i\hbar}{2}\gamma\hat{a}\hat{a}^\dagger = \omega_{QHO}\hat{a}^\dagger\hat{a} - \frac{i\hbar}{2}\Gamma\hat{a}^\dagger\hat{a} - \frac{i\hbar}{2}\gamma(\hat{a}^\dagger\hat{a} + 1)$$
$$\text{(E.2)}$$

$$\hat{H}_{eff}^\dagger = \omega_{QHO}\hat{a}^\dagger\hat{a} + \frac{i\hbar}{2}\Gamma\hat{a}^\dagger\hat{a} + \frac{i\hbar}{2}\gamma\hat{a}\hat{a}^\dagger = \omega_{QHO}\hat{a}^\dagger\hat{a} + \frac{i\hbar}{2}\Gamma\hat{a}^\dagger\hat{a} + \frac{i\hbar}{2}\gamma(\hat{a}^\dagger\hat{a} + 1)$$
$$\text{(E.3)}$$

Introducing all of this in (E.1), we arrive at the master equation of the damped harmonic oscillator:

$$\frac{\partial \rho_{QHO}(t)}{\partial t} = \frac{-i}{\hbar}[H_{QHO}, \hat{\rho}_{QHO}(t)] + \hat{D}(\hat{\rho}_{QHO}(t)) \qquad \text{(E.4)}$$

where $\hat{D}(\hat{\rho}_{QHO}(t))$ is named the dissipator of the oscillator:

$$\hat{D}(\hat{\rho}_{QHO}(t)) = \Gamma\hat{a}\hat{\rho}_{QHO}(t)\hat{a}^\dagger + \gamma\hat{a}^\dagger\hat{\rho}_{QHO}(t)\hat{a} - \frac{1}{2}\{\Gamma\hat{a}^\dagger\hat{a} + \gamma\hat{a}\hat{a}^\dagger, \hat{\rho}_{QHO}(t)\}$$

(E.5)

Now we focus on computing the populations and coherences of $\hat{\rho}_{QHO}(t)$. For the populations we obtain :

$$\frac{\partial\rho_{QHO,nn}(t)}{\partial t} = \frac{-i\omega_{QHO}}{\hbar}\left(\langle n \mid \hat{a}^\dagger\hat{a}\hat{\rho}_{QHO} \mid n\rangle - \langle n \mid \hat{\rho}_{QHO}\hat{a}^\dagger\hat{a} \mid n\rangle\right) + \langle n \mid \hat{D}(\hat{\rho}_{QHO}(t)) \mid n\rangle$$

(E.6)

Where the terms between brackets vanishes since:
$\langle n \mid \hat{a}^\dagger\hat{a}\hat{\rho}_{QHO} \mid n\rangle = \langle n \mid \hat{\rho}_{QHO}\hat{a}^\dagger\hat{a} \mid n\rangle = n\langle n \mid \hat{\rho}_{QHO} \mid n\rangle$ and they cancel out. Following all the algebra we arrive at an expression for the expectation value of the dissipator in the Fock basis given by:

$$\langle n \mid \hat{D}(\hat{\rho}_{QHO}(t)) \mid n\rangle = \Gamma(n+1)\langle n+1 \mid \hat{\rho}_{QHO}(t) \mid n+1\rangle + \gamma n\langle n-1 \mid \hat{\rho}_{QHO}(t) \mid n-1\rangle - $$
$$ - \Gamma n\langle n \mid \hat{\rho}_{QHO}(t) \mid n\rangle - (n+1)\gamma\langle n \mid \hat{\rho}_{QHO}(t) \mid n\rangle \quad \text{(E.7)}$$

Putting this again in Eq.(E.6) we can notice that if we focus on computing the populations of the evolve density operator, the first tho terms vanishes when we only consider the $\mid n\rangle$ Fock state, and at the end what we obtain is:

$$\rho_{QHO,nn}(t) = \rho_{QHO,nn}(0)e^{-(n\Gamma+(n+1)\gamma)t}$$

(E.8)

whereas if I am interested in computing the coherences:

$$\frac{\partial\rho_{QHO,nm}(t)}{\partial t} = \frac{-i\omega_{QHO}}{\hbar}\left(\langle n \mid \hat{a}^\dagger\hat{a}\hat{\rho}_{QHO} \mid m\rangle - \langle n \mid \hat{\rho}_{QHO}\hat{a}^\dagger\hat{a} \mid m\rangle\right) + \langle n \mid \hat{D}(\hat{\rho}_{QHO}(t)) \mid m\rangle$$

(E.9)

Where now the term between brackets do not vanish: $\langle n \mid \hat{a}^\dagger\hat{a}\hat{\rho}_{QHO} \mid m\rangle - \langle n \mid \hat{\rho}_{QHO}\hat{a}^\dagger\hat{a} \mid m\rangle = (n-m)\langle n \mid \hat{\rho}_{QHO} \mid m\rangle$. And in this case the last term is given by:

$$\langle n \mid \hat{D}(\hat{\rho}_{QHO}(t)) \mid m\rangle = \Gamma(n+1)(m+1)\langle n+1 \mid \hat{\rho}_{QHO}(t) \mid m+1\rangle + $$
$$\gamma nm\langle n-1 \mid \hat{\rho}_{QHO}(t) \mid n-1\rangle - -\frac{\Gamma}{2}(n+m)n\langle n \mid \hat{\rho}_{QHO}(t) \mid m\rangle - \frac{\gamma}{2}(n+m+1)\langle n \mid \hat{\rho}_{QHO}(t) \mid m\rangle$$

(E.10)

The expression for the coherences is:

$$\rho_{QHO,nm}(t) = \rho_{QHO,nm}(0)e^{i\omega(n-m)t}e^{-(\frac{\Gamma}{2}(n+m)+\frac{\gamma}{2}(n+m+1))t}$$

(E.11)

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But as we start considering a pure state for the oscillator, a coherent state $\rho(0) = | \alpha_o \rangle \langle \alpha_o |$, $\rho_{QHO,nm}(0)$ vanishes and just the populations survive, therefore there is not superposition.

Therefore, what we will have, it will be a exponential decay of the probability of finding the QHO in a coherent state.

We can rewire the density operator of our system taking into account only the populations as:

$$\rho_{QHO}(t) = \rho_{QHO,nn}(0)e^{-(n\Gamma+(n+1)\gamma)t} \, | \, n \rangle \langle n \, | \qquad \text{(E.12)}$$

Where:

$$\rho_{QHO,nn}(0) = \langle n \, || \, \alpha(0) \rangle \langle \alpha(0) \, || \, n \rangle = P(n) = \frac{| \, \alpha \, |^{2n} \, e^{-|\alpha|^2}}{n!} \qquad \text{(E.13)}$$

This is a Poissonian distribution that indicate us the probability of finding n photons in a coherent state.

$$\rho_{QHO}(t) = P(n)e^{-(n\Gamma+(n+1)\gamma)t} \, | \, n \rangle \langle n \, | \qquad \text{(E.14)}$$

Taking this into account we now study the evolution of the full system:

2 Master equation full system

Now we study how the effect of the coupling between the oscillator and the environment affects the dynamics of the full system.

Firstly, we write the master equation for the full evolve density operator $\rho(t)$::

$$\frac{\partial \rho(t)}{\partial t} = \frac{-i}{\hbar}[\hat{H}_{eff}, \hat{\rho(t)}]^* + \sum_{j=1} L_j \rho(t) \, L_j^\dagger \qquad \text{(E.15)}$$

Where in this case $\hat{H}_{eff}$ is given by:

$$\hat{H}_{eff} = \hat{H}_1 - \frac{i\hbar}{2} \sum_{j=1} L_j^\dagger L_j \qquad \text{(E.16)}$$

H_1 is the Hamiltonian of the closed system already studied $H_1 = H_{TLS} + H_{QHO} + H_{int}$ and L_j are the same jump operators defined above, since only the QHO sees the environment. Following LEMBAS, now we have to choose a basis to compute the dynamics and to study the thermodynamic properties. Starting with the spin, we trace over the oscillator, arriving at:

$$\frac{\partial \rho_{TLS}(t)}{\partial t} = \frac{-i}{\hbar}Tr_{QHO}\{[H_{TLS} + H_{QHO} + H_{int}, \hat{\rho}(t)]\} + Tr_{QHO}\{\hat{D}(\hat{\rho}(t))\} \qquad \text{(E.17)}$$

where $\hat{D}(\hat{\rho}(t))$ is the dissipator, but now of the full system:

$$\hat{D}(\hat{\rho}(t)) = \Gamma\hat{a}\hat{\rho}(t)\hat{a}^{\dagger} + \gamma\hat{a}^{\dagger}\hat{\rho}(t)\hat{a} - \frac{1}{2}\{\Gamma\hat{a}^{\dagger}\hat{a} + \gamma\hat{a}\hat{a}^{\dagger}, \hat{\rho}(t)\} \qquad \text{(E.18)}$$

.

Likewise, we can trace over the spin to study the dynamics of the oscillator.

3   Work and heat exchange in a TLS

Using the same derivation that in the closed system we try to find an expression for the energy exchange in a closed system. Considering initial pure states for both systems, we start computing the change in the internal energy for the spin:

$$dU = \frac{d}{dt}Tr_{TLS}\{\hat{H}'_{TLS}\rho\hat{T}_{LS}\}dt = Tr_{TLS}\{\dot{\hat{H}}'_{TLS}\rho\hat{T}_{LS} + \hat{H}'_{TLS}\rho\dot{\hat{T}}_{LS}\} \quad \text{(E.19)}$$

Where $\hat{H}'_{TLS} = \hat{H}_{TLS} + \hat{H}_{1,TLS}^{eff}$.

$$dU = Tr_{TLS}\{(\dot{\hat{H}}_{TLS} + \dot{\hat{H}}_{1,TLS}^{eff})\rho\hat{T}_{LS} + \hat{H}'_{TLS}\rho\dot{\hat{T}}_{LS}\}dt \qquad \text{(E.20)}$$

Since $\hat{H}_{TLS}$ does not depend on time, the first term on the right hand side vanishes, and thus

$$dU = Tr_{TLS}\{\dot{\hat{H}}_{1,TLS}^{eff}\rho\hat{T}_{LS} + \hat{H}'_{TLS}\rho\dot{\hat{T}}_{LS}\}dt \qquad \text{(E.21)}$$

Introducing, the expression obtained in the previous section for the evolve density operator of the TLS and making use of several commutation relations we arrive at the following expression for the change in the internal energy for the spin:

$$dU = Tr_{TLS}\left\{(\dot{\hat{H}}_{1,TLS}^{eff})\hat{\rho}_{TLS} - i[\hat{H}'_A, \hat{H}_{2,TLS}^{eff}]\hat{\rho}_{TLS}\right\} + Tr_{TLS}\left\{\hat{H}'_{TLS}Tr_{QHO}\{\hat{D}(\rho(t))\}\right\}dt \tag{E.22}$$

Where we can identify in the right hand side of the equation the work, related with the unitary dynamics:

$$\dot{W}_{TLS} = Tr_{TLS}\left\{(\dot{\hat{H}}_{1,TLS}^{eff})\hat{\rho}_{TLS} - i[\hat{H}'_A, \hat{H}_{2,TLS}^{eff}]\hat{\rho}_{TLS}\right\} \qquad \text{(E.23)}$$

and the heat flux:

$$\dot{Q}_{TLS} = Tr_{TLS}\left\{\hat{H}'_{TLS}Tr_{QHO}\{\hat{D}(\rho(t))\}\right\} \qquad \text{(E.24)}$$

We see that this term leads to a non-unitary dynamics for the spin since it depends on a mixture of states. To be able to compute these terms we need the evolve state of the full system, given by:

$$\hat{\rho}(t) = P(n)e^{-(n\Gamma+(n+1)\gamma)t}\hat{\rho}_{TLS}(0) \otimes \hat{D}(\alpha/2) \mid n\rangle\langle n \mid \hat{D}^\dagger(\alpha/2) \qquad (E.25)$$

From this expression we can obtain the reduced states of both systems. For the spin $\hat{\rho}_{TLS}(t) = P(n)e^{-(n\Gamma+(n+1)\gamma)t}\hat{\rho}_{TLS}(0)$ and for the oscillator $\hat{\rho}_{QHO}(t) = P(n)e^{-(n\Gamma+(n+1)\gamma)t}\hat{D}(\alpha/2) \mid n\rangle\langle n \mid \hat{D}^\dagger(\alpha/2)$ and we see that even starting in pure states both systems are correlated after the evolution.

Now we focus on computing the work and heat fluxes in the basis of the TLS. Following exactly the same method that we did in the case of the closed system, we start evaluating the effective Hamiltonian, then we divide it in two parts, one that commutes with the free Hamiltonian and another that does not, and finally we arrive at the following expression for the work flux:

$$\dot{W}_{TLS} = 2g^2 P^2(n)e^{-2(n\Gamma+(n+1)\gamma)t}\left(-(n\Gamma+(n+1)\gamma)+sin(\omega_{QHO}t)\right) \text{ (E.26)}$$

Where remember that $P(n)$ is the Poissonian distribution, and with Γ and γ the rates of decaying and absorption due to the coupling.

Likewise, we arrive at an expression for the heat flux:

$$\dot{Q}_{TLS} = Tr_{TLS}\left\{\hat{H}'_{TLS}Tr_{QHO}\{\hat{D}(\rho(t))\}\right\}dt = Tr_{TLS}\left\{\hat{H}'_{TLS}\hat{D}(\rho_{TLS}(t))\right\}$$
$$(E.27)$$

where $\hat{H}'_{TLS} = \hat{H}_{TLS} + \hat{H}_{1,TLS}^{eff}$ .We can prove that this terms vanishes since $Tr_{QHO}\{\hat{D}(\rho(t))\} = 0$:

$$Tr_{QHO}\{\hat{D}(\rho(t))\} = \Gamma Tr_{QHO}\{\hat{a}\hat{\rho}(t)\hat{a}^\dagger\}+\gamma Tr_{QHO}\{\hat{a}^\dagger\hat{\rho}(t)\hat{a}\}-\frac{\Gamma}{2}Tr_{QHO}\{\hat{a}^\dagger\hat{a}\hat{\rho}(t)\}-$$
$$\frac{\gamma}{2}Tr_{QHO}\{\hat{a}\hat{a}^\dagger\hat{\rho}(t)\} - \frac{\Gamma}{2}Tr\{\hat{\rho}(t)\hat{a}^\dagger\hat{a}\} - \frac{\gamma}{2}Tr_{QHO}\{\hat{\rho}(t)\hat{a}\hat{a}^\dagger\} \quad (E.28)$$

Using the cyclic properties of the trace, we can rewrite the above expression as:

$$Tr_{QHO}\{\hat{D}(\rho(t))\} = \Gamma Tr_{QHO}\{\hat{\rho}(t)\hat{a}^\dagger\hat{a}\}+\gamma Tr_{QHO}\{\hat{\rho}(t)\hat{a}\hat{a}^\dagger\}-\frac{\Gamma}{2}Tr_{QHO}\{\hat{\rho}(t)\hat{a}^\dagger\hat{a}\}-$$
$$\frac{\gamma}{2}Tr_{QHO}\{\hat{\rho}(t)\hat{a}\hat{a}^\dagger\} - \frac{\Gamma}{2}Tr\{\hat{\rho}(t)\hat{a}^\dagger\hat{a}\} - \frac{\gamma}{2}Tr_{QHO}\{\hat{\rho}(t)\hat{a}\hat{a}^\dagger\} \quad (E.29)$$

And thus we see that this term vanishes $Tr_{QHO}\{\hat{D}(\rho(t))\} = 0$. Therefore in the heat flux into the the TLS is $\dot{Q}_{TLS} = 0$.

4 Work and heat exchange in a damped QHO

Now we are going to study what happens with the oscillator.Tracing over the TLS in oder to study the dynamics of the QHO we arrive at:

$$\frac{\partial \rho_{QHO}(t)}{\partial t} = \frac{-i}{\hbar} Tr_{TLS}\left\{[H_{TLS} + H_{QHO} + H_{int}, \hat{\rho}(t)]\right\} + Tr_{TLS}\left\{\hat{D}(\hat{\rho}(t))\right\}$$
(E.30)

Likewise that in the other case we arrive at the following expressions for the change in the internal energy:

$$dU = Tr_{QHO}\left\{(\dot{\hat{H}}_{1,QHO}^{eff})\hat{\rho}_{QHO} - i[\hat{H}'_A, \hat{H}_{2,QHO}^{eff}]\hat{\rho}_{QHO}\right\} + Tr_{QHO}\left\{\hat{H}'_{QHO}Tr_{TLS}\{\hat{D}(\rho(t))\}\right\}dt$$
(E.31)

Where we can distinguish between the work flux:

$$\dot{W}_{QHO} = Tr_{QHO}\left\{(\dot{\hat{H}}_{1,QHO}^{eff})\hat{\rho}_{QHO} - i[\hat{H}'_{QHO}, \hat{H}_{2,QHO}^{eff}]\hat{\rho}_{QHO}\right\} \quad \text{(E.32)}$$

And the heat flux:

$$\dot{Q}_{QHO} = Tr_{QHO}\left\{\hat{H}'_{QHO}Tr_{TLS}\{\hat{D}(\rho(t))\}\right\} = Tr_{QHO}\left\{\hat{H}_{QHO}\hat{D}(\rho_{QHO}(t))\right\}$$
(E.33)

We do not show all the steps here because it is redundant since we follow the the same process that we have done in all the previous sections. All the calculations that could appear ,have been done before. Therefore the work perform on the damped harmonic oscillator is given by:

$$\dot{W}_{QHO} = -2g^2 P^2(n)e^{-2(n\Gamma + (n+1)\gamma)t}\sin(\omega_{QHO}t) \quad \text{(E.34)}$$

We observe that $\dot{W}_{QHO} = -\dot{W}_{TLS}$, that is what we obtained in the closed system as well. However, in this case we have not got a oscillatory behavior since he amplitude of such oscillations decay in time. And the expression for the heat flux into the oscillator is given by:

$$\dot{Q}_{QHO} = Tr_{QHO}\left\{\hat{H}_{QHO}\hat{D}(\rho_{QHO}(t))\right\} \quad \text{(E.35)}$$

Appendix F

Numerical Methodology for computing Local thermodynamics

In this section we explain the numerical methodology followed to compute the local thermodynamical concepts using LEMBAS. This method is acceptable for closed systems independently on the interaction Hamiltonian.

We use a quantum toolbox in python,QuTiP[16], that includes several functions to solve the dynamics and time-evolution given a Hamiltonian and a state. Therefore, by defining the initial density operator for our system, choosing a Hamiltonian and an interval of time in which we consider that the systems interact, the program give us directly the evolve density operator of the full system for every period of time.

As LEMBAS is based in the local dynamics we have to trace over each of these density operator to work with the reduced density states. Once we have this, we define functions for the effective Hamiltonians of each subsystem, as in Eq.(A.12). Then we have to split those Hamiltonians in two parts, one that commute with the Hamiltonian of the system considered and another that does not. To do this, we firstly extract the eigenvectors of the bare Hamiltonians and form a matrix and its transpose with them. With this two matrix we can diagonalize any Hamiltonian in the chosen basis, and thus we obtain the commuting part of the effective Hamiltonian of a system A, $\hat{H}_{1,A}^{eff}$. The non-commuting will be given simply as $\hat{H}_{2,A}^{eff} = \hat{H}_A^{eff} - \hat{H}_{1,A}^{eff}$.

Following the expressions for work Eq.(A.31) and heat Eq(A.38), we define two functions like these. Looking at them we can see that we still need to compute the time derivative of $\hat{H}_{1,A}^{eff}$, and the correlated terms C_{AB} to solve those equations. For $\dot{\hat{H}}_{1,A}^{eff}$ we need to create a loop that does the

derivative along the list of matrices(in the full interval) for element. For computing C_{AB} we only need the evolution density operator and the tensor product of the reduced states as in Eq.(D.15).

To sum up, just studying the dynamics of a closed system for a given Hamiltonian, independently of if we deal with a commuting or non commuting Hamiltonian and defining the functions for the heat and work fluxes we can obtained results as in the graphs presented above.

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