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Quantum thermodynamics: a modified Otto engine

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RICHARD QUINTILIANO MATOS

Quantum thermodynamics: a modified Otto engine

Dissertation presented to the Graduate Program in Physics (PPGF) at the Institute of Physics(IF) of the Federal University of Goiás(UFG), as part of the requirements for obtaining the Master's degree in physics.

Area: Quantum thermodynamics.

Advisor: Prof. Dr. Norton G. de Almeida.

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Ata nº 208 da sessão de Defesa de Dissertação de Richard Quintiliano Matos, que confere o título de Mestre em Física, na área de concentração em Física.

Aos 02 dias do mês de março de 2023, a partir das 14h00min, por meio de videoconferência, realizou-se a sessão pública de Defesa de Dissertação intitulada “Quantum thermodynamics: A modified Otto engine”. Os trabalhos foram instalados pelo Orientador, Professor Doutor Norton Gomes de Almeida (IF/UFG), com a participação dos demais membros da Banca Examinadora: Professor Doutor Gentil Dias de Moraes Neto (Zhejiang Normal University / China), membro titular externo; e Professor Doutor Rafael de Morais Gomes (IF/UFG), membro titular interno. Durante a arguição, os membros da banca não fizeram sugestão de alteração do título do trabalho. A Banca Examinadora reuniu-se em sessão secreta a fim de concluir o julgamento da Dissertação, tendo sido o candidato aprovado pelos seus membros. Proclamados os resultados pelo Professor Doutor Norton Gomes de Almeida, Presidente da Banca Examinadora, foram encerrados os trabalhos e, para constar, lavrou-se a presente ata que é assinada pelos membros da Banca Examinadora, aos 02 dias do mês de março de 2023.

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There is a theory which states that if ever anyone discovers exactly what the Universe is for and why it is here, it will instantly disappear and be replaced by something even more bizarre and inexplicable. There is another theory which states that this has already happened.

DOUGLAS ADAMS

Dedico este trabalho aos meus pais, pilares da minha formação como ser humano.

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Abstract

Quantum thermodynamics is an emerging area that arouses the interest of many scientists and engineers. Although it is a new and incomplete theory, it comes with surprising results.

We propose to study a quantum engine that utilizes thermal reservoirs as baths but an unusual system as working fluid, a *squeezed* harmonic oscillator. The fluid was chosen as an educated guess to study if an engine working solely with a quantum resource could surpass Carnot's limit. The problem was solved analytically and then simulated using the qutip library to python, we showed that this engine is capable of working in Carnot's regime. Furthermore, we calculated the Shortcut to adiabaticity to the evolving hamiltonian so we could improve the system's power without losing efficiency.

This kind of machine serves the purpose of showing that one cannot surpass Carnot's limit if one is using thermal reservoirs.

Key-words

Thermal engines, Thermodynamics, Quantum mechanics.

Resumo

A termodinâmica quântica é uma área emergente que desperta o interesse de muitos cientistas e engenheiros. Embora seja uma teoria nova e incompleta, ela apresenta resultados surpreendentes. Propomos estudar um motor quântico que utiliza reservatórios térmicos como banhos, mas um sistema incomum como fluido de trabalho, um oscilador harmônico comprimido. O fluido foi escolhido como um palpite para estudar se um motor trabalhando apenas com um recurso quântico poderia ultrapassar o limite de Carnot. O problema foi resolvido analiticamente e depois simulado usando a biblioteca qutip para python, mostramos que esta engine é capaz de funcionar no regime de Carnot. Além disso, calculamos o Atalho para adiabaticidade para o hamiltoniano evolutivo para que possamos melhorar a potência do sistema sem perder eficiência. Este tipo de máquina serve para mostrar que não se pode ultrapassar o limite de Carnot se estivermos usando reservatórios térmicos.

Palavras-Chave

Motores térmicos, Termodinâmica, Mecânica Quântica.

Contents

1 Introduction

This chapter will provide a brief introduction to the research by first discussing a background plus context, followed by the problem we face, the goals of the research, general objectives and questions, the importance of it, and finally, the limitations.

Carnot was the first one to describe the ideal quantum thermodynamics cycle, the one that would have the highest efficiency among all possible cycles [1]. Said machine would work on a quasi-static process, i.e., at zero power, all processess would happen so slowly that the whole cycle would be reversible, and most interesting, its efficiency doesn't depend on the working fluid [2]. Since the development of the first quantum thermal machines/engines [3, 4], it's been a dream to find a thermal machine that surpasses the classical limit imposed by Carnot by utilizing quantum resources both in the baths and working fluid. This search for *beyond Carnot efficiency* is motivated by the fact that there was not a quantum theory in Carnot's epoch when classical thermodynamics was developed. This can be done either by using a genuine quantum bath [5–8] or by using a working fluid that carries quantum properties[1] [9, 10]. So, it was very shocking when the results of [11] announced that the Carnot's limit could be broken using squeezing reservoirs, in which case, the efficiency would approach 1(100%) for a large enough squeezing parameter.

Another result showing the advantage of quantum thermal machines over their classical counterparts when using squeezed reservoirs as a quantum resource [12–14] was obtained in [15] where the authors showed that close to unitary efficiency can also be achieved for non-zero power even without techniques like a *shortcut to adiabaticity*(STA) [16–21] or quantum lubricants [9, 22]. The first, STA, is a technique that allows a gain in potency without a loss in efficiency as it mimics the slow evolution for

[1] as coherence or entanglement.

the system [2] while the second one, lubricants, increase the efficiency by using coherences. Moreover, in [5], the authors found a counter-intuitive phenomenon happening with an Otto engine coupled to a negative temperature reservoir, where higher efficiency was achieved the faster the compression and expansion strokes were performed. The authors in [23] showed that negative effective temperatures increase power over positive temperatures. In [24], the authors demonstrate that fermionic reservoir coolers can cool systems better than bosonic reservoirs, even if the fermionic reservoir has a strictly positive temperature.

Having said that, it's clear that quantum resources reservoirs outperform regular thermal reservoirs. That raises the question "*what would be the effects of quantum resources as working fluid ?*". In our particular case, the question we are trying to answer is a little simpler "*what would be the effects of squeezing on harmonic oscillator working fluid ?*". To answer this question, we are going to study an Otto cycle coupled with traditional thermal baths where we directly apply the squeezing. This differs from previous works as we are using thermal states reservoir and applying the quantum resource to the working fluid instead. that's why the thermodynamic quantities are going to be functions of the squeezing parameter. We will show that is possible to obtain an engine with an efficiency that is arbitrarily close to Carnot. We also show, in an alternative way from [25] that Carnot's efficiency cannot be exceeded.

This work is organized in the following way. In 2, a set of necessary tools will be presented, 2.1 will present the Master's equation formalism for open quantum systems, which is widely used in thermodynamics, 2.2 will present a brief insight into the concepts of quantum thermodynamics used in these work and 2.3 will present the formalism of shortcuts to adiabaticity. In chapter 3 we presented the model of the

[2] The quantum adiabatic evolution.

cycle we are using as an engine. C presents the cycle along with the technicalities on how to solve it, section 3.2 shows the results of the simulation in C, 3.3 presents the maximum efficiency an engine operating between thermal reservoirs can achieve, then we proceed to calculate the STA for the squeezed harmonic oscillator on 3.4. In the end, we present the conclusions in 4.

2 Theoretical Basis

2.1 Open Quantum Systems

2.1.1 Closed System Evolutions

First of all, we begin by presenting a short introduction to closed systems as a starting point on our way through the open system's dynamics. The evolution of a closed system is given by Schrodinger's equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle = -iH(t)\left|\psi(t)\right\rangle, \tag{2.1}$$

where $|\psi\rangle$ is a vector in a Hilbert space $\mathcal{H}$ that completely describes the system and is evolved by the Hamiltonian H, which is an operator that acts on this same space.

The solution to that equation is obtained by direct integration

$$\left|\psi(t)\right\rangle = \mathcal{U}(t,t_0)\left|\psi(t_0)\right\rangle. \tag{2.2}$$

$\mathcal{U}$ is called evolution operator since it evolves a $|\psi\rangle$ from a time t_0 to a future time t. Moreover, the evolution operator must obey a Schrodinger type equation[1]

$$\frac{\mathrm{d}\mathcal{U}(t,t_0)}{\mathrm{d}t} = -iH(t)\mathcal{U}(t,t_0). \tag{2.3}$$

If the Hamiltonian commutes with itself for any two different times, then the explicit shape of $\mathcal{U}$ is [2]

$$\mathcal{U}(t,t_0) = exp\left\{-i\int_{t_0}^{t} H(s)ds\right\}. \tag{2.4}$$

[1] It's obvious from substituting 2.2 in 2.1

[2] In the case where the Hamiltonian doesn't commute with itself at different times, *i.e.*,$[H(t_1), H(t_2)] \neq 0$, then, we must have a time-ordered integral, see [26].

Another way to describe quantum mechanics is by defining a density operator (or density matrix)

$$\rho(t) \equiv \sum_i p_i \left|\psi_i(t)\right\rangle \left\langle\psi_i(t)\right|, \tag{2.5}$$

that will describe the system and take the role of $|\psi\rangle$. This is a more general way of describing these systems because it takes into account the possibility of mixed states [27]. This operator ρ must be positive because its entries represents probabilities and its trace is direct to calculate:

$$\begin{aligned}
\mathrm{Tr}\{\rho\} &= \mathrm{Tr}\left\{\sum_i p_i \left|\psi_i(t)\right\rangle \left\langle\psi_i(t)\right|\right\}, && \text{(2.6a)}\\
&= \sum_i p_i \,\mathrm{Tr}\{\left|\psi_i(t)\right\rangle \left\langle\psi_i(t)\right|\}, && \text{(2.6b)}\\
&= \sum_i p_i, && \text{(2.6c)}\\
&= 1. && \text{(2.6d)}
\end{aligned}$$

The evolution of ρ is given by:

$$\begin{aligned}
\rho(t) &= \sum_i p_i \left|\psi_i(t)\right\rangle \left\langle\psi_i(t)\right|, && \text{(2.7a)}\\
&= \sum_i p_i \mathcal{U}(t,t_0) \left|\psi_i(t_0)\right\rangle \left\langle\psi_i(t_0)\right| \mathcal{U}^\dagger(t,t_0), && \text{(2.7b)}\\
&= \mathcal{U}(t,t_0) \left(\sum_i p_i \left|\psi_i(t_0)\right\rangle \left\langle\psi_i(t_0)\right|\right) \mathcal{U}^\dagger(t,t_0), && \text{(2.7c)}\\
\rho(t) &= \mathcal{U}(t,t_0)\rho(t_0)\mathcal{U}^\dagger(t,t_0). && \text{(2.7d)}
\end{aligned}$$

By deriving 2.7d, it's possible to write a well known equation, the Liouville - Von Neumann equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -i[H(t),\rho(t)]. \tag{2.8}$$

With the help of super-operators [3], equation 2.8 is written as:

[3] Linear maps that act on linear operators and return linear operators/ Automorphism. [28].

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \mathcal{L}(t)\rho(t), \tag{2.9}$$

where $\mathcal{L}$ is the Liouville super-operator that acts on ρ and returns $-i[H(t), \rho(t)]$[4].

2.1.2 Required theorems

We need to state two important theorems without proof (but the proof is available in [29]):

Choi's Theorem :

A linear map $\mathcal{V} : B(\mathcal{H}) \to B(\mathcal{H})$ is completely positive iff it can be expressed as shown below:

$$\mathcal{V}\rho = \sum_i V_i^\dagger \rho V_i, \tag{2.10}$$

where $V_i \in B(\mathcal{H})$ (positive).

Choi-Kraus Theorem :

A linear map $\mathcal{V} : B(\mathcal{H}) \to B(\mathcal{H})$ is completely positive and trace-preserving iff it has the following form:

$$\mathcal{V}\rho = \sum_i V_i^\dagger \rho V_i, \tag{2.11}$$

where $V_i \in B(\mathcal{H})$ (positive) have the property of:

$$\sum_i V_i V_i^\dagger = \mathcal{I}. \tag{2.12}$$

All these operators V_i that forms completely positive and trace-preserving maps are called *Kraus Operators*. It's important to note that Kraus operators can be time-dependent with the conditions that those properties are true at all times.

[4] $\mathcal{L}(t)\rho(t)$ is to be interpreted as $\mathcal{L}(\rho)$, i.e. $\mathcal{L}$ is not just multiplied in the left.

2.1.3 Mathematical deduction of the Lindblad equation

Here, we follow the path in [29–31] to describe an open system in quantum mechanics. First of all, we ask *What is the most general way to make a markovian map that maps density operator to density operator ?*

The first step consists in realizing that such transformation must be completely positive [5] as the eigenstates of the density operator are always positive because it represent probabilities. Another important property is that it must preserve the trace of ρ so the total probability conserves [6]. This is to show the importance of the theorems in section 2.1.2.

From equation 2.9, we write the general form of $\mathcal{L}$ that have the required properties.

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \mathcal{L}\rho(t). \tag{2.13}$$

This map may be thought of with an analogy to the unitary evolution operator as $\rho(t) = \mathcal{V}(t-t_0)\rho(t_0) = e^{\mathcal{L}t}\rho(t_0)$.

We have begun by writing a base for Fock-Liouville's space (equivalent to the Hilbert space but for super-operators) that has a dimension of d^2 if the Hilbert space has the dimension of d. This base F_i is required to be orthonormal with i in range 1 to d^2, so:

$$\langle F_i|F_j\rangle = Tr[F_i^\dagger F_j] = \delta_{i,j}. \tag{2.14}$$

We then choose the last base vector to be $F_{d^2} = \frac{\mathcal{I}}{\sqrt{d}}$, it's easy to notice from 2.14, that the trace of all other F_i is equal to zero :

$$\langle F_{d^2}|F_j\rangle = Tr\left[\frac{\mathcal{I}}{\sqrt{d}}F_j\right] = \frac{1}{\sqrt{d}}Tr[F_j] = 0. \tag{2.15}$$

[5] $\mathcal{V}\otimes\mathcal{I}_B : B(\mathcal{H}_A)\otimes B(\mathcal{H}_B) \to B(\mathcal{H}_A)\otimes B(\mathcal{H}_B)$, if the input ρ is positive, so is the output.

[6] $\sum_i p_i = 1$

The operators V_i of the map $\mathcal{V}(t)$ may be described in this base as:

$$V_l = \sum_{i=1}^{d^2} \langle F_i | V_l \rangle \, F_i, \tag{2.16}$$

and the map is:

$$\mathcal{V}(t)\rho = \sum_{i,j}^{d^2} c_{i,j}(t) F_i \rho F_j^\dagger, \tag{2.17}$$

where $c_{i,j}$ is:

$$c_{i,j} = \sum_{l=1}^{d^2} \langle F_i | V_l(t) \rangle \, \langle V_l(t) | F_j \rangle \, . \tag{2.18}$$

The original problem of discovering a form of $\mathcal{L}$ can be found in writing the derivative of ρ:

$$\mathcal{L}(t)\rho(t) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[\rho(t+\varepsilon) - \rho(t) \right] = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[\mathcal{V}(\varepsilon)\rho(t) - \rho(t) \right], \tag{2.19}$$

from now on, I will leave the explicit dependency in time of rho out of notation (it still depends on time, it's just implicit in notation). In the base we choose (The explicit sum is made in Appendix A):

$$\mathcal{L}\rho = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[\sum_{i=1}^{d^2} \sum_{j=1}^{d^2} c_{i,j}(\varepsilon) F_i \rho F_j^\dagger - \rho \right], \tag{2.20}$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[\frac{c_{d^2,d^2}(\varepsilon) - d}{d} \rho + \frac{1}{\sqrt{d}} \sum_{i=1}^{d^2-1} \left\{ c_{i,d^2}(\varepsilon) F_i \rho + c_{d^2,i}(\varepsilon) \rho F_i^\dagger \right\} + \sum_{i=1}^{d^2-1} \sum_{j=1}^{d^2-1} c_{i,j}(\varepsilon) F_i \rho F_j^\dagger \right]. \tag{2.21}$$

The limit is applied and the quantities that depend on it are redefined as follows:

$$\begin{aligned} a_{d^2,d^2} &= \lim_{\varepsilon\to 0} \frac{c_{d^2,d^2}(\varepsilon) - d}{\varepsilon}, \\ a_{i,d^2} &= \lim_{\varepsilon\to 0} \frac{c_{i,d^2}(\varepsilon)}{\varepsilon}, \\ a_{d^2,j} &= \lim_{\varepsilon\to 0} \frac{c_{d^2,j}(\varepsilon)}{\varepsilon}, \\ a_{i,j} &= \lim_{\varepsilon\to 0} \frac{c_{i,j}(\varepsilon)}{\varepsilon}, \end{aligned} \tag{2.22}$$

equation 2.20 is then:

$$\mathcal{L}\rho = \frac{a_{d^2,d^2}}{d}\rho + \frac{1}{\sqrt{d}}\sum_{i=1}^{d^2-1}\left\{a_{i,d^2}F_i\rho + a_{d^2,j}\rho F_i^\dagger\right\} + \sum_{i,j=1}^{d^2-1} a_{i,j}F_i\rho F_j^\dagger \tag{2.23}$$

Summing over i and defining a new operator F:

$$F \equiv \frac{1}{\sqrt{d}}\sum_{i=1}^{d^2} a_{i,d^2}F_i, \tag{2.24}$$

in such a way that:

$$\mathcal{L}\rho = \frac{a_{d^2,d^2}}{d}\rho + F\rho + \rho F^\dagger + \sum_{i,j=1}^{d^2-1} a_{i,j}F_i\rho F_j^\dagger. \tag{2.25}$$

To recover the form of the Liouville - Von Neumann equation, we rewrite F in a hermitian part and an anti-hermitian part:

$$F = \frac{F+F^\dagger}{2} + i\frac{F-F^\dagger}{2i} \equiv G - iH, \tag{2.26a}$$

$$F^\dagger = \frac{F+F^\dagger}{2} + i\frac{F^\dagger-F}{2i} \equiv G + iH. \tag{2.26b}$$

Replacing the dependencies on F with the new definitions, we get:

$$F\rho + \rho F^\dagger = (G - iH)\rho + \rho(G + iH), \tag{2.27a}$$

$$= G\rho + \rho G - iH\rho + i\rho H, \tag{2.27b}$$

$$= \{G, \rho\} - i[H, \rho]. \tag{2.27c}$$

Making a change of variables, it is possible to embed the first term of the equation 2.25 in the anti-commutator:

$$G' = G + \frac{a_{d^2,d^2}\mathcal{I}}{2d}, \tag{2.28}$$

$$\mathcal{L}\rho = -i[H,\rho] + \{G,\rho\} + \sum_{i,j=1}^{d^2-1} a_{i,j} F_i \rho F_j^\dagger. \tag{2.29}$$

With the condition that the trace of ρ must remain constant:

$$Tr\left\{\mathcal{L}\rho\right\} = Tr\left\{\frac{\mathrm{d}}{\mathrm{d}t}\rho\right\} = \frac{\mathrm{d}}{\mathrm{d}t} Tr\left\{\rho\right\} = 0, \tag{2.30}$$

$$0 = Tr\left\{-iH\rho + i\rho H + G\rho + \rho G + \sum_{i,j=1}^{d^2-1} a_{i,j} F_i \rho F_j^\dagger\right\}, \tag{2.31a}$$

$$= Tr\left\{-iH\rho + iH\rho + G\rho + G\rho + \sum_{i,j=1}^{d^2-1} a_{i,j} F_j^\dagger F_i \rho\right\}, \tag{2.31b}$$

$$= Tr\left\{\left(2G + \sum_{i,j=1}^{d^2-1} a_{i,j} F_j^\dagger F_i\right)\rho\right\}, \tag{2.31c}$$

so:

$$2G + \sum_{i,j=1}^{d^2-1} a_{i,j} F_j^\dagger F_i = 0, \tag{2.32}$$

or:

$$G = -\frac{1}{2}\sum_{i,j=1}^{d^2-1} a_{i,j} F_j^\dagger F_i. \tag{2.33}$$

The most general form of the Liouville super-operator $\mathcal{L}$ that describes the evolution of density operators is called the Lindblad equation :

$$\mathcal{L}\rho = -i[H,\rho] + \sum_{i,j=1}^{d^2} a_{i,j} F_i \rho F_j^\dagger - \frac{1}{2} a_{i,j}\left\{F_j^\dagger F_i, \rho\right\}. \tag{2.34}$$

Finally, the matrix formed by the elements $a_{i,j}$ is diagonalizable since it is Hermitian (as $c_{j,i} = c_{i,j}^*$, the same goes for $a_{j,i}$). On the basis that diagonalizes it:

$$\mathcal{L}\rho = -i[H,\rho] + \sum_{k=1}^{d^2} \Gamma_i \left(L_i \rho L_i^\dagger - \frac{1}{2} \left\{ L_i^\dagger L_i, \rho \right\} \right), \tag{2.35}$$

the problem here is that the H and L_i aren't unique.

2.1.4 Microscopic derivation

For a more tangible deduction and to define the formats that H and L_i should have, it is customary to use a microscopic deduction: We start with the following Interaction Hamiltonian:

$$H = H_S \otimes \mathcal{I}_R + \mathcal{I}_S \otimes H_R + \alpha H_{SR}, \tag{2.36}$$

where H_S is the system's Hamiltonian, H_R is the reservoir's and H_{SR} is the coupling one.

The whole evolution equation can be written in the *interaction picture*[7] as (Note that we are making the temporal dependencies explicit again):

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_T(t) = -i[H_I(t), \rho_T(t)]. \tag{2.37}$$

By direct integration, we arrive at:

$$\rho_T(t) = \rho_T(0) - i\alpha \int_0^t [H_I(t'), \rho_T(t')] dt', \tag{2.38}$$

that can be iterated to:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_T(t) = -i\alpha[H_I(t), \rho_T(0)] - \alpha^2 \int_0^t dt' [H_I(t), [H_I(t'), \rho_T(t')]]. \tag{2.39}$$

[7]The interaction picture is defined as:

$$\rho_T = e^{i(H_S+H_R)t} \rho_{T,Sch} e^{-i(H_S+H_R)t},$$
$$H_I = e^{i(H_S+H_R)t} H_{SR} e^{-i(H_S+H_R).t}$$

Rewriting $\rho_T(t')$ as:

$$\rho_T(t') = \rho_T(t) - i\alpha \int_t^{t'} [H_I(t''), \rho(t'')]dt'', \tag{2.40}$$

and substituting in equation 2.39:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\rho_T(t) = -i\alpha[H_I(t), \rho_T(0)] - \alpha^2 \int_0^t [H_I(t), [H_I(t'), \rho_T(t)]]dt' + \\ + i\alpha^3 \int_0^t dt' \int_t^{t'} dt''[H_I(t), [H_I(t'), [H_I(t'', \rho(t''))]]], \end{aligned} \tag{2.41}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_T(t) = -i\alpha[H_I(t), \rho_T] - \alpha^2 \int_0^t [H_I(t), [H_I(t'), \rho_T(t)]]dt' + \mathcal{O}(\alpha^3). \tag{2.42}$$

In the weak interaction limit, we consider only terms to the second-order, as α^3 is much smaller than α^2 . As we are trying to write an equation that describes just the system's evolution, we take the partial trace over the reservoirs variables, $\rho = Tr_R\{\rho_T\}$, the same would work if we needed the evolution of the reservoir alone ($\sigma = Tr_S\{\rho_T\}$).

$$\frac{\mathrm{d}}{\mathrm{d}t}Tr_R\{\rho_T(t)\} = \frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -i\alpha Tr_R[H_I(t), \rho_T] - \alpha^2 \int_0^t dt' Tr_R[H_I(t), [H_I(t'), \rho_T(t)]]. \tag{2.43}$$

It is assumed that the reservoir is much larger than the system so in the weak interaction condition, we consider σ constant:

$$Tr_S\{\rho_T(t)\} = \sigma(t) \approx \sigma. \tag{2.44}$$

Also, we assumed that σ is a steady state of H_R :

$$[\sigma, H_R] = 0. \tag{2.45}$$

H_{SR} is written as:

$$H_{SR} = \sum_l S_l \otimes R_l \tag{2.46}$$

So, the interaction picture Hamiltonian H_I is just:

$$H_I(t) = \sum_l \hat{S}_l(t) \otimes \hat{R}_l(t), \tag{2.47}$$

where:

$$\hat{S}_l(t) = e^{iH_S t} S_l e^{-iH_S t}, \tag{2.48}$$

$$\hat{R}_l(t) = e^{iH_R t} R_l e^{-iH_R t}, \tag{2.49}$$

The averages of R_l in σ are chosen to be zero ($\langle R_l \rangle_\sigma = Tr\{\sigma R_l\} = 0$), which is always possible by making a change called "*Lamb Shift*" on the total Hamiltonian [32]. With this, it is easy to see that the average in σ of $\hat{R}_l$ in the interaction picture is also null:

$$\begin{aligned} Tr\left\{\sigma \hat{R}_l\right\} &= Tr\left\{\sigma e^{iH_R t} R_l e^{-iH_R t}\right\}, \\ &= Tr\left\{e^{-iH_R t} \sigma e^{iH_R t} R_l\right\}, \\ &= Tr\left\{\sigma e^{-iH_R t} e^{iH_R t} R_l\right\}, \\ &= Tr\{\sigma R_l\} = 0, \end{aligned} \tag{2.50}$$

because of this, the average of H_I in σ is zero:

$$Tr_R\{\sigma H_I(t)\} = \sum_l \hat{S}_l(t) Tr\left\{\sigma \hat{R}_l(t)\right\} = 0. \tag{2.51}$$

It's also possible to show that the second order averages in R vanish with a characteristic time τ_C [32], in such a way that the integrand in 2.43 is not null only in the proximity of $\tau = \tau_C$, where $\tau = t - t'$.

So, we may write 2.43 as:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\alpha^2 \int_0^\infty d\tau Tr_R[H_I(t), [H_I(t-\tau), \rho_T(t)]]. \tag{2.52}$$

The next assumption made is that the correlations disappear very quickly (of the order of magnitude of τ_C), *i.e.* in times smaller than the characteristic times of the system, in such a way that we can consider :

$$\rho_T(t) = \rho(t) \otimes \sigma(t) + \rho_{corr} \approx \rho(t) \otimes \sigma(t) \approx \rho(t) \otimes \sigma, \tag{2.53}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\alpha^2 \int_0^\infty d\tau Tr_R[H_I(t), [H_I(t-\tau), \rho(t) \otimes \sigma]], \tag{2.54}$$

$$\begin{aligned}[H_I(t), [H_I(t-\tau), \rho(t) \otimes \sigma]] = {} & H_I(t)H_I(t-\tau)\rho(t) \otimes \sigma \\ & - H_I(t)\rho(t) \otimes \sigma H_I(t-\tau) \\ & - H_I(t-\tau)\rho(t) \otimes \sigma H_I(t) \\ & + \rho(t) \otimes \sigma H_I(t-\tau)H_I(t).\end{aligned} \tag{2.55}$$

Using the equation 2.47 :

$$\begin{aligned}[H_I(t), [H_I(t-\tau), \rho(t) \otimes \sigma]] = {} & \sum_{l,k} \hat{S}_l(t)\hat{S}_k(t-\tau)\rho(t) \otimes \hat{R}_l(t)\hat{R}_k(t-\tau)\sigma \\ & - \hat{S}_l(t)\rho(t)\hat{S}_k(t-\tau) \otimes \hat{R}_l(t)\sigma\hat{R}_k(t-\tau) \\ & - \hat{S}_k(t-\tau)\rho(t)\hat{S}_l(t) \otimes \hat{R}_k(t-\tau)\sigma\hat{R}_l(t) \\ & + \rho(t)\hat{S}_k(t-\tau)\hat{S}_l(t) \otimes \sigma\hat{R}_k(t-\tau)\hat{R}_l(t).\end{aligned} \tag{2.56}$$

Using the spectral theorem :

$$S_l(\omega) = \sum_{\varepsilon'-\varepsilon=\omega} P_\varepsilon S_l P_{\varepsilon'}, \tag{2.57}$$

where P_ε are the energy projectors[8]. So:

$$[H_S, S_l(\omega)] = \sum_{\varepsilon'-\varepsilon=\omega} H_S P_\varepsilon S_l P_{\varepsilon'} - P_\varepsilon S_l P_{\varepsilon'} H_S, \tag{2.58a}$$

$$= \sum_{\varepsilon'-\varepsilon=\omega} \varepsilon P_\varepsilon S_l P_{\varepsilon'} - P_\varepsilon S_l P_{\varepsilon'} \varepsilon', \tag{2.58b}$$

$$= -\omega S_l(\omega), \tag{2.58c}$$

and

$$[H_S, S_l^\dagger(\omega)] = \sum_{\varepsilon'-\varepsilon=\omega} H_S P_{\varepsilon'} S_l^\dagger P_\varepsilon - P_{\varepsilon'} S_l^\dagger P_\varepsilon H_S, \tag{2.59a}$$

$$= \sum_{\varepsilon'-\varepsilon=\omega} \varepsilon' P_{\varepsilon'} S_l^\dagger P_\varepsilon - P_\varepsilon S_l^\dagger P_\varepsilon \varepsilon, \tag{2.59b}$$

$$= \omega S_l(\omega). \tag{2.59c}$$

From this, we calculate:

$$\hat{S}_l(t) = e^{iH_S t} S_l(\omega) e^{-iH_S t}, \tag{2.60a}$$

$$= S_l(\omega) + it[H_S, S_l(\omega)] + \frac{(it)^2}{2!}[H_S, [H_S, S_l(\omega)]] + ..., \tag{2.60b}$$

$$= S_l(\omega) - it\omega S_l(\omega) - \frac{t^2\omega^2}{2!} S_l(\omega) + ..., \tag{2.60c}$$

$$= e^{-i\omega t} S_l(\omega), \tag{2.60d}$$

and

$$\hat{S_l}^\dagger(t) = = e^{iH_S t} S_l^\dagger(\omega) e^{-iH_S t}, \tag{2.61a}$$

$$= S_l^\dagger(\omega) + it[H_S, S_l^\dagger(\omega)] + \frac{(it)^2}{2!}[H_S, [H_S, S_l^\dagger(\omega)]] + ..., \tag{2.61b}$$

$$= S_l^\dagger(\omega) + it\omega S_l^\dagger(\omega) - \frac{t^2\omega^2}{2!} S_l^\dagger(\omega) + ..., \tag{2.61c}$$

$$= e^{i\omega t} S_l^\dagger(\omega). \tag{2.61d}$$

[8] $H_S P_\varepsilon = \varepsilon P_\varepsilon$.

It's also possible to prove that the systems Hamiltonian H_S and $S_l^\dagger(\omega)S_k(\omega)$ commute, which will be useful further ahead when we obtain the evolution in a Lindblad form.

$$
\begin{aligned}
[H_S, S_l^\dagger(\omega)S_k(\omega)] &= H_S S_l^\dagger(\omega)S_k(\omega) - S_l^\dagger(\omega)S_k(\omega)H_S, && \text{(2.62a)}\\
&= H_S S_l^\dagger(\omega)S_k(\omega) - S_l^\dagger(\omega)\left\{H_S S_k(\omega) - [H_S, S_k(\omega)]\right\}, && \text{(2.62b)}\\
&= H_S S_l^\dagger(\omega)S_k(\omega) - S_l^\dagger(\omega)\left\{H_S S_k(\omega) - \omega S_k(\omega)\right\}, && \text{(2.62c)}\\
&= H_S S_l^\dagger(\omega)S_k(\omega) - S_l^\dagger(\omega)H_S S_k(\omega) - \omega S_l^\dagger S_k(\omega), && \text{(2.62d)}\\
&= H_S S_l^\dagger(\omega)S_k(\omega) - \left\{H_S S_l^\dagger(\omega) - [H_S, S_l^\dagger]\right\} S_k(\omega) - \omega S_l^\dagger S_k(\omega), && \text{(2.62e)}\\
&= H_S S_l^\dagger(\omega)S_k(\omega) - H_S S_l^\dagger(\omega)S_k(\omega) + \omega S_l^\dagger S_k(\omega) - \omega S_l^\dagger S_k(\omega), && \text{(2.62f)}\\
&= 0. && \text{(2.62g)}
\end{aligned}
$$

Also, it's easy to show that $S_l^\dagger(\omega) = S_l(-\omega)$:

$$
\begin{aligned}
S_l^\dagger(\omega) &= \sum_{\varepsilon-\varepsilon'=\omega} P_{\varepsilon'}^\dagger S_l^{\dagger\dagger} P_\varepsilon^\dagger, && \text{(2.63a)}\\
&= \sum_{\varepsilon-\varepsilon'=\omega} P_{\varepsilon'} S_l P_\varepsilon, && \text{(2.63b)}\\
&= \sum_{\varepsilon-\varepsilon'=-\omega} P_\varepsilon S_l P_{\varepsilon'} = S_l(-\omega). && \text{(2.63c)}
\end{aligned}
$$

Substituting $S_k(\omega)$ in $\hat{S}_k(t-\tau)$ and $S_l^\dagger(\omega')$ in $\hat{S}_l(t)$:

$$
\begin{aligned}
[H_I(t),[H_I(t-\tau),\rho(t)\otimes\sigma]] = \sum_{l,k,\omega,\omega'} & e^{i\omega' t} S_l^\dagger(\omega') e^{-i\omega(t-\tau)} S_k(\omega)\rho(t)\otimes \hat{R}_l(t)\hat{R}_k(t-\tau)\sigma \\
& - e^{-i\omega(t-\tau)} S_k(\omega)\rho(t) e^{i\omega' t} S_l^\dagger(\omega')\otimes \hat{R}_k(t-\tau)\sigma\hat{R}_l(t) \\
& + h.c., \\
= \sum_{l,k,\omega,\omega'} & e^{i(\omega'-\omega)t} e^{i\omega\tau} S_l^\dagger(\omega') S_k(\omega)\rho(t)\otimes \hat{R}_l(t)\hat{R}_k(t-\tau)\sigma \\
& - e^{i(\omega'-\omega)t} e^{i\omega\tau} S_k(\omega)\rho(t) S_l^\dagger(\omega')\otimes \hat{R}_k(t-\tau)\sigma\hat{R}_l(t) \\
& + h.c..
\end{aligned}
\tag{2.64}
$$

Using this commutator in 2.54 :

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\alpha^2 \int_0^\infty d\tau Tr_R\{ \sum_{l,k,\omega,\omega'} & e^{i(\omega'-\omega)t} e^{i\omega\tau} S_l^\dagger(\omega') S_k(\omega)\rho(t)\otimes \hat{R}_l(t)\hat{R}_k(t-\tau)\sigma \\
& - e^{i(\omega'-\omega)t} e^{i\omega\tau} S_k(\omega)\rho(t) S_l^\dagger(\omega')\otimes \hat{R}_k(t-\tau)\sigma\hat{R}_l(t) \\
& + h.c.\}.
\end{aligned}
\tag{2.65}
$$

The partial trace in R ignores the system:

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\alpha^2 \int_0^\infty d\tau \sum_{l,k,\omega,\omega'} & e^{i(\omega'-\omega)t} S_l^\dagger(\omega') S_k(\omega)\rho(t) e^{i\omega\tau} Tr\{\hat{R}_l(t)\hat{R}_k(t-\tau)\sigma\} \\
& - e^{i(\omega'-\omega)t} S_k(\omega)\rho(t) S_l^\dagger(\omega') e^{i\omega\tau} Tr\{\hat{R}_k(t-\tau)\sigma\hat{R}_l(t)\} \\
& + h.c..
\end{aligned}
\tag{2.66}
$$

As the trace is invariant under cyclic commutation, the 2 traces shown above are the same. Also, the terms of the system don't depend on τ, so we can write:

$$
\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \sum_{l,k,\omega,\omega'} \Gamma_{lk}(\omega) \left\{ \hat{S}_k(\omega)\rho(t)\hat{S}_l{}^\dagger(\omega') - \hat{S}_l{}^\dagger(\omega')\hat{S}_k(\omega)\rho(t) \right\} + h.c., \tag{2.67}
$$

where $\Gamma_{lk}(\omega)$ was defined as:

$$\Gamma_{lk}(\omega) \equiv \int_0^\infty d\tau \alpha^2 e^{i\omega\tau} Tr\{\hat{R}_l(t)\hat{R}_k(t-\tau)\sigma\} = \int_0^\infty d\tau \alpha^2 e^{i\omega\tau} Tr\{\hat{R}_l(\tau)R_k\sigma\}. \quad (2.68)$$

Note that R_k in the last equation is the Schrodinger one, *i.e.*, $R_l = \hat{R}_l(0)$. We then separate $\Gamma_{lk}(\omega)$ into real and imaginary parts as follows:

$$\Gamma_{lk}(\omega) = \frac{1}{2}\gamma_{lk}(\omega) + i\pi_{lk}(\omega), \quad (2.69)$$

γ and π are given by:

$$\begin{aligned} \gamma_{lk}(\omega) &= \Gamma_{lk}(\omega) + \Gamma^*_{kl}(\omega), \\ \pi_{lk}(\omega) &= \frac{\Gamma_{lk}(\omega) - \Gamma^*_{kl}(\omega)}{2i}. \end{aligned} \quad (2.70)$$

With that:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \sum_{l,k,\omega} &\left\{\frac{1}{2}\gamma_{lk}(\omega) + i\pi_{lk}(\omega)\right\}[\hat{S}_k(\omega)\rho(t), \hat{S}_l{}^\dagger(\omega)] + \\ &+ \left\{\frac{1}{2}\gamma_{lk}(\omega) - i\pi_{lk}(\omega)\right\}[\hat{S}_k(\omega), \rho(t)\hat{S}_l{}^\dagger(\omega)], \end{aligned} \quad (2.71)$$

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = &\sum_{l,k,\omega} \frac{\gamma_{lk}(\omega)}{2}\{\hat{S}_k(\omega)\rho(t)\hat{S}_l{}^\dagger(\omega) - \hat{S}_l{}^\dagger(\omega)\hat{S}_k(\omega)\rho(t) + \\ &+ \hat{S}_k(\omega)\rho(t)\hat{S}_l{}^\dagger(\omega) - \rho(t)\hat{S}_l{}^\dagger(\omega)\hat{S}_k(\omega)\} + \\ &+ i\pi_{lk}(\omega)\{\hat{S}_k(\omega)\rho(t)\hat{S}_l{}^\dagger(\omega) - \hat{S}_l{}^\dagger(\omega)\hat{S}_k(\omega)\rho(t) - \\ &- \hat{S}_k(\omega)\rho(t)\hat{S}_l{}^\dagger(\omega) + \rho(t)\hat{S}_l{}^\dagger(\omega)\hat{S}_k(\omega)\}, \end{aligned} \quad (2.72)$$

$$\begin{aligned} &= \sum_{l,k,\omega} \gamma_{lk}(\omega)\left\{\hat{S}_k(\omega)\rho(t)\hat{S}_l{}^\dagger(\omega) - \frac{1}{2}\left\{\hat{S}_l{}^\dagger(\omega)\hat{S}_k(\omega), \rho(t)\right\}\right\} - \\ &- i\pi_{lk}(\omega)\left[\hat{S}_l{}^\dagger(\omega)\hat{S}_k(\omega), \rho(t)\right]. \end{aligned} \quad (2.73)$$

That may be written as:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -i\left[H_{LS}, \rho(t)\right] + \mathcal{D}[\rho(t)], \quad (2.74)$$

where the first term is written as H_{LS} because it represents a shift in the total energy and could be written as part of an effective Hamiltonian as $H_{eff} = H_S + H_{LS}$ in Schrodinger's picture. The only thing left to do is to write H_{LS} and $\mathcal{D}[\rho(t)]$ explicitly:

$$H_{LS} = \sum_{l,k,\omega} \pi_{lk}(\omega) \hat{S}_l^{\dagger}(\omega) \hat{S}_k(\omega), \tag{2.75}$$

$$\mathcal{D}[\rho(t)] = \sum_{l,k,\omega} \gamma_{lk}(\omega) \left\{ \hat{S}_k(\omega) \rho(t) \hat{S}_l^{\dagger}(\omega) - \frac{1}{2} \left\{ \hat{S}_l^{\dagger}(\omega) \hat{S}_k(\omega), \rho(t) \right\} \right\}. \tag{2.76}$$

Moreover, the matrix γ_{lk} is hermitian[9] and can be diagonalized to the Lindblad form in equation 2.35.

$$\mathcal{D}[\rho(t)] = \sum_{i,\omega} \Gamma_i(\omega) \left\{ \hat{S}_i(\omega) \rho(t) \hat{S}_i^{\dagger}(\omega) - \frac{1}{2} \left\{ \hat{S}_i^{\dagger}(\omega) \hat{S}_i(\omega), \rho(t) \right\} \right\}. \tag{2.77}$$

As a last remark, the term $\mathcal{D}[\bullet]$ is called dissipator since it can be shown that the purity of a system ($\mathrm{Tr}(\rho^2)$) decreases in contrast to a unitary evolution, where it's constant [30].

Furthermore, there is a state called steady state that represents the limit where everything that could happen already happened and so the system is constant in time, or mathematically:

$$\rho_{ss} = \lim_{t \to \infty} \rho(t), \tag{2.78}$$

it is always possible to find a steady state for the evolution of ρ by $\mathcal{L}$ [29, 33, 34] but it's not always unique [35]. The problem with the non-uniqueness of the steady state would be a problem in the models of machines in thermodynamics because the system would never *thermalize*[10], on the bright side, this is the exception [29].

[9] Note that γ_{lk} is real by definition and $\gamma_{lk} = \gamma_{kl}$.

[10] would never achieve thermal stability.

2.2 Quantum Thermodynamics

Quantum thermodynamics is the study of how energy flows as work and heat in quantum systems and it's a relatively new area of physics. The first definitions of heat and work in the quantum regime were described by Allicki [36] but he was not the first one to realize quantum systems could be engines or machines [3], since then, it has been an area studied with great interest.

The first step towards a quantum theory of thermodynamics is to realize how to divide the change in energy in heat and work[11]. In usual quantum mechanics, the energy is

$$E = \langle H \rangle = \mathrm{Tr}\{H\rho\}, \tag{2.79}$$

so, the differential of energy is given by:

$$dE = \mathrm{Tr}\{dH\rho + Hd\rho\}. \tag{2.80}$$

We defined the first term as work and the other as heat. The idea behind this is that we can completely control the Hamiltonian and thus the energy change that comes out of it is work. The other part is then the heat, which makes sense in some way since the experimentalist doesn't control the change in the state, it happens as a response from the system. So

$$dW = \mathrm{Tr}\{dH\rho\}, \tag{2.81}$$

and

$$dQ = \mathrm{Tr}\{Hd\rho\}, \tag{2.82}$$

[11] We want to point out that this division is not always valid, for a more general formulation, read [37–40]. But in the regime we are using it, it's good, as made in [41].

or, in a more useful way

$$W(t) = \int_0^t \mathrm{Tr}\left\{\frac{\mathrm{d}H}{\mathrm{d}\tau}\rho\right\}d\tau, \tag{2.83}$$

$$Q(t) = \int_0^t \mathrm{Tr}\left\{H\frac{\mathrm{d}\rho}{\mathrm{d}\tau}\right\}d\tau. \tag{2.84}$$

In this model, the first law of thermodynamics is straightforward:

$$dU = dW + dQ, \tag{2.85}$$

or

$$\Delta U = \int_0^t \mathrm{Tr}\left\{\frac{\mathrm{d}H}{\mathrm{d}\tau}\rho\right\}d\tau + \int_0^t \mathrm{Tr}\left\{H\frac{\mathrm{d}\rho}{\mathrm{d}\tau}\right\}d\tau. \tag{2.86}$$

If we analyze a system without a reservoir, i.e., a close system evolving in a unitary way, we can write:

$$\frac{\mathrm{d}\langle E\rangle}{\mathrm{d}t} = \mathrm{Tr}\left\{\frac{\mathrm{d}\rho}{\mathrm{d}t}H + \rho\frac{\mathrm{d}H}{\mathrm{d}t}\right\}, \tag{2.87}$$

but

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left\{\mathcal{U}\rho(t_0)\mathcal{U}^\dagger\right\}, \tag{2.88}$$

$$= \frac{\mathrm{d}\mathcal{U}}{\mathrm{d}t}\rho(t_0)\mathcal{U}^\dagger + \mathcal{U}\rho(t_0)\frac{\mathrm{d}\mathcal{U}^\dagger}{\mathrm{d}t}, \tag{2.89}$$

$$= -iH\mathcal{U}\rho\mathcal{U}^\dagger + i\mathcal{U}\rho\mathcal{U}^\dagger H, \tag{2.90}$$

so

$$\frac{\mathrm{d}\langle E\rangle}{\mathrm{d}t} = \mathrm{Tr}\left\{-iH\mathcal{U}\rho\mathcal{U}^\dagger H + i\mathcal{U}\rho\mathcal{U}^\dagger H^2 + \rho\frac{\mathrm{d}H}{\mathrm{d}t}\right\}, \tag{2.91}$$

$$= \mathrm{Tr}\left\{\rho\frac{\mathrm{d}H}{\mathrm{d}t}\right\} = \frac{\mathrm{d}W}{\mathrm{d}t}, \tag{2.92}$$

so, as was expected, the closed system doesn't trade heat and all changes in the total energy of the system are due to work[12].

[12]Note too that unitary transformation doesn't alter Von Neumann's entropy [27].

On the other hand, if we study a system interacting with a reservoir but with a constant hamiltonian, the power is

$$\frac{\mathrm{d}\langle E\rangle}{\mathrm{d}t} = \mathrm{Tr}\left\{\frac{\mathrm{d}\rho}{\mathrm{d}t}H + \rho\cancelto{0}{\frac{\mathrm{d}H}{\mathrm{d}t}}\right\}, \tag{2.93}$$

$$= \mathrm{Tr}\left\{\frac{\mathrm{d}\rho}{\mathrm{d}t}H\right\} = \frac{\mathrm{d}Q}{\mathrm{d}t}, \tag{2.94}$$

the energy transfer in this case is just heat.

2.3 Shortcut to adiabaticity

In quantum mechanics, the concept of adiabaticity is related to the one in thermodynamics in the sense that both describe the slow evolution of systems. For a slow-driven Hamiltonian, the transitions between instantaneous eigenstates are close to zero.

The method of shortcuts to adiabaticity consists in adding another hamiltonian to the original so the system can evolve as an instantaneous eigenstate of the original hamiltonian at any speed we like. The method used in this work was developed in [16–21].

So, if the eigenvalue equation to the original hamiltonian ($H_0(t)$) is:

$$H_0(t)\left|n(t)\right\rangle = E_n(t)\left|n(t)\right\rangle, \tag{2.95}$$

where H_0 is:

$$H_0(t) = \sum_n E_n(t)\left|n(t)\right\rangle\!\left\langle n(t)\right|. \tag{2.96}$$

In the limit of adiabatic evolution, the systems state is described as;

$$\left|\psi_n(t)\right\rangle = e^{i\xi_n(t)}\left|n(t)\right\rangle, \tag{2.97}$$

the phase $\xi_n(t)$ may be found by substituting equations 2.96 e 2.97 in 2.95.

$$\mathcal{H}_0(t)\left|\psi_n(t)\right\rangle = i\partial_t\left|\psi_n(t)\right\rangle, \tag{2.98}$$

$$\sum_m E_m(t)\left|m(t)\right\rangle\!\left\langle m(t)\right| e^{i\xi_n(t)}\left|n(t)\right\rangle = i\partial_t(e^{i\xi_n(t)}\left|n(t)\right\rangle), \tag{2.99}$$

$$\sum_m E_m(t)e^{i\xi_n(t)}\left\langle m(t)|n(t)\right\rangle\left|n(t)\right\rangle = i\{i\dot{\xi_n}(t)\left|n(t)\right\rangle + \partial_t\left|n(t)\right\rangle\}e^{i\xi_n(t)}, \tag{2.100}$$

$$\sum_m \delta_{nm}(t)E_m(t)e^{i\xi_n(t)}\left|n(t)\right\rangle = i\{i\dot{\xi_n}(t)\left|n(t)\right\rangle + \left|\partial_t n(t)\right\rangle\}e^{i\xi_n(t)}, \tag{2.101}$$

$$E_n(t)e^{i\xi_n(t)}\left|n(t)\right\rangle = i\{i\dot{\xi_n}(t)\left|n(t)\right\rangle + \left|\partial_t n(t)\right\rangle\}e^{i\xi_n(t)}. \tag{2.102}$$

Multiplying in the left by $\langle n(t)|\, e^{-i\xi_n(t)}$ one find:

$$\dot{\xi_n}(t) = -E_n(t) + i\,\langle n(t)|\partial_t n(t)\rangle\,, \tag{2.103}$$

finally, to obtain ξ_n, just integrate:

$$\xi_n(t) = -\int_0^t E_n(t')dt' + i\int_0^t \langle n(t')|\partial_{t'} n(t')\rangle\, dt'. \tag{2.104}$$

From Schrodinger's equation to the evolution operator ($\mathcal{U}(t)$, we can find the Hamiltonian given the evolution:

$$\mathcal{H}(t)\mathcal{U}(t) = i\hbar\partial_t\mathcal{U}(t), \tag{2.105a}$$

$$\mathcal{H}(t) = i\hbar\dot{\mathcal{U}}(t)\mathcal{U}^\dagger(t). \tag{2.105b}$$

The evolution operator can be easily inferred as:

$$\mathcal{U}(t) = \sum_n \exp(i\xi_n)\,|n(t)\rangle\,\langle n(0)|\,. \tag{2.106}$$

To calculate the Hamiltonian 2.105b, we need $\dot{\mathcal{U}}$ and $\mathcal{U}^\dagger$:

$$\dot{\mathcal{U}}(t) = \partial_t\left\{\sum_n e^{i\xi_n(t)}\,|n(t)\rangle\langle n(0)|\right\} \tag{2.107a}$$

$$= \sum_n\left\{i\dot{\xi}_n(t)e^{i\xi_n(t)}\,|n(t)\rangle\langle n(0)| + e^{i\xi_n(t)}\,|\partial_t n(t)\rangle\langle n(0)|\right\}, \tag{2.107b}$$

$$= \sum_n\left\{i\dot{\xi}_n(t)\,|n(t)\rangle\langle n(0)| + |\partial_t n(t)\rangle\langle n(0)|\right\}e^{i\xi_n(t)}, \tag{2.107c}$$

$$\mathcal{U}^\dagger(t) = \left\{\sum_n e^{i\xi_n(t)}\,|n(t)\rangle\langle n(0)|\right\}^\dagger, \tag{2.108a}$$

$$= \sum_n e^{-i\xi_n(t)}\,|n(0)\rangle\langle n(t)|\,. \tag{2.108b}$$

Putting 2.107c and 2.108b in 2.105b:

$$\mathcal{H}(t) = i\hbar \sum_{n,m} \left\{ i\dot{\xi}_n \left|n(t)\right\rangle\!\left\langle n(0)\right| + \left|\partial_t n(t)\right\rangle\!\left\langle n(0)\right| \right\} e^{i\xi_n(t)} e^{-i\xi_m(t)} \left|m(0)\right\rangle\!\left\langle m(t)\right|, \quad (2.109a)$$

$$= i\hbar \sum_{n,m} e^{i(\xi_n(t)-\xi_m(t))} \left\{ i\dot{\xi}_n(t) \left|n(t)\right\rangle\!\left\langle m(t)\right| \delta_{n,m}(t) + \left|\partial_t n(t)\right\rangle\!\left\langle m(t)\right| \delta_{n,m}(t) \right\}, \quad (2.109b)$$

$$= i\hbar \sum_{n} \left\{ i\dot{\xi}_n(t) \left|n(t)\right\rangle\!\left\langle n(t)\right| + \left|\partial_t n(t)\right\rangle\!\left\langle n(t)\right| \right\}, \quad (2.109c)$$

finally, replace 2.103 in 2.109c:

$$\mathcal{H}(t) = i\hbar \sum_{n} \left\{ i \left[-\frac{1}{\hbar} E_n(t) + i \left\langle n(t)|\partial_t n(t)\right\rangle \right] \left|n(t)\right\rangle\!\left\langle n(t)\right| + \left|\partial_t n(t)\right\rangle\!\left\langle n(t)\right| \right\}, \quad (2.110a)$$

$$= \sum_n E_n(t) \left|n(t)\right\rangle\!\left\langle n(t)\right| + i\hbar \sum_n \left\{ \left|\partial_t n(t)\right\rangle \left\langle n(t)\right| - \left\langle n(t)|\partial_t n(t)\right\rangle \left|n(t)\right\rangle\!\left\langle n(t)\right| \right\}, \quad (2.110b)$$

$$= \mathcal{H}_0(t) + \mathcal{H}_{CD}(t), \quad (2.110c)$$

where :

$$\mathcal{H}_{CD}(t) = i\hbar \sum_n \left\{ \left|\partial_t n(t)\right\rangle \left\langle n(t)\right| - \left\langle n(t)|\partial_t n(t)\right\rangle \left|n(t)\right\rangle\!\left\langle n(t)\right| \right\}, \quad (2.111)$$

CD here comes from *Counterdiabatic Driving* since it works by removing the non-adiabatic part of the evolution.

There is yet another, more natural way to write $\mathcal{H}_{CD}$ by calculating it's the matrix

elements $\langle m(t)|\,\mathcal{H}_{CD}\,|o(t)\rangle$:

$$\langle m(t)|\,\mathcal{H}_{CD}\,|o(t)\rangle = i\hbar\,\langle m(t)|\sum_n \{|\partial_t n(t)\rangle\,\langle n(t)| - \langle n(t)|\partial_t n(t)\rangle\,|n(t)\rangle\langle n(t)|\}\,|o(t)\rangle\,, \tag{2.112}$$

$$= i\hbar\sum_n \langle m(t)|\partial_t n(t)\rangle\,\langle n(t)|o(t)\rangle - \langle n(t)|\partial_t n(t)\rangle\,\langle m(t)|n(t)\rangle\,\langle n(t)|o(t)\rangle\,, \tag{2.113}$$

$$= i\hbar\sum_n \langle m(t)|\partial_t n(t)\rangle\,\delta_{no}(t) - \langle n(t)|\partial_t n(t)\rangle\,\delta_{mn}(t)\delta_{no}(t), \tag{2.114}$$

$$= i\hbar\,\{\langle m(t)|\partial_t o(t)\rangle - \langle o(t)|\partial_t o(t)\rangle\,\delta_{mo}(t)\}\,. \tag{2.115}$$

It's easy to see that $\mathcal{H}_{CD}$ has no diagonal terms, i.e., $\langle n(t)|\,\mathcal{H}_{CD}\,|n(t)\rangle = 0 \quad \forall \quad n$. From the eigenvalue equation to the Hamiltonian, one can obtain:

$$\mathcal{H}_0(t)\,|n(t)\rangle = E_n(t)\,|n(t)\rangle\,, \tag{2.116}$$

$$\dot{\mathcal{H}}_0(t)\,|n(t)\rangle + \mathcal{H}_0(t)\,|\partial_t n(t)\rangle = \dot{E}_n(t)\,|n(t)\rangle + E_n(t)\,|\partial_t n(t)\rangle\,. \tag{2.117}$$

Multiplying in the left by $\langle m(t)|$ for a $m \neq n$:

$$\langle m(t)|\,\dot{\mathcal{H}}_0(t)\,|n(t)\rangle + \langle m(t)|\,\mathcal{H}_0(t)\,|\partial_t n(t)\rangle = \dot{E}_n(t)\cancelto{0}{\langle m(t)|n(t)\rangle} + E_n(t)\,\langle m(t)|\partial_t n(t)\rangle\,, \tag{2.118}$$

$$\langle m(t)|\,\dot{\mathcal{H}}_0(t)\,|n(t)\rangle = \{E_n(t) - E_m(t)\}\,\langle m(t)|\partial_t n(t)\rangle\,, \tag{2.119}$$

$$\langle m(t)|\partial_t n(t)\rangle = \frac{\langle m(t)|\,\dot{\mathcal{H}}_0(t)\,|n(t)\rangle}{E_n(t) - E_m(t)}. \tag{2.120}$$

We can finally write the counter driving hamiltonian as:

$$\mathcal{H}_{CD}(t) = \sum_{n,m} |m(t)\rangle\langle m(t)| \, \mathcal{H}_{CD}(t) \, |n(t)\rangle\langle n(t)| \,, \tag{2.121}$$

$$= \sum_{\substack{m,n \\ m\neq n}} |m(t)\rangle \left\{ i\hbar \, \langle m(t)|\partial_t n(t)\rangle \right\} \langle n(t)| \,, \tag{2.122}$$

$$= i\hbar \sum_{\substack{m,n \\ m\neq n}} |m(t)\rangle \, \frac{\langle m(t)| \, \dot{\mathcal{H}}_0 \, |n(t)\rangle}{E_n(t) - E_m(t)} \, \langle n(t)| \,. \tag{2.123}$$

2.4 Squeezing

It's well known that non-commuting operators must obey the uncertainty principle

$$\Delta A \Delta B \geq \frac{1}{2} \left| \langle [A, B] \rangle \right|, \tag{2.124}$$

that limits the minimum uncertainty on measurements.We can apply this to the position and momentum operators to obtain the usual:

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \tag{2.125}$$

There are states for which this uncertainty can achieve the equality, for example, the coherent states for the harmonic oscillator. The coherent states are defined as

$$\hat{a} \left| \alpha \right\rangle = \alpha \left| \alpha \right\rangle, \tag{2.126}$$

i.e., the eigenstates of the ladder operators.

The uncertainty to the position is:

$$\begin{aligned}
(\Delta x)^2 &= \left\langle x^2 \right\rangle - \left\langle x \right\rangle^2, && (2.127)\\
&= \frac{\hbar}{2m\omega} \left\langle \alpha \right| \left(\hat{a} + \hat{a}^\dagger \right)^2 \left| \alpha \right\rangle - \frac{\hbar}{2m\omega} \left\langle \alpha \right| \left(\hat{a} + \hat{a}^\dagger \right) \left| \alpha \right\rangle^2, && (2.128)\\
&= \frac{\hbar}{2m\omega} \left(\left\langle \alpha \right| \left(\hat{a}^2 + \hat{a}^{\dagger 2} + 2\hat{a}^\dagger \hat{a} + 1 \right) \left| \alpha \right\rangle - (\alpha + \bar{\alpha})^2 \right), && (2.129)\\
&= \frac{\hbar}{2m\omega} \left((\alpha + \bar{\alpha})^2 + 1 - (\alpha + \bar{\alpha})^2 \right), && (2.130)\\
&= \frac{\hbar}{2m\omega}. && (2.131)
\end{aligned}$$

Same can be calculated for momentum:

$$\begin{aligned}
(\Delta p)^2 &= \left\langle p^2 \right\rangle - \left\langle p \right\rangle^2, && (2.132)\\
&= -\frac{\hbar m\omega}{2} \left\langle \alpha \right| \left(\hat{a} - \hat{a}^\dagger \right)^2 \left| \alpha \right\rangle + \frac{\hbar m\omega}{2} \left\langle \alpha \right| \left(\hat{a} - \hat{a}^\dagger \right) \left| \alpha \right\rangle^2, && (2.133)\\
&= -\frac{\hbar m\omega}{2} \left(\left\langle \alpha \right| \left(\hat{a}^2 + \hat{a}^{\dagger 2} - 2\hat{a}^\dagger \hat{a} - 1 \right) \left| \alpha \right\rangle - (\alpha + \bar{\alpha})^2 \right), && (2.134)\\
&= -\frac{\hbar m\omega}{2} \left((\alpha - \bar{\alpha})^2 - 1 - (\alpha - \bar{\alpha})^2 \right), && (2.135)\\
&= \frac{\hbar m\omega}{2}. && (2.136)
\end{aligned}$$

So, their product is:

$$\Delta x \Delta p = \frac{\hbar}{2}. \tag{2.137}$$

There is yet another way of looking at this, we can use the electric operator of a single mode electromagnetic wave:

$$\hat{E}(t) = \frac{E_0}{2}\left(\hat{a}e^{-i\omega t} + \hat{a}^\dagger e^{i\omega t}\right), \tag{2.138}$$

or:

$$\hat{E}(t) = E_0\left(\hat{X}_1 \cos\omega t + \hat{X}_2 \sin\omega t\right), \tag{2.139}$$

here, the operators $\hat{X}_1$ and $\hat{X}_2$ are called quadratures of the field and are given by:

$$\hat{X}_1 = \frac{\hat{a} + \hat{a}^\dagger}{2} \tag{2.140}$$

$$\hat{X}_2 = \frac{\hat{a} - \hat{a}^\dagger}{2i} \tag{2.141}$$

they must obey a similar uncertainty principle given by:

$$\Delta X_1 \Delta X_2 \geq \frac{1}{4}, \tag{2.142}$$

for coherent states of light, the equality is true and the quadrature fluctuations are equal to one another

$$\left\langle (\Delta X_1)^2 \right\rangle = \left\langle (\Delta X_2)^2 \right\rangle = \frac{1}{4}. \tag{2.143}$$

These minimum uncertainty is called vacuum uncertainty (as the vacuum states are a form of obtain this equality). There is a way to still obtain a smaller uncertainty in the way that we squeeze the uncertainty on the quadratures, one gets smaller but the other must become greater, since the uncertainty principle must remain true.

These squeezed states are defined by the squeezing operator:

$$|\psi_S\rangle = \hat{S}(\zeta)\,|\psi\rangle\,, \tag{2.144}$$

ζ is equal to $re^{i\theta}$, where r is called squeezing parameter and θ represents the angle between the squeezing axis and the quadrature axis, furthermore, the operator itself is defined as:

$$\hat{S}(r,\theta) = \exp\left\{\frac{1}{2}(\zeta^*\hat{a}^2 - \zeta\hat{a}^{\dagger 2})\right\}. \tag{2.145}$$

it's useful to calculate the application of the squeezing operator in the ladder operators:

$$\hat{S}^\dagger \hat{a} \hat{S} = \hat{a}\cosh r - \hat{a}^\dagger e^{i\theta}\sinh r, \tag{2.146}$$

$$\hat{S}^\dagger \hat{a}^\dagger \hat{S} = \hat{a}^\dagger\cosh r - \hat{a}e^{-i\theta}\sinh r. \tag{2.147}$$

We then, calculate the variance in the quadratures for the squeezed vacuum state:

$$(\Delta X_1)^2 = \left\langle X_1^2\right\rangle - \left\langle X_1\right\rangle^2, \tag{2.148}$$

$$= \left\langle\zeta\right| X_1^2 \left|\zeta\right\rangle - \left\langle\zeta\right| X_1 \left|\zeta\right\rangle^2, \tag{2.149}$$

$$= \frac{1}{4}\left\langle 0\right| \hat{S}^\dagger(\hat{a}+\hat{a}^\dagger)^2\hat{S}\left|0\right\rangle - \frac{1}{4}\left\langle 0\right| \hat{S}^\dagger(\hat{a}+\hat{a}^\dagger)\hat{S}\left|0\right\rangle^2, \tag{2.150}$$

$$= \frac{1}{4}\left\langle 0\right| \hat{S}^\dagger(\hat{a}^2+\hat{a}^{\dagger 2}+2\hat{a}^\dagger\hat{a}+1)\hat{S}\left|0\right\rangle - \tag{2.151}$$

$$- \frac{1}{4}\left\langle 0\right| \left(\hat{a}(\cosh r - e^{-i\theta}\sinh r) + \hat{a}^\dagger(\cosh r - e^{i\theta}\sinh r)\right)\left|0\right\rangle^2,$$

$$= \frac{1}{4}\left\langle 0\right| (\hat{S}^\dagger\hat{a}\hat{S})^2 + 2(\hat{S}^\dagger\hat{a}^\dagger\hat{S})^2 + (\hat{S}^\dagger\hat{a}^\dagger\hat{S}\hat{S}^\dagger\hat{a}\hat{S}) + 1\left|0\right\rangle, \tag{2.152}$$

$$= (\cosh^2 r + \sinh^2 r - 2\cosh r\sinh r\cos\theta) \tag{2.153}$$

$$(\Delta X_2)^2 = \left\langle X_2^2 \right\rangle - \left\langle X_2 \right\rangle^2, \tag{2.154}$$

$$= \langle\zeta| X_2^2 |\zeta\rangle - \langle\zeta| X_2 |\zeta\rangle^2, \tag{2.155}$$

$$= -\frac{1}{4} \langle 0| \hat{S}^\dagger (\hat{a} - \hat{a}^\dagger)^2 \hat{S} |0\rangle + \frac{1}{4} \langle 0| \hat{S}^\dagger (\hat{a} - \hat{a}^\dagger) \hat{S} |0\rangle^2, \tag{2.156}$$

$$= -\frac{1}{4} \langle 0| \hat{S}^\dagger (\hat{a}^2 + \hat{a}^{\dagger 2} - 2\hat{a}^\dagger \hat{a} - 1) \hat{S} |0\rangle + \tag{2.157}$$

$$+ \frac{1}{4} \langle 0| \left(\hat{a}(\cosh r + e^{-i\theta} \sinh r) - \hat{a}^\dagger (\cosh r + e^{i\theta} \sinh r)\right) |0\rangle^2,$$

$$= -\frac{1}{4} \langle 0| (\hat{S}^\dagger \hat{a} \hat{S})^2 + (\hat{S}^\dagger \hat{a}^\dagger \hat{S})^2 - 2(\hat{S}^\dagger \hat{a}^\dagger \hat{S} \hat{S}^\dagger \hat{a} \hat{S}) - 1 |0\rangle, \tag{2.158}$$

$$= (\cosh^2 r + \sinh^2 r + 2 \cosh r \sinh r \cos\theta) \tag{2.159}$$

When we consider the case when $\theta = 0$:

$$(\Delta X_1)^2 = \frac{1}{4} e^{-2r}, \tag{2.160}$$

$$(\Delta X_2)^2 = \frac{1}{4} e^{2r}, \tag{2.161}$$

it's then obvious that as the first quadrature X_1 is compressed(*squeezed*) by a factor of e^{-2r}[13], the second one is stretched by a factor of e^{-2r}, hence the name of the operation.

[13] r is always positive.

3 The Problem and Solution

3.1 The engine

It's possible to create a quantum heat engine with almost any system, we just need to make sure it's gaining energy from the baths and using it to make useful things, to perform work.

The system we chose to study is a harmonic oscillator with constant frequency in which we applied the *Squeezing Operator* and coupled it to two thermal baths at different temperatures.

3.1.1 Squeezed Otto Cycle

First of all, we will define the cycle we are using.

- 1 - *Adiabatic compression:*

We have begun by using the thermal state (Gibbs's state) for the harmonic oscillator (which hamiltonian will be represented as $\hat{H}_{ho}$) with temperature defined by β_h and frequency ω, then applied squeezing on it while not in contact with any reservoir:

$$\begin{aligned} \hat{H}_{ho} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \implies \hat{H}_{sho} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + \chi\left(\hat{a}^{\dagger 2} + \hat{a}^2\right), \\ \hat{\rho}_1 = \frac{e^{-\beta_h\hat{H}_{ho}}}{Z_h} \overset{\hat{U}}{\Longrightarrow} \hat{\rho}_2 = \hat{U}\hat{\rho}_1\hat{U}^\dagger. \end{aligned} \tag{3.1}$$

This step is called compression because the effective frequency of the oscillator is decreased and so are the energy gaps in the hamiltonian. This can be seen by diagonalizing the Hamiltonian of the Squeezed harmonic oscillator(H_{sho}).

- 2 - *Contact with the cold reservoir(β_c):*

Subsequently to the unitary evolution, contact was established between the system and

the cold reservoir and we allowed the system to thermalize again (now with the cold temperature reservoir).

$$\hat{H}_{sho} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + \chi\left(\hat{a}^{\dagger 2} + \hat{a}^2\right) \implies \hat{H}_{sho} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + \chi\left(\hat{a}^{\dagger 2} + \hat{a}^2\right),$$
$$\hat{\rho}_2 = \hat{U}\hat{\rho}_1\hat{U}^\dagger \overset{\hat{U}}{\Longrightarrow} \hat{\rho}_3 = \frac{e^{-\beta_c\hat{H}_{sho}}}{Z_c}. \tag{3.2}$$

• 3 - *Adiabatic expansion:*

The third step is done by turning off the squeezing, and returning to the harmonic oscillator Hamiltonian (H_{ho}) :

$$\hat{H}_{sho} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + \chi\left(\hat{a}^{\dagger 2} + \hat{a}^2\right) \implies \hat{H}_{ho} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right),$$
$$\hat{\rho}_3 = \frac{e^{-\beta_c\hat{H}_{sho}}}{Z_c} \overset{\hat{V}=\hat{U}^\dagger}{\Longrightarrow} \hat{\rho}_4 = \hat{V}\hat{\rho}_3\hat{V}^\dagger. \tag{3.3}$$

• 4 - *Contact with the hot reservoir(β_h):*

The system is finally thermalized with the hot reservoir returning to the initial state:

$$\hat{H}_{ho} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \implies \hat{H}_{ho} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right),$$
$$\hat{\rho}_4 = \hat{V}\hat{\rho}_3\hat{V}^\dagger \overset{\hat{U}}{\Longrightarrow} \hat{\rho}_1 = \frac{e^{-\beta_h\hat{H}_{ho}}}{Z_h}. \tag{3.4}$$

As we were studying only the effects of the pumping in the engine, we do not change the oscillator's frequency ω throughout the calculations.

3.1.2 Diagonalizing of $\hat{H}_{sho}$

To calculate the energy in steps 2 and 3, we diagonalize the Hamiltonian $\hat{H}_{sho}$ applying a Bogoliubov transformation, which consists in defining a new operator $\hat{b}$ as:

$$\hat{b} = \mu\hat{a} + \nu\hat{a}^\dagger, \tag{3.5}$$

here, it can be shown that $\hat{b}$ has the same properties as $\hat{a}$ so it's also a ladder operator in a different Hilbert space. We select the constants μ and ν so the Hamiltonian has no quadratic terms and so we can write:

$$\hat{H}_{sho} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + \chi\left(\hat{a}^{\dagger 2} + \hat{a}^2\right) = \hbar\Omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right), \tag{3.6}$$

where:

$$\Omega = \omega\sqrt{1 - \left(\frac{2\chi}{\omega}\right)^2}, \tag{3.7}$$

which is plotted below:

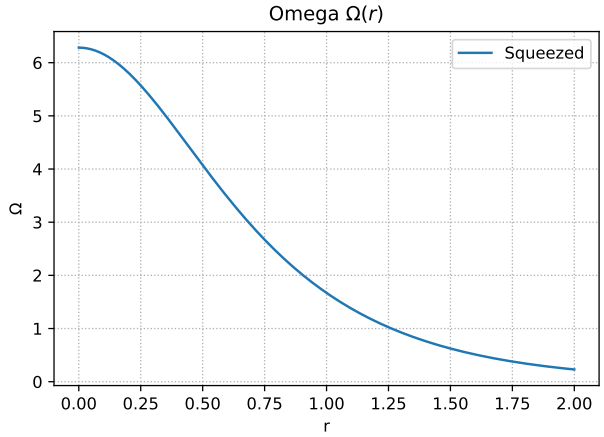


Figure 1: Given some ω(taken here as $\omega = 2\pi$), this plot shows that Ω is always smaller than ω, which is the reason steps 1 and 3 are compression and expansion respectively, also, Ω never actually hits zero.

It's possible to write this in terms of the squeezing by realizing that the hamiltonian can actually by written as:

$$\hat{H}_{sho} = \frac{\Omega}{\omega}\hat{S}^\dagger(r)\hat{H}_{ho}\hat{S}(r). \tag{3.8}$$

Using this, the relation between r and χ, and r and Ω are:

$$\chi = \frac{\omega}{2}\operatorname{sech} 2r, \tag{3.9}$$

$$\Omega = \omega \tanh 2r. \tag{3.10}$$

These relations are used to plot the graphs as function of r instead of χ (see above.).

3.1.3 The energy of each ρ

The energies calculated are:

$$\langle H\rangle_1 = Tr\left\{\rho_1 \hat{H}_{ho}\right\} = \frac{\hbar\omega}{2}\coth\left(\frac{\beta_h\omega}{2}\right), \tag{3.11}$$

$$\langle H\rangle_2 = Tr\left\{\rho_2 \hat{H}_{sho}\right\} = \frac{\hbar Q_1^*\Omega}{2}\coth\left(\frac{\beta_h\omega}{2}\right), \tag{3.12}$$

$$\langle H\rangle_3 = Tr\left\{\rho_3 \hat{H}_{sho}\right\} = \frac{\hbar\Omega}{2}\coth\left(\frac{\beta_c\Omega}{2}\right), \tag{3.13}$$

$$\langle H\rangle_4 = Tr\left\{\rho_4 \hat{H}_{ho}\right\} = \frac{\hbar Q_2^*\omega}{2}\coth\left(\frac{\beta_c\Omega}{2}\right), \tag{3.14}$$

where Q_i^* is the adiabaticity parameter[1] that characterizes the speed of the transformation (or the quantum adiabaticity to it) and Ω is the effective frequency of the squeezed Hamiltonian [42–44].

3.1.4 Thermodynamic quantities

It's easy to perceive that all the energy traded in steps 1 and 3 is work since it's done by unitary transformations as in 2.92.

$$\begin{aligned}\langle W\rangle_{compression} &= \langle H\rangle_2 - \langle H\rangle_1, \\ &= \frac{\hbar}{2}\left(Q_1^*\Omega - \omega\right)\coth\left(\frac{\beta_h\omega}{2}\right),\end{aligned} \tag{3.15}$$

[1] Obtained in B

$$\begin{aligned}\langle W\rangle_{expansion} &= \langle H\rangle_4 - \langle H\rangle_3\,, \\ &= \frac{\hbar}{2}\left(Q_2^*\omega - \Omega\right)\coth\left(\frac{\beta_c\Omega}{2}\right),\end{aligned} \tag{3.16}$$

In the same way, it's natural to identify the energy change in steps 2 and 4 as heat given that they're due to thermal reservoirs and there's not a transformation on the system's Hamiltonian as in 2.94.

$$\begin{aligned}\langle Q\rangle_{cold} &= \langle H\rangle_3 - \langle H\rangle_2\,, \\ &= \frac{\hbar\Omega}{2}\left\{\coth\left(\frac{\beta_c\Omega}{2}\right) - Q_1^*\coth\left(\frac{\beta_h\omega}{2}\right)\right\},\end{aligned} \tag{3.17}$$

$$\begin{aligned}\langle Q\rangle_{hot} &= \langle H\rangle_1 - \langle H\rangle_4\,, \\ &= \frac{\hbar\omega}{2}\left\{\coth\left(\frac{\beta_h\omega}{2}\right) - Q_2^*\coth\left(\frac{\beta_c\Omega}{2}\right)\right\}.\end{aligned} \tag{3.18}$$

The efficiency calculated is :

$$\eta = 1 - \frac{\Omega}{\omega}\mathcal{F}, \tag{3.19}$$

and

$$\mathcal{F} = \left\{\frac{\coth\left(\frac{\beta_c\Omega}{2}\right) - Q_1^*\coth\left(\frac{\beta_h\omega}{2}\right)}{Q_2^*\coth\left(\frac{\beta_c\Omega}{2}\right) - \coth\left(\frac{\beta_h\omega}{2}\right)}\right\}. \tag{3.20}$$

In the slow regime [2] $Q_i^* = 1, i = 1, 2$; and we may write:

$$\eta = 1 - \frac{\Omega}{\omega}, \tag{3.21}$$

or, as a function of the parameter of squeezing r

$$\eta = 1 - \operatorname{sech} 2r. \tag{3.22}$$

One might think that if $r \to \infty$ then $\eta \to 1$, but there is a superior limit to r given by the engine condition, i.e., $W_{total} < 0$ and $Q_h > 0$. The superior limit of r is

$$r_{max} = \frac{1}{2}\cosh^{-1}\frac{T_h}{T_c}, \tag{3.23}$$

[2] Adiabatic change.

if $r > r_{max}$, then $W > 0$ and $Q < 0$, the system would transfer heat to the hot reservoir.

That is to be compared with the traditional Otto engine with a harmonic oscillator (where the frequency is a function of time) [43], even though the efficiency looks the same, the terms mean different things. We achieve this efficiency by altering the effective frequency of the system by applying squeezing while they change the actual frequency. It's important to realize that there is no Otto engine if the frequency doesn't change.

Yet on the quasi-static limit, we may plot 3.22 for further study, figure 2 is a plot of η versus r for $Q_1^* = Q_2^* = 1$, $\omega = 2\pi$, $T_h = 10$ and $T_c = 1$. This result is in agreement with [45, 46] in which anharmonicity can improve the performance of quantum thermal machines.

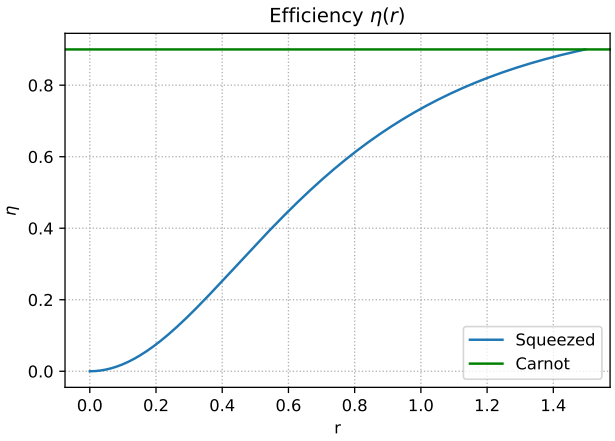


Figure 2: This is the graph of the adiabatic case, where $Q_1^* = Q_2^* = 1$, and the parameters of the system are $\omega = 2\pi$,$T_h = 10$, and $T_c = 1$. We lined the Carnot's engine efficiency for comparison.

3.1.5 High and Low-Temperature Limits

Now, we maximize the power in the adiabatic regime $Q^*_{1,2} = 1$ and make the high-temperature approximation $T_i \to \infty$ or $\beta_i \to 0^+$, for small values, $\coth x \approx \frac{1}{x}$ and we can write:

$$W = \frac{1}{\beta_h}\left\{\frac{\Omega}{\omega} - 1\right\} + \frac{1}{\beta_c}\left\{\frac{\omega}{\Omega} - 1\right\}, \tag{3.24}$$

the condition for maximum power then is $\frac{\omega}{\Omega} = \sqrt{\frac{\beta_h}{\beta_c}}$ and the efficiency is equal to the Curzon-Ahlborn [47]

$$\eta = 1 - \sqrt{\frac{\beta_h}{\beta_c}}. \tag{3.25}$$

For the low temperature limit, $\beta_c \to \infty$ [3]

$$\eta = 1 - \sqrt{\frac{\beta_h \Omega}{2}}, \tag{3.26}$$

this is an interesting result if we compare it with Eq.(12) [43] because it shows that in this limit [4], even after reducing the lowest frequency, is possible to increase the efficiency even without changing the frequency, just by applying a squeezing to it.

On the other hand, if we make a sudden change approach $Q^*_{1,2} = \frac{(\omega^2+\Omega^2)}{2\omega\Omega}$, in the high-temperature limit, we recover the results on [43]

$$\eta = \frac{1 - \sqrt{\frac{T_c}{T_h}}}{2 + \sqrt{\frac{T_c}{T_h}}}, \tag{3.27}$$

and in the low-temperature regime

$$\eta = \frac{1 - \sqrt{\frac{\beta_h \Omega}{2}}}{2 + \sqrt{\frac{\beta_h \Omega}{2}}}. \tag{3.28}$$

For a sudden change, the maximum efficiency possible is $\frac{1}{2}$ in the limit where $\beta_h \to 0^+, T_h \to \infty$.

[3] we also considered $\beta_h \omega >> 1$, i.e., $\beta_h << \beta_c$

[4] $Q^*_1 = Q^*_2 = 1$, $\beta_c \to \infty$ and $\beta_h \to 0^+$.

3.2 Simulations

The graph for a general $Q^*_{1,2}$ is helpful to compare with computational results, so it's plotted below:

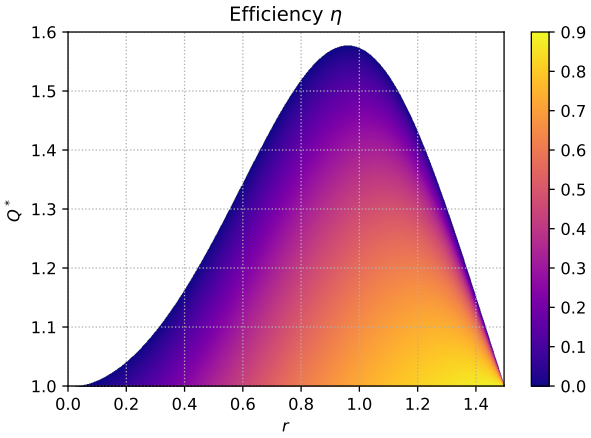


Figure 3: This graph shows the efficiency for $\omega = 2\pi$, $T_h = 10$ and $T_c = 1$.

Next, we study the effect of non-adiabaticity in unitary strokes performed at non-zero power in a general way using numerical methods in Python and the QuTip toolbox [48–50]. We run the unitary strokes with a linear variation in time, i.e., $\chi(t) = \chi_0 \left(\frac{t}{\tau}\right)$ and $\chi(t) = \chi_0 \left(1 - \frac{t}{\tau}\right)$ where τ is a constant that defines how fast this change happens. The program is displayed in appendix C and was run for different r. Time represents the total time taken in both compression and expansion strokes (taken to be the same).

The values were chosen to be $r = 0,4$, $r = 0,8$‘, and $r = 1,2$ and they're plotted below.

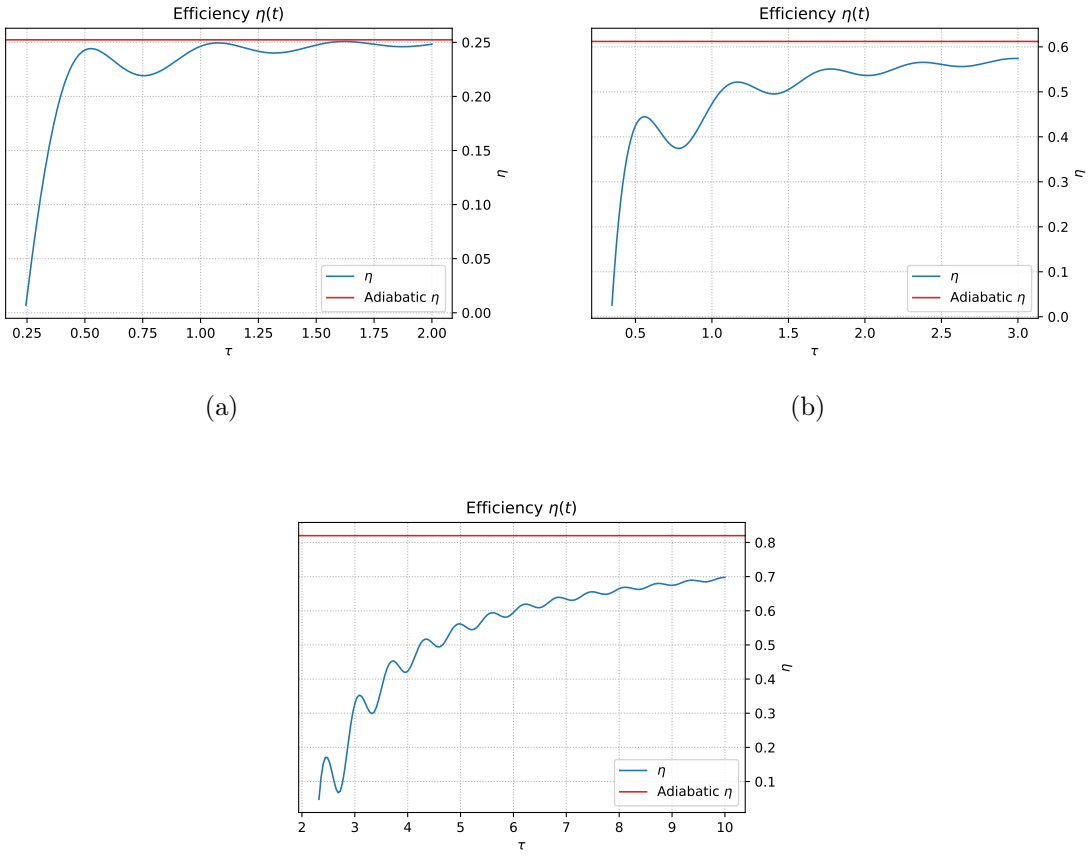
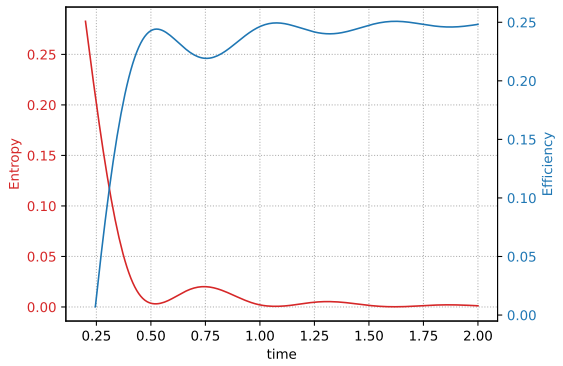


Figure 4: In these plots, the red trace represents the maximum efficiency given a squeezing parameter r (infinitely slow strokes). (a) r=0,4 (b) r=0,8 and (c) r=1,2.

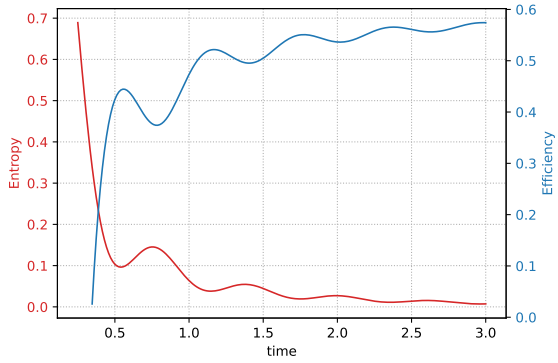
We needed an explanation for the oscillatory comportment of efficiency with the time taken by the unitary evolution strokes. The answer came in the form of entropy production as written in [51]. It's necessary to mention that Von Neumann entropy is invariant over unitary transformations so

This oscillatory comportment can be explained by plotting the entropy changes for different strokes, here, we plotted it for the unitary strokes $S_{expansion} + S_{compression}$ that was calculated as shown in [51] since the Von Neumann entropy is invariant for unitary transformations. The entropy were calculated as a relative entropy between the

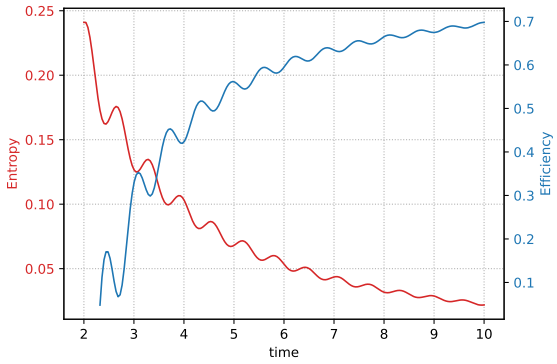
real state (state after the evolution) and a hypothetical equilibrium state that would happen if the evolution took an infinite amount of time to occur.



(a)



(b)



(c)

Figure 5: In these plots, the red trace represents the maximum efficiency given a squeezing parameter r (infinitely slow strokes). (a) r=0,4 (b) r=0,8 and (c) r=1,2.

As one should hope, the entropy increases as the efficiency decrease, which relates the relative entropy with work lost for *inner friction*, as the author [51] calls the irreversible work that should be lost in the engine.

3.3 Theorem

In this section, we will take advantage of this diagonalization method applied to this work to prove that Carnot's efficiency can't be exceeded for thermal reservoir cycles. Note that is already done in [25] making use of fluctuation relations involving the nonequilibrium work and heat exchanged with the reservoir, we are following an alternative path. The theorem will be stated as:

It is not possible to extract an efficiency η greater than Carnot efficiency η_{carnot} from an Otto cycle without resorting to quantum (non-thermal) reservoirs.

To prove this theorem we will make use of a well-known result in which any hermitian operator can be diagonalized, e.g., the Bogoliubov transformation that diagonalizes our Hamiltonian. In other words, is always possible to write:

$$H(a, a^\dagger) = \Omega b^\dagger b, \tag{3.29}$$

Now, if we assume only thermal reservoirs and the Otto cycle, the efficiency η is given by Eq.(3.19) and it is always greater when we keep the QHO frequency fixed. We therefore must show that $\eta \leq \eta_{carnot}$. Taking into account the engine condition $\langle Q \rangle_{hot} > 0$, we can write

$$\frac{\hbar\omega}{2}\left\{\coth\left(\frac{\beta_h\omega}{2}\right) - Q_2^* \coth\left(\frac{\beta_c\Omega}{2}\right)\right\} > 0, \tag{3.30}$$

from which we obtain

$$\frac{\coth\left(\frac{\beta_h\omega}{2}\right)}{\coth\left(\frac{\beta_c\Omega}{2}\right)} > Q_2^* \geq 1, \tag{3.31}$$

and therefore $\coth\left(\frac{\beta_h\omega}{2}\right) \geq \coth\left(\frac{\beta_c\Omega}{2}\right)$, or, equivalently:

$$\frac{\beta_h}{\beta_c} \leq \frac{\Omega}{\omega}. \tag{3.32}$$

Now, multiply both sides by the term in parentheses on the right-hand side by $\mathcal{F}$ of

Eq.(3.20)

$$\frac{\beta_h}{\beta_c}\mathcal{F} \leq \frac{\Omega}{\omega}\mathcal{F} \tag{3.33}$$

and rearranging to

$$1 - \frac{\beta_h}{\beta_c}\mathcal{F} \geq 1 - \frac{\Omega}{\omega}\mathcal{F}, \tag{3.34}$$

we can see that the right-hand side in the above inequality is just η, as given by Eq.(3.19):

$$1 - \frac{\beta_h}{\beta_c}\left\{\frac{\coth\left(\frac{\beta_c\Omega}{2}\right) - Q_1^*\coth\left(\frac{\beta_h\omega}{2}\right)}{Q_2^*\coth\left(\frac{\beta_c\Omega}{2}\right) - \coth\left(\frac{\beta_h\omega}{2}\right)}\right\} \geq \eta. \tag{3.35}$$

Consider now the following inequality:

$$(Q_1^* - 1)\coth\left(\frac{\beta_h\omega}{2}\right) + (Q_2^* - 1)\coth\left(\frac{\beta_c\Omega}{2}\right) \geq 0, \tag{3.36}$$

which is obvious since $Q_i^* \geq 1$, $i = 1, 2$, and the coth function is always positive for positive inputs. Then, from the above equation, we obtain

$$\frac{Q_1^*\coth\left(\frac{\beta_h\omega}{2}\right) - \coth\left(\frac{\beta_c\Omega}{2}\right)}{\coth\left(\frac{\beta_h\omega}{2}\right) - Q_2^*\coth\left(\frac{\beta_c\Omega}{2}\right)} \geq 1. \tag{3.37}$$

Multiplying both sides by β_h/β_c and rearranging:

$$1 - \frac{\beta_h}{\beta_c}\left\{\frac{Q_1^*\coth\left(\frac{\beta_h\omega}{2}\right) - \coth\left(\frac{\beta_c\Omega}{2}\right)}{\coth\left(\frac{\beta_h\omega}{2}\right) - Q_2^*\coth\left(\frac{\beta_c\Omega}{2}\right)}\right\} \leq 1 - \frac{\beta_h}{\beta_c}. \tag{3.38}$$

Note that the right-hand side in the above equation is just η_{carnot}. Finally, we use Eq.(3.35) to complete the prove:

$$\eta \leq 1 - \frac{\beta_h}{\beta_c}\left\{\frac{Q_1^*\coth\left(\frac{\beta_h\omega}{2}\right) - \coth\left(\frac{\beta_c\Omega}{2}\right)}{\coth\left(\frac{\beta_h\omega}{2}\right) - Q_2^*\coth\left(\frac{\beta_c\Omega}{2}\right)}\right\} \leq \eta_{carnot}. \tag{3.39}$$

or

$$\eta \leq \eta_{Carnot} \tag{3.40}$$

3.4 STA Hamiltonian

There is a way to increase the power of the engine without losing efficiency, it's called a shortcut to adiabaticity. The method revolves around adding a hamiltonian to the model so it evolves in a fast way but following the quantum adiabatic evolution of the original system. [52]

3.4.1 Counterdiabatic Driving

The *STA* method seeks to alter the original problem in a way to make the system evolve to be always an eigenstate of the instantaneous Hamiltonian. In the diagonal base, the Hamiltonian can be written as:

$$\hat{\mathcal{H}}_0 = \sum_n E_n(t) \left|n(t)\right\rangle\!\left\langle n(t)\right| . \tag{3.41}$$

We are searching for the Hamiltonian that makes our system be described by the ket:

$$\left|\psi_n(t)\right\rangle = e^{i\xi_n(t)} \left|n(t)\right\rangle . \tag{3.42}$$

The Hamiltonian to be summed in the original to achieve this is:

$$\hat{\mathcal{H}}_{CD} = i \sum_n \left\{ \left|\partial_t n(t)\right\rangle\!\left\langle n(t)\right| - \left\langle n(t)|\partial_t n(t)\right\rangle \left|n(t)\right\rangle\!\left\langle n(t)\right| \right\} . \tag{3.43}$$

3.4.2 $|\partial_t n(t)\rangle$

The problem here is to apply the STA method to the squeezed harmonic oscillator which is given by the following Hamiltonian:

$$\hat{\mathcal{H}} = \Omega(t) \left(\hat{b}_t^\dagger \hat{b}_t + \frac{1}{2} \right) , \tag{3.44}$$

where:

$$\Omega(t) = \Omega_t = \sqrt{\Omega^2 - 4\chi(t)^2}. \tag{3.45}$$

The operators $\hat{b}^\dagger$ and $\hat{b}$ are called instantaneous operators because they change with time but are written in the base that diagonalizes the time-dependent Hamiltonian.

The instantaneous eigenstates of it are given by:

$$\langle x|n\rangle_t = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\Omega_t}{\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{m\Omega_t x^2}{2}\right) H_n\left(\sqrt{m\Omega_t}x\right). \tag{3.46}$$

here, x is not the physical position but has the same properties in the same way that $\hat{b}$ isn't the destruction operator but has the same properties of it.

The time derivative of it is:

$$\begin{aligned}\langle x|\partial_t n\rangle_t = &\frac{1}{\sqrt{2^n n!}}\frac{1}{4}\frac{m\dot{\Omega}_t}{\pi}\left(\frac{m\Omega_t}{\pi}\right)^{-\frac{3}{4}} \exp\left(-\frac{m\Omega_t x^2}{2}\right) H_n\left(\sqrt{m\Omega_t}x\right) + \\ &+ \frac{1}{\sqrt{2^n n!}}\left(\frac{m\Omega_t}{\pi}\right)^{\frac{1}{4}}\left(-\frac{m\dot{\Omega}_t x^2}{2}\right)\exp\left(-\frac{m\Omega_t x^2}{2}\right) H_n\left(\sqrt{m\Omega_t}x\right) + \\ &+ \frac{1}{\sqrt{2^n n!}}\left(\frac{m\Omega_t}{\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{m\Omega_t x^2}{2}\right)\partial_t H_n\left(\sqrt{m\Omega_t}x\right).\end{aligned} \tag{3.47}$$

Using the following property of Hermite polynomial:

$$\partial_x H_n(x) = 2nH_{n-1}(x), \tag{3.48}$$

and rearranging some terms:

$$\begin{aligned}\langle x|\partial_t n\rangle_t = &\frac{\dot{\Omega}_t}{4\Omega_t}\left\{\frac{1}{\sqrt{2^n n!}}\left(\frac{m\Omega_t}{\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{m\Omega_t x^2}{2}\right) H_n\left(\sqrt{m\Omega_t}x\right)\right\} - \\ &- \frac{\dot{\Omega}_t}{\Omega_t}\frac{m\Omega_t x^2}{2}\left\{\frac{1}{\sqrt{2^n n!}}\left(\frac{m\Omega_t}{\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{m\Omega_t x^2}{2}\right) H_n\left(\sqrt{m\Omega_t}x\right)\right\} + \\ &+ \frac{1}{\sqrt{2^n n!}}\left(\frac{m\Omega_t}{\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{m\Omega_t x^2}{2}\right)\left\{2nH_{n-1}\left(\sqrt{m\Omega_t}x\right)\sqrt{\frac{m}{\Omega_t}}\frac{x\dot{\Omega}_t}{2}\right\}.\end{aligned} \tag{3.49}$$

The terms in braces are equal to $\langle x|n(t)\rangle$:

$$\begin{aligned}\langle x|\partial_t n(t)\rangle = &\frac{\dot{\Omega}_t}{\Omega_t}\left(\frac{1}{4} - \frac{m\Omega_t x^2}{2}\right)\langle x|n\rangle_t + \\ &+ \frac{\dot{\Omega}_t}{\Omega_t}\sqrt{\frac{m\Omega_t}{2}}x\sqrt{n}\left\{\frac{1}{\sqrt{2^{n-1}(n-1)!}}\left(\frac{m\Omega_t}{\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{m\Omega_t x^2}{2}\right) H_{n-1}\left(\sqrt{m\Omega_t}x\right)\right\}.\end{aligned} \tag{3.50}$$

Again, the term in braces is just $\langle x|n-1\rangle_t$:

$$\langle x|\partial_t n\rangle_t = \frac{\dot{\omega}_t}{\omega_t}\left(\frac{1}{4} - \frac{m\omega_t x^2}{2}\right)\langle x|n\rangle_t + \frac{\dot{\omega}_t}{\omega_t}\sqrt{\frac{m\omega_t}{2}}x\sqrt{n}\,\langle x|n-1\rangle_t\,. \tag{3.51}$$

Removing the x bra:

$$|\partial_t n\rangle_t = \frac{\dot{\Omega}_t}{\Omega_t}\left(\frac{1}{4} - \frac{m\Omega_t\hat{x}^2}{2}\right)|n\rangle_t + \frac{\dot{\Omega}_t}{\Omega_t}\sqrt{\frac{m\Omega_t}{2}}\hat{x}\sqrt{n}\,|n-1\rangle_t\,. \tag{3.52}$$

Using that $\sqrt{n}\,|n-1\rangle_t = \hat{b}\,|n\rangle_t$:

$$|\partial_t n\rangle_t = \frac{\dot{\Omega}_t}{\Omega_t}\left(\frac{1}{4} - \frac{m\Omega_t\hat{x}^2}{2}\right)|n\rangle_t + \frac{\dot{\Omega}_t}{\Omega_t}\sqrt{\frac{m\Omega_t}{2}}\hat{x}\hat{b}\,|n\rangle_t\,, \tag{3.53}$$

$$= \frac{\dot{\Omega}_t}{\Omega_t}\left\{\frac{1}{4} - \frac{m\Omega_t\hat{x}^2}{2} + \sqrt{\frac{m\Omega_t}{2}}\hat{x}\hat{b}\right\}|n\rangle_t\,. \tag{3.54}$$

It's possible to write $\hat{x}$ e $\hat{x}^2$ as functions of $\hat{b}$ and $\hat{b}^\dagger$:

$$\hat{x} = \sqrt{\frac{1}{2m\Omega_t}}\left(\hat{b} + \hat{b}^\dagger\right), \tag{3.55}$$

$$\hat{x}^2 = \frac{1}{2m\Omega_t}\left(\hat{b} + \hat{b}^\dagger\right)\left(\hat{b} + \hat{b}^\dagger\right), \tag{3.56}$$

$$= \frac{1}{2m\Omega_t}\left(\hat{b}^2 + \hat{b}^{\dagger 2} + \hat{b}^\dagger\hat{b} + \hat{b}\hat{b}^\dagger\right), \tag{3.57}$$

and, as $\hat{b}\hat{b}^\dagger = \hat{b}^\dagger\hat{b} + 1$:

$$\hat{x}^2 = \frac{1}{2m\Omega_t}\left(\hat{b}^2 + \hat{b}^{\dagger 2} + 2\hat{b}^\dagger\hat{b} + 1\right). \tag{3.58}$$

So :

$$|\partial_t n\rangle_t = \frac{\dot{\Omega}_t}{\Omega_t}\left\{\cancel{\frac{1}{4}} - \frac{1}{4}\left(\hat{b}^2 + \hat{b}^{\dagger 2} + 2\hat{b}^\dagger\hat{b} + \cancel{1}\right) + \frac{1}{2}\left(\hat{b} + \hat{b}^\dagger\right)\hat{b}\right\}|n\rangle_t\,, \tag{3.59}$$

$$= \frac{\dot{\Omega}_t}{4\omega_t}\left\{-\hat{b}^2 - \hat{b}^{\dagger 2} \cancel{- 2\hat{b}^\dagger\hat{b}} + 2\hat{b}^2 + \cancel{2\hat{b}^\dagger\hat{b}}\right\}|n\rangle_t\,, \tag{3.60}$$

$$= \frac{\dot{\Omega}_t}{4\Omega_t}\left\{\cancel{2\hat{b}^2} \overset{\hat{b}^2}{\nearrow} \cancel{- \hat{b}^2} - \hat{b}^{\dagger 2}\right\}|n\rangle_t\,, \tag{3.61}$$

$$= \frac{\dot{\Omega}_t}{4\Omega_t}\left\{\hat{b}^2 - \hat{b}^{\dagger 2}\right\}|n\rangle_t\,. \tag{3.62}$$

3.4.3 $\langle n|\partial_t n\rangle_t$

The operators in $|\partial_t n\rangle_t$ are quadratic, so this calculation is trivial :

$$\langle n|\partial_t n\rangle_t = \langle n|_t \left\{ \frac{\dot{\Omega}_t}{4\Omega_t} \left(\hat{b}^2 - \hat{b}^{\dagger 2}\right) |n\rangle_t \right\}, \tag{3.63}$$

$$= \frac{\dot{\Omega}_t}{4\Omega_t} \left\{ \cancelto{0}{\langle n|\hat{b}^2|n\rangle_t} - \cancelto{0}{\langle n|\hat{b}^{\dagger 2}|n\rangle_t} \right\}, \tag{3.64}$$

$$= 0. \tag{3.65}$$

3.4.4 $\mathcal{H}_{CD}$

Applying what e found to $\mathcal{H}_{CD}$:

$$\mathcal{H}_{CD} = i \sum_n \left\{ |\partial_t n\rangle\langle n|_t - \cancelto{0}{\langle n|\partial_t n\rangle_t} |n\rangle\langle n|_t \right\}, \tag{3.66}$$

$$= i \sum_n \frac{\dot{\Omega}_t}{4\Omega_t} \left\{ \hat{b}^2 - \hat{b}^{\dagger 2} \right\} |n\rangle\langle n|_t \,, \tag{3.67}$$

$$= i \frac{\dot{\Omega}_t}{4\Omega_t} \left\{ \hat{b}^2 - \hat{b}^{\dagger 2} \right\} \cancelto{\mathbb{I}}{\sum_n |n\rangle\langle n|_t}. \tag{3.68}$$

So :

$$\mathcal{H}_{CD} = i \frac{\dot{\Omega}_t}{4\Omega_t} \left\{ \hat{b}^2 - \hat{b}^{\dagger 2} \right\}, \tag{3.69}$$

or, back in the original base:

$$\mathcal{H}_{CD} = i \frac{\dot{\Omega}_t}{4\Omega_t} (\mu^2 - \nu^2)(a^2 - a^{\dagger 2}), \tag{3.70}$$

$$\mathcal{H}_{CD} = i \frac{\dot{\Omega}_t}{4\Omega_t} (a^2 - a^{\dagger 2}). \tag{3.71}$$

By using this Hamiltonian, it's possible to have an adiabatic engine even if we make the evolution fast. So, it increases the power of the engine.

4 Conclusion

In this work, we presented the formulation of open quantum systems usually used in quantum thermodynamics [28–35]. A little introduction to quantum thermodynamics [3, 36–41] and how to improve its power by applying shortcut to adiabaticity [16–19, 21, 43].

We then proceeded to study a modified quantum harmonic oscillator by making it a working fluid on an engine operating between two thermal reservoirs. We achieved an analytical result on efficiency that shows that the squeezed engine can achieve Carnot's efficiency for some squeezing parameter r if the engine runs on a quasi-static cycle.

Also, we provide a form of calculation for the STA for the squeezing harmonic oscillator that surprisingly is just to apply another second-order hamiltonian that will force the system to evolve in an "adiabatically" way, adiabatically here means in a quantum way.

Last but not least, we ran the cycle through simulations on QuTip and showed the results. Our results showed an interesting oscillatory pattern that is unexpected, since the longer it takes, closer to adiabaticity we should be. The oscillatory pattern implies that the efficiency may drop even if we make the operation a little longer. The explanation for this is given by the authors in [51] which shows that inner friction can waste some energy and this is proven by the entropy production plot, when the efficiency decreases the entropy increases. This is yet another point that shows that Von Neumann's entropy is not always the thermodynamics entropy.

Appendix A Separation of the terms in section 2.1.3

The sum made here is:

$$\sum_{i}^{d^2}\sum_{j}^{d^2} c_{i,j}(\varepsilon)F_i\rho F_j^\dagger \tag{A.1}$$

To facilitate the understanding in the way we wrote the terms of the sum in 2.20 one may imagine the sum over i and j are actually over all the elements of a square matrix of dimensions d^2 x d^2 :

$$\begin{pmatrix} c_{1,1}F_1\rho F_1^\dagger & c_{1,2}F_1\rho F_2^\dagger & ... & c_{1,d^2}F_1\rho F_{d^2}^\dagger \\ c_{2,1}F_2\rho F_1^\dagger & c_{2,2}F_2\rho F_2^\dagger & ... & c_{2,d^2}F_2\rho F_{d^2}^\dagger \\ ... & ... & ... & ... \\ c_{d^2,1}F_{d^2}\rho F_1^\dagger & c_{d^2,2}F_{d^2}\rho F_2^\dagger & ... & c_{d^2,d^2}F_{d^2}\rho F_{d^2}^\dagger \end{pmatrix} \tag{A.2}$$

Remembering $F_{d^2} = \frac{\mathcal{I}}{\sqrt{d}}$, so:

$$\begin{pmatrix} c_{1,1}F_1\rho F_1^\dagger & c_{1,2}F_1\rho F_2^\dagger & ... & \frac{1}{\sqrt{d}}c_{1,d^2}F_1\rho \\ c_{2,1}F_2\rho F_1^\dagger & c_{2,2}F_2\rho F_2^\dagger & ... & \frac{1}{\sqrt{d}}c_{2,d^2}F_2\rho \\ ... & ... & ... & ... \\ \frac{1}{\sqrt{d}}c_{d^2,1}\rho F_1^\dagger & \frac{1}{\sqrt{d}}c_{d^2,2}\rho F_2^\dagger & ... & \frac{1}{d}c_{d^2,d^2}\rho \end{pmatrix} \tag{A.3}$$

From where the terms are separated by "order "[1] of F in the problem, in zero order we have the last term:

$$\frac{1}{d}c_{d^2,d^2}\rho \tag{A.4}$$

In the first order, we have all the terms of the last row and column (except for the term d^2 x d^2 which was already counted in zero order):

$$\sum_{i=1}^{d^2-1}\frac{1}{\sqrt{d}}\left\{c_{i,d^2}F_i\rho + c_{d^2,i}\rho F_i^\dagger\right\} \tag{A.5}$$

[1] Order here refers to which power of F appears in the term in question.

Here, a sum in j should have appeared, but as the terms do not intersect (and they are *dummy indices*), $j = i$ is made in the second summation.

In second order we have all the other terms (the sums now go up to $d^2 - 1$ to disregard the last row and column):

$$\sum_{i=1}^{d^2-1} \sum_{j=1}^{d^2-1} c_{i,j} F_i \rho F_j^\dagger$$

Finally, one has:

$$\sum_{i}^{d^2} \sum_{j}^{d^2} c_{i,j}(\varepsilon) F_i \rho F_j^\dagger = \frac{1}{d} c_{d^2,d^2} \rho + \sum_{i=1}^{d^2-1} \frac{1}{\sqrt{d}} \left\{ c_{i,d^2} F_i \rho + c_{d^2,i} \rho F_i^\dagger \right\} + \sum_{i=1}^{d^2-1} \sum_{j=1}^{d^2-1} c_{i,j} F_i \rho F_j^\dagger \tag{A.6}$$

Appendix B Husimi Parameter (nonadibatic factor)

Husimi [42] proposed a way to calculate the energy of the time dependent harmonic oscillator that is described by the following Schrodinger equation:

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\partial_{x'}^2\psi + \frac{m}{2}\omega^2(t)x'^2\psi. \tag{B.1}$$

Furthermore, it's well known that the propagator must obey this same equation:

$$i\hbar\partial_t K = -\frac{\hbar^2}{2m}\partial_{x'}^2 K + \frac{m}{2}\omega^2(t)x'^2 K. \tag{B.2}$$

It was solved by proposing a Gaussian solution with time dependent terms that could be adjusted to the specific solution:

$$K = \exp\left\{\frac{i}{2\hbar}\left(a(t)x'^2 + 2b(t)x' + c(t)\right)\right\}. \tag{B.3}$$

Applying B.3 to B.1 and separating the polynomial terms:

$$\left\{\frac{\dot{a}}{2} + \frac{a^2}{2m} + \frac{m\omega^2}{2}\right\}x'^2 + \left\{\dot{b} + \frac{ab}{m}\right\}x' + \left\{\dot{c} + \frac{b^2}{2m} - \frac{i\hbar a}{2m}\right\} = 0. \tag{B.4}$$

As this polynomial is zero for whatever x', then its coefficients have to cancel independently and generate three differential equations:

$$\frac{\dot{a}}{m} = -\frac{a}{m^2} - \omega^2, \tag{B.5}$$

$$\dot{b} = -\frac{ab}{m}, \tag{B.6}$$

$$\dot{c} = \frac{i\hbar a}{m} - \frac{b^2}{m}. \tag{B.7}$$

The first equation is a Riccati equation that can be transformed into something more familiar with the transformation $a = m\frac{\dot{X}}{X}$:

$$\left\{\frac{\ddot{X}X - \dot{X}^2}{X^2}\right\} = -\frac{\dot{X}^2}{X^2} - \omega^2, \tag{B.8}$$

$$\ddot{X} = -\omega^2 X. \tag{B.9}$$

The equation in b can be solved by direct integration:

$$\dot{b} = -\frac{\dot{X}b}{X}, \tag{B.10}$$

$$\frac{\dot{b}}{b} = -\frac{\dot{X}}{X}, \tag{B.11}$$

$$\int \frac{\dot{b}}{b}dt = -\int \frac{\dot{X}}{X}dt, \tag{B.12}$$

$$\int \frac{1}{b}db = -\int \frac{1}{X}dX, \tag{B.13}$$

$$\ln(b) = -\ln(X) + \ln(\kappa), \tag{B.14}$$

$$b = \frac{\kappa}{X}. \tag{B.15}$$

where κ represents the degree of freedom given by the constant of integration.

Same can be done in c:

$$\dot{c} = i\hbar\frac{\dot{X}}{X} - \frac{1}{m}\frac{\kappa^2}{X^2}, \tag{B.16}$$

$$c = i\hbar\ln(X) - \frac{1}{m}\int \frac{\kappa^2}{X^2}dt. \tag{B.17}$$

It's also well known that the Wronskian of the two solutions of a second order ODE (here X and Y) is constant (Abel's Theorem). Without loss of generality, we can say that this constant is -1 (redefining the functions X and Y, if necessary, since, if X is a solution, aX is also a solution)

$$W(X,Y) = X\dot{Y} - \dot{X}Y = \theta = -1. \tag{B.18}$$

An interesting fact that will come in handy later is:

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{Y}{X} = \frac{\dot{Y}X - Y\dot{X}}{X^2} = -\frac{1}{X^2}, \tag{B.19}$$

Substituting in B.17:

$$c = i\hbar \ln(X) + \frac{\kappa}{m}\frac{Y}{X} + C. \tag{B.20}$$

Putting $a(t)$, $b(t)$ and $c(t)$ back in B.3 :

$$K = \exp\left(\frac{i}{2\hbar}\left\{\frac{m\dot{X}x'^2}{X} + \frac{2\kappa x'}{X} + i\hbar\ln(X) + \frac{\kappa^2}{m}\frac{Y}{X} + C\right\}\right), \tag{B.21}$$

$$= e^{\frac{-\ln(X)}{2}} e^{\frac{iC}{2\hbar}} \exp\left(\frac{im}{2\hbar X}\left\{\dot{X}x'^2 + 2x'\frac{\kappa}{m} + \frac{\kappa^2}{m^2}Y\right\}\right). \tag{B.22}$$

In the limit $t \to t_0$ we must obtain:

$$K(x', t; x, t_0) = \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}} \exp\left(\frac{im(x'-x)^2}{2\hbar(t-t_0)}\right). \tag{B.23}$$

that is the propagator to a free particle. From here we discover the values of the constants κ and C.

$$K = \sqrt{\frac{m}{2i\pi\hbar X}} \exp\left(\frac{im}{2\hbar X}\left\{\dot{X}x'^2 - 2x'x + x^2Y\right\}\right), \tag{B.24}$$

and, in this limit $X(t \approx t_0) \approx t - t_0$, $X(t_0) = 0$, $\dot{X}(t_0) = 1$ and $Y(t_0) = 1$, that are the boundary condition.

With this, we wish to calculate the probability of starting with a state $|n\rangle$ and end up with $|m\rangle$ after evolving the state with this propagator, i.e. :

$$P_{n\to m} = |\langle m|\,\mathcal{U}(t, t_0)\,|n\rangle\,|^2, \tag{B.25}$$

which can be written as follows by inserting completeness relations for x and x_0:

$$P_{n\to m} = \left|\iint \langle m|x\rangle\,\langle x|\,\mathcal{U}(t, t_0)\,|x_0\rangle\,\langle x_0|n\rangle\,dxdx_0\right|^2. \tag{B.26}$$

Identifying the terms, we get:

$$P_{n\to m} = \left|\iint \psi_m^*(x)K(x, t; x_0, t_0)\psi_n(x_0)dxdx_0\right|^2 \tag{B.27}$$

Or, using that the squared modulus of a complex number is just that number multiplied by its conjugate:

$$P_{n\to m} = \iiiint \psi_m^*(x)K(x,t;x_0,t_0)\psi_n(x_0)\psi_m(x')K^*(x',t;x_0',t_0)\psi_n^*(x_0')dxdx_0dx'dx_0' \tag{B.28}$$

To simplify the problem, we use the method of generating functions[1] and we write the generator as follows form:

$$P(u,v) = \sum_{n,m} u^n v^m P_{n\to m}. \tag{B.29}$$

From B.28 we can write:

$$\begin{aligned} P(u,v) = \iiiint dxdx'dx_0dx_0'K(x,t;x_0,t_0)K^*(x',t;x_0',t_0). \\ \cdot\left\{\sum_n u^n\psi_n(x_0)\psi_n^*(x_0')\right\}\left\{\sum_m u^m\psi_m^*(x)\psi_m(x')\right\}. \end{aligned} \tag{B.30}$$

To move forward, one employs the well-known identity of Hermite polynomials [54]:

$$\frac{1}{\sqrt{\pi(1-z^2)}}\exp\left(-\frac{(1-z^2)(\bar{x}^2+\bar{x_0}^2)-4zxx_0}{2(1-z^2)}\right) = \sum_{n=0}^{\infty} z^n\psi_n(x)\psi_n^*(x_0), \tag{B.31}$$

where $\bar{x} = x/\sqrt{\hbar/m\omega_0}$.

For simplicity, the adopted units will be the natural units of the system where $\hbar = m = \omega_0 = 1$. Replacing B.31 in B.30:

$$\begin{aligned} P(u,v) = \frac{1}{\pi\sqrt{(1-u^2)(1-v^2)}}\iiiint K(x,t;x_0,t_0)K^*(x',t;x_0',t_0) \\ \exp\left(-\frac{(1+u^2)(x_0^2+x_0'^2)-4ux_0x_0'}{2(1-u^2)} - \frac{(1+v^2)(x^2+x'^2)-4vxx'}{2(1-v^2)}\right)dxdx_0dx'dx_0'. \end{aligned} \tag{B.32}$$

[1] Link in Wikipedia on the topic [53]

Finally, this integral is a multidimensional Gaussian (4-D) that has a tabulated solution:

$$\int ... \int \exp\left(-\frac{1}{2}\sum_{rs} A_{rs}x_r x_s\right) dx_1 ... dx_n = \sqrt{\frac{(2\pi)^n}{\det(A)}}. \tag{B.33}$$

With that in hand, we identify the terms of the matrix A and calculate its determinant:

$$P(u,v) = \sqrt{\frac{2}{Q(1-u^2)(1-v^2) + (1+u^2)(1+v^2) - 4uv}}. \tag{B.34}$$

where :

$$Q = \frac{1}{2}\left\{X^2 + \dot{X}^2 + Y^2 + \dot{Y}^2\right\}. \tag{B.35}$$

This Q is already the nonadiabaticity parameter.

B.1 case 1 : $v = 1$

If $v = 1$:

$$P(u,1) = \sqrt{\frac{2}{Q(1-u^2)(1-1) + (1+u^2)(1+1) - 4u}}, \tag{B.36}$$

$$= \sqrt{\frac{2}{2 - 4u + u^2}}, \tag{B.37}$$

$$= \sqrt{\frac{2}{2(1-u)^2}}, \tag{B.38}$$

$$= \frac{1}{1-u}. \tag{B.39}$$

The equation B.39 is equivalent to:

$$\sum_m P_{n\to m} = 1. \tag{B.40}$$

Comparing with the definition of $P(u,v)$:

$$P(u,1) = \sum_n u^n \sum_m P_{n\to m}, \tag{B.41}$$

$$= \sum_n u^n, \tag{B.42}$$

$$= \frac{1}{1-u}. \tag{B.43}$$

B.2 Case 2 : Time independent ω

For the unperturbed case, the solutions for X and Y are known:

$$X = -\dot{Y} = \sin t \quad , \quad \dot{X} = Y = \cos(t). \tag{B.44}$$

It's easy to see that:

$$Q = \frac{1}{2}\left\{\sin^2 t + \cos^2(t) + \sin^2 t + \cos^2(t)\right\}, \tag{B.45}$$

$$= 1. \tag{B.46}$$

Substituting in B.29:

$$P(u,v)_{Q=1} = \sqrt{\frac{2}{(1-u^2)(1-v^2)+(1+u^2)(1+v^2)-4uv}}, \tag{B.47}$$

$$= \sqrt{\frac{2}{1+u^2v^2-v^2-u^2+1+u^2v^2+u^2+v^2-4uv}}, \tag{B.48}$$

$$= \sqrt{\frac{2}{2+2u^2v^2-4uv}}, \tag{B.49}$$

$$= \sqrt{\frac{1}{(1-uv)^2}}, \tag{B.50}$$

$$= \frac{1}{1-uv}. \tag{B.51}$$

This case is equivalent to the transitionless case, i.e. $P_{n\to m} = \delta_{nm}$:

$$P(u,1) = \sum_{n,m} u^n v^m P_{n\to m}, \tag{B.52}$$

$$= \sum_{n,m} u^n v^m \delta_{nm}, \tag{B.53}$$

$$= \sum_{n} \{uv\}^n, \tag{B.54}$$

$$= \frac{1}{1-uv}. \tag{B.55}$$

B.3 Case 3 : $P(-u,-v)$

Substituting $u \to -u$ and $v \to -v$ in B.34, one realises that:

$$P(-u,-v) = \sqrt{\frac{2}{Q(1-(-u)^2)(1-(-v)^2)+(1+(-u)^2)(1+(-v)^2)-4(-u)(-v)}}, \tag{B.56}$$

$$= \sqrt{\frac{2}{Q(1-u^2)(1-v^2)+(1+u^2)(1+v^2)-4uv}}, \tag{B.57}$$

$$= P(u,v). \tag{B.58}$$

Doing the same in B.29 :

$$P(-u,-v) = \sum_{n,m} \{-u\}^n \{-v\}^m P_{n\to m}, \tag{B.59}$$

$$= \sum_{n,m} \{-1\}^{n+m} u^n v^m P_{n\to m}. \tag{B.60}$$

As $P(-u,-v) = P(u,n)$, so:

$$\sum_{n,m} (-1)^{n+m} u^n v^m P_{n\to m} = \sum_{n,m} u^n v^m P_{n\to m}, \tag{B.61}$$

$$\sum_{n,m} \left\{(-1)^{n+m} - 1\right\} u^n v^m P_{n\to m} = 0. \tag{B.62}$$

As u and v can be any, for the equality to be satisfied, all terms of the sum must be zero. This implies that the transition probability to states of different parities must be zero.:

$$P_{n\to m} = 0 \qquad \text{, if m and n have different parities.} \tag{B.63}$$

B.4 Consequences

We calculate the derivative of $P(u,v)$ with respect to v and then set $v = 1$ in the equation B.34:

$$\frac{\partial P(u,v)}{\partial v}|_{v=1} = -\frac{2^{-1/2}\left\{-2vQ(1-u^2)+2v(1+u^2)-4u\right\}}{(Q(1-u^2)(1-v^2)+(1+u^2)(1+v^2)-4uv)^{3/2}}|_{v=1}, \tag{B.64}$$

$$= -\frac{2^{-1/2\left\{-2Q(1-u^2)+2(1+u^2)-4u\right\}}}{(2(1+u^2)-4u)^{3/2}}, \tag{B.65}$$

$$= -\frac{-Q(1-u)(1+u)+(1-u)^2}{2(1-u)^3}, \tag{B.66}$$

$$= \frac{1}{2(1-u)^2}\left\{Q(1+u)-(1-u)\right\}. \tag{B.67}$$

in the other relation:

$$\frac{\partial P(u,v)}{\partial v}|_{v=1} = \sum_{n,m} u^n m v^{m-1} P_{n\to m}|_{v=1}, \tag{B.68}$$

$$= \sum_n u^n \sum_m m P_{n\to m}, \tag{B.69}$$

$$= \sum_n u^n \langle m \rangle_n . \tag{B.70}$$

where $\langle m \rangle_n$ is the average quantum number for a state m given that the system started at n.

On the other hand, we have that :

$$\frac{\mathrm{d}}{\mathrm{d}u}\sum_{n=0}^{\infty} u^n = \frac{\mathrm{d}}{\mathrm{d}u}\frac{1}{1-u}, \tag{B.71}$$

$$\sum_{n=1}^{\infty} n u^{n-1} = \frac{1}{(1-u)^2}. \tag{B.72}$$

Substituting B.72 in B.67 and usingB.70:

$$\frac{1}{2}\sum_{n=1}^{\infty} nu^{n-1}\left\{Q(1+u)-(1-u)\right\} = \sum_{n=0}^{\infty} u^n \left\langle m\right\rangle_n , \tag{B.73}$$

$$\frac{1}{2}\left\{\sum_{n=1}^{\infty} nu^{n-1}Q + \sum_{n=1}^{\infty} nu^{n}Q + \sum_{n=1}^{\infty} nu^{n} - \sum_{n=1}^{\infty} nu^{n-1}\right\} = \sum_{n=0}^{\infty} u^n \left\langle m\right\rangle_n . \tag{B.74}$$

Changing the dummy indices from $n-1$ to n and realizing that we can sum the term with $n=0$ for the remaining terms (since it is equivalent to summing zero):

$$\frac{1}{2}\left\{\sum_{n=0}^{\infty}(n+1)u^{n}Q + \sum_{n=0}^{\infty} nu^{n}Q + \sum_{n=0}^{\infty} nu^{n} - \sum_{n=0}^{\infty}(n+1)u^{n}\right\} = \sum_{n=0}^{\infty} u^n \left\langle m\right\rangle_n , \tag{B.75}$$

$$\sum_{n=0}^{\infty} u^n \left\{\frac{2nQ+Q-1}{2}\right\} = \sum_{n=0}^{\infty} u^n \left\langle m\right\rangle_n , \tag{B.76}$$

Or, isolating $\langle m\rangle_n$:

$$\left\langle m\right\rangle_n = \left\{n+\frac{1}{2}\right\}Q - \frac{1}{2} \tag{B.77}$$

Rewriting the energy to the oscillators:

$$\langle E_f\rangle = \frac{\omega_f}{\omega_0} Q E_0 \tag{B.78}$$

Appendix C Program in python using Qutip

```
#Library imports
import qutip as qt
import numpy as np
import matplotlib.pyplot as plt
#Constants
dim = 30                                        # Fock space dimension
n_loops_tau = 200                               # loops for evolution
    time
n_loops_ec = 200                                # loops for solver
r_max = 0.4                                     # r utilized
omega_h = 2*np.pi                               # \omega, no squeezing
    frequency
chi_max = (1/2)*omega_h*np.tanh(2*r_max)        # maximum squeezing (
    function of r)
omega_c = np.sqrt(omega_h**2 - 4*chi_max**2)    # \Omega, diagonal
    frequency
gamma = 1                                       # Decay rate
T_c = 1                                         # Cold reservoir
    temperature
T_h = 10                                        # Hot reservoir
    temperature
beta_c = 1/T_c                                  # Inverse cold
    temperature
beta_h = 1/T_h                                  # Inverse hot
    temperature
n_c = 1/(np.exp((1/T_c)*omega_c) - 1)           # Ocupaton number on
    cold reservoir
n_h = 1/(np.exp((1/T_h)*omega_h) - 1)           # Ocupation number on
    ho reservoir
```

```
tau_list = np.linspace(0.3, 2.5, n_loops_tau) # time list
eta_max = 1-omega_c/omega_h                    # Max eff given r
eta_carnot = 1- T_c/T_h                        # Eff Carnot
# Hamiltonian and operators
a = qt.destroy(dim)                              # annihilation
    operator
b = np.cosh(r_max)*a + np.sinh(r_max)*a.dag()    # annihilation
    operator in b
H_c = omega_c*(b.dag()*b + (1/2)*qt.qeye(dim))   # Squeezed
    hamiltonian
H_h = omega_h*(a.dag()*a + (1/2)*qt.qeye(dim))   # Harmonic oscillator
     hamiltonian
#colapse operators
gamma_mod = gamma*np.exp(2*r_max)                # moddified gamma
C_ops_c = [np.sqrt(gamma_mod*(n_c + 1))*b, np.sqrt(gamma_mod*n_c)*b.
    dag()]
C_ops_h = [np.sqrt(gamma*(n_h + 1))*a, np.sqrt(gamma*n_h)*a.dag()]
#Important functions
def Coeff_exp(t, args):     # Expansion coefficient
    t_exp = (1 - t/tau)
    return t_exp
def Coeff_comp(t, args):    # Compression coefficient
    t_comp = (t/tau)
    return t_comp
def logrho(a):              #Log for the matrix terms
    if a > 0:
        return np.log(a)
    else:
        return 0
def entropy(rho_1,rho_2):  #Relative entropy
```

```
45      S_rel=0
46      for i in range(dim-1):
47          p_1 = ((qt.fock(dim,i).dag())*rho_1*(qt.fock(dim,i)).full())
    [0][0].real
48          p_2 = ((qt.fock(dim,i).dag())*rho_2*(qt.fock(dim,i)).full())
    [0][0].real
49          S = (p_1*logrho(p_1) - p_1*logrho(p_2)).real
50          S_rel = S_rel + S
51      return(S_rel)
52  #lists
53  W_exp_list = []
54  W_comp_list = []
55  Q_h_list = []
56  Q_c_list = []
57  S_exp_list=[]
58  S_comp_list=[]
59  S_uni_list=[]
60  eta_list = []
61  W_net_list = []
62  #Time dependent hamiltonians
63  H_exp_t = [omega_h*(a.dag()*a + (1/2)*qt.qeye(dim)),[chi_max*(a.dag()
    **2 + a**2),Coeff_exp]]
64  H_comp_t = [omega_h*(a.dag()*a+(1/2)*qt.qeye(dim)),[chi_max*(a.dag()
    **2 + a**2),Coeff_comp]]
65  #Starting rho
66  rho_1 = (-(1/T_c)*H_c).expm()/((-(1/T_c)*H_c).expm()).tr()
67  #The cycle
68  for i in range(n_loops_tau):
69      tau = tau_list[i]
70      t_ec_list = np.linspace(0,tau,n_loops_ec)
```

```
    #expansion
    result_exp = qt.mesolve(H_exp_t, rho_1, t_ec_list, [], [])
    rho_2 = result_exp.states[-1]       #Real state after expansion
    W_exp = ((H_h*rho_2 - H_c*rho_1).tr()).real
    W_exp_list.append(W_exp)
    sigma_exp = (-(beta_c*omega_c/omega_h)*H_h).expm()/((-(beta_c*
omega_c/omega_h)*H_h).expm()).tr()
    #"reversible adiabatic statte" where beta_c' = beta_c*omega_c/
omega_h
    S_exp= entropy(rho_2,sigma_exp)
    S_exp_list.append(S_exp)
    #Heating
    rho_3 = qt.steadystate(H_h, C_ops_h)
    Q_h = (((H_h*rho_3) - (H_h*rho_2)).tr()).real
    Q_h_list.append(Q_h)
    #S_h = entropy(rho_2,rho_3)
    #S_h_list.append(S_h)
    #Compression
    result_comp = qt.mesolve(H_comp_t, rho_3, t_ec_list, [], [])
    rho_4 = result_comp.states[-1]
    W_comp = ((H_c*rho_4 - H_h*rho_3).tr()).real
    W_comp_list.append(W_comp)
    sigma_comp = (-(beta_h*omega_h/omega_c)*H_c).expm()/((-(beta_h*
omega_h/omega_c)*H_c).expm()).tr()
    S_comp= entropy(rho_4,sigma_comp).real
    S_comp_list.append(S_comp)
    #Cooling
    Q_c = (((H_c*rho_1) - (H_c*rho_4)).tr()).real
    Q_c_list.append(Q_h)
    #S_c = entropy(rho_4,rho_1)
```

```
98      #S_c_list.append(S_c)
99  #writting S_uni
100 for i in range(n_loops_tau):
101     S_uni = S_comp_list[i]+S_exp_list[i]
102     S_uni_list.append(S_uni)
103 #Writting eta
104 for i in range(n_loops_tau):
105     W_net = W_exp_list[i] + W_comp_list[i]
106     W_net_list.append(W_net)
107     if W_net < 0:
108         if Q_h_list[i] > 0:
109             eta = - W_net/Q_h_list[i]
110             eta_list.append(eta.real)
111         else:
112             eta_list.append(np.nan)
113     else:
114         eta_list.append(np.nan)
115 #Plotting
116 fig, ax1 = plt.subplots()
117 plt.grid(linestyle=':')
118 color = 'tab:red'
119 ax1.set_xlabel('time')
120 ax1.set_ylabel('Entropy', color=color)
121 ax1.plot(tau_list, S_uni_list, color=color)
122 ax1.tick_params(axis='y', labelcolor=color)
123 ax2 = ax1.twinx()  # instantiate a second axes that shares the same x-
    axis
124 color = 'tab:blue'
125 ax2.set_ylabel('Efficiency', color=color)  # we already handled the x-
    label with ax1
```

```
126 ax2.plot(tau_list, eta_list, color=color)
127 ax2.tick_params(axis='y', labelcolor=color)
128
129 fig.tight_layout()  # otherwise the right y-label is slightly clipped
130 plt.show()
```

References

[1] S. Carnot, "Réflexions sur la puissance motrice du feu et sur les machines propres à développer cette puissance," in *Annales scientifiques de l'École Normale Supérieure*, vol. 1, pp. 393–457, 1872. [Cited on page 1.]

[2] H. B. Callen, "Thermodynamics and an introduction to thermostatistics," 1998. [Cited on page 1.]

[3] H. E. Scovil and E. O. Schulz-DuBois, "Three-level masers as heat engines," *Physical Review Letters*, vol. 2, no. 6, p. 262, 1959. [Cited on pages 1, 20, and 48.]

[4] J. Geusic, E. Schulz-DuBios, and H. Scovil, "Quantum equivalent of the carnot cycle," *Physical Review*, vol. 156, no. 2, p. 343, 1967. [Cited on page 1.]

[5] R. J. de Assis, T. M. de Mendonça, C. J. Villas-Boas, A. M. de Souza, R. S. Sarthour, I. S. Oliveira, and N. G. de Almeida, "Efficiency of a quantum otto heat engine operating under a reservoir at effective negative temperatures," *Physical Review Letters*, vol. 122, no. 24, p. 240602, 2019. [Cited on pages 1 and 2.]

[6] P. Li and B. Jia, "Particle-exchange heat engine working between bosonic and fermionic reservoirs," *Physical Review E*, vol. 83, no. 6, p. 062104, 2011. [Cited on page 1.]

[7] J. S. Wright, T. Gould, A. R. Carvalho, S. Bedkihal, and J. A. Vaccaro, "Quantum heat engine operating between thermal and spin reservoirs," *Physical Review A*, vol. 97, no. 5, p. 052104, 2018. [Cited on page 1.]

[8] A. Nüßeler, I. Dhand, S. F. Huelga, and M. B. Plenio, "Efficient simulation of open quantum systems coupled to a fermionic bath," *Physical Review B*, vol. 101, no. 15, p. 155134, 2020. [Cited on page 1.]

[9] P. A. Camati, J. F. Santos, and R. M. Serra, "Coherence effects in the performance of the quantum otto heat engine," *Physical Review A*, vol. 99, no. 6, p. 062103, 2019. [Cited on page 1.]

[10] M. Herrera, J. H. Reina, I. D'Amico, and R. M. Serra, "Experimental correlation-boosted quantum engine," *arXiv preprint arXiv:2211.11449*, 2022. [Cited on page 1.]

[11] J. Roßnagel, O. Abah, F. Schmidt-Kaler, K. Singer, and E. Lutz, "Nanoscale heat engine beyond the carnot limit," *Physical review letters*, vol. 112, no. 3, p. 030602, 2014. [Cited on page 1.]

[12] R. Long and W. Liu, "Performance of quantum otto refrigerators with squeezing," *Physical Review E*, vol. 91, no. 6, p. 062137, 2015. [Cited on page 1.]

[13] J. Klaers, S. Faelt, A. Imamoglu, and E. Togan, "Squeezed thermal reservoirs as a resource for a nanomechanical engine beyond the carnot limit," *Physical Review X*, vol. 7, no. 3, p. 031044, 2017. [Cited on page 1.]

[14] J. Wang, J. He, and Y. Ma, "Finite-time performance of a quantum heat engine with a squeezed thermal bath," *Physical Review E*, vol. 100, no. 5, p. 052126, 2019. [Cited on page 1.]

[15] R. J. de Assis, J. S. Sales, U. C. Mendes, and N. G. de Almeida, "Two-level quantum otto heat engine operating with unit efficiency far from the quasi-static regime under a squeezed reservoir," *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 54, no. 9, p. 095501, 2021. [Cited on page 1.]

[16] M. V. Berry, "Transitionless quantum driving," *Journal of Physics A: Mathematical and Theoretical*, vol. 42, no. 36, p. 365303, 2009. [Cited on pages 1, 23, and 48.]

[17] X. Chen, A. Ruschhaupt, S. Schmidt, A. del Campo, D. Guéry-Odelin, and J. G. Muga, "Fast optimal frictionless atom cooling in harmonic traps: Shortcut to adiabaticity," *Physical review letters*, vol. 104, no. 6, p. 063002, 2010. [Cited on pages 1, 23, and 48.]

[18] A. del Campo, "Shortcuts to adiabaticity by counterdiabatic driving," *Physical review letters*, vol. 111, no. 10, p. 100502, 2013. [Cited on pages 1, 23, and 48.]

[19] S. Deffner, C. Jarzynski, and A. del Campo, "Classical and quantum shortcuts to adiabaticity for scale-invariant driving," *Physical Review X*, vol. 4, no. 2, p. 021013, 2014. [Cited on pages 1, 23, and 48.]

[20] O. Abah and E. Lutz, "Performance of shortcut-to-adiabaticity quantum engines," *Physical Review E*, vol. 98, no. 3, p. 032121, 2018. [Cited on pages 1 and 23.]

[21] D. Guéry-Odelin, A. Ruschhaupt, A. Kiely, E. Torrontegui, S. Martínez-Garaot, and J. G. Muga, "Shortcuts to adiabaticity: Concepts, methods, and applications," *Reviews of Modern Physics*, vol. 91, no. 4, p. 045001, 2019. [Cited on pages 1, 23, and 48.]

[22] S. Lee, M. Ha, J.-M. Park, and H. Jeong, "Finite-time quantum otto engine: Surpassing the quasistatic efficiency due to friction," *Physical Review E*, vol. 101, no. 2, p. 022127, 2020. [Cited on page 1.]

[23] J. Nettersheim, S. Burgardt, Q. Bouton, D. Adam, E. Lutz, and A. Widera, "Power of a quasi-spin quantum otto engine at negative effective temperature," *arXiv preprint arXiv:2207.09272*, 2022. [Cited on page 2.]

[24] G. G. Damas, R. J. de Assis, and N. G. de Almeida, "Cooling with fermionic thermal reservoirs," *Phys. Rev. E*, vol. 107, p. 034128, Mar 2023. [Cited on page 2.]

[25] M. Campisi, "Fluctuation relation for quantum heat engines and refrigerators," *Journal of Physics A: Mathematical and Theoretical*, vol. 47, no. 24, p. 245001, 2014. [Cited on pages 2 and 42.]

[26] M. C. Baldiotti, "Mecânica quântica." http://www.uel.br/pessoal/baldiotti/2FIS030.pdf, 2013. [Cited on page 4.]

[27] J. Von Neumann, *Mathematical foundations of quantum mechanics: New edition*, vol. 53. Princeton university press, 2018. [Cited on pages 5 and 21.]

[28] J. Preskill, *Lecture Notes for Physics 229 : Quantum Information and Computation*. California Institute of Technology, 1998. [Cited on pages 5 and 48.]

[29] D. Manzano, "A short introduction to the lindblad master equation," *AIP Advances*, vol. 10, no. 2, p. 025106, 2020. [Cited on pages 6, 7, 19, and 48.]

[30] H.-P. Breuer, F. Petruccione, *et al.*, *The theory of open quantum systems*. Oxford University Press on Demand, 2002. [Cited on pages 7, 19, and 48.]

[31] G. Lindblad, "On the generators of quantum dynamical semigroups," *Communications in Mathematical Physics*, vol. 48, pp. 119–130, 1976. [Cited on pages 7 and 48.]

[32] C. Cohen-Tannoudji, J. Dupont-Roc, and G. Grynberg, *Atom-Photon Interactions: Basic Processes and Applications*. 1998. [Cited on pages 13 and 48.]

[33] D. Nigro, "On the uniqueness of the steady-state solution of the lindblad–gorini–kossakowski–sudarshan equation," *Journal of Statistical Mechanics: Theory and Experiment*, vol. 2019, no. 4, p. 043202, 2019. [Cited on pages 19 and 48.]

[34] B. Baumgartner and H. Narnhofer, "Analysis of quantum semigroups with gks–lindblad generators: Ii. general," *Journal of Physics A: Mathematical and Theoretical*, vol. 41, no. 39, p. 395303, 2008. [Cited on pages 19 and 48.]

[35] V. V. Albert, "Lindbladians with multiple steady states: theory and applications," *arXiv preprint arXiv:1802.00010*, 2018. [Cited on pages 19 and 48.]

[36] R. Alicki, "The quantum open system as a model of the heat engine," *Journal of Physics A: Mathematical and General*, vol. 12, no. 5, p. L103, 1979. [Cited on pages 20 and 48.]

[37] E. B. Botosso, J. S. Sales, and N. G. de Almeida, "A comment on a possible inadequacy of new redefinitions of heat and work in quantum thermodynamics," *arXiv preprint arXiv:2107.03369*, 2021. [Cited on pages 20 and 48.]

[38] E. B. Bottosso *et al.*, "A possible inadequacy of a recent proposal for redefining heat and work in quantum thermodynamics," 2021. [Cited on pages 20 and 48.]

[39] M. N. Bera, A. Riera, M. Lewenstein, and A. Winter, "Generalized laws of thermodynamics in the presence of correlations," *Nature communications*, vol. 8, no. 1, p. 2180, 2017. [Cited on pages 20 and 48.]

[40] S. Alipour, A. Rezakhani, A. Chenu, A. Del Campo, and T. Ala-Nissila, "Entropy-based formulation of thermodynamics in arbitrary quantum evolution," *Physical Review A*, vol. 105, no. 4, p. L040201, 2022. [Cited on pages 20 and 48.]

[41] J. Gemmer, M. Michel, and G. Mahler, *Quantum thermodynamics: Emergence of thermodynamic behavior within composite quantum systems*, vol. 784. Springer, 2009. [Cited on pages 20 and 48.]

[42] K. Husimi, "Miscellanea in elementary quantum mechanics, ii," *Progress of Theoretical Physics*, vol. 9, no. 4, pp. 381–402, 1953. [Cited on pages 35 and 51.]

[43] O. Abah, J. Rossnagel, G. Jacob, S. Deffner, F. Schmidt-Kaler, K. Singer, and E. Lutz, "Single-ion heat engine at maximum power," *Physical review letters*, vol. 109, no. 20, p. 203006, 2012. [Cited on pages 35, 37, 38, and 48.]

[44] J. Roßnagel, O. Abah, F. Schmidt-Kaler, K. Singer, and E. Lutz, "Nanoscale heat engine beyond the carnot limit," *Physical review letters*, vol. 112, no. 3, p. 030602, 2014. [Cited on page 35.]

[45] U. C. Mendes, J. S. Sales, and N. G. de Almeida, "Quantum otto thermal machines powered by kerr nonlinearity," *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 54, no. 17, p. 175504, 2021. [Cited on page 37.]

[46] S. Karar, S. Datta, S. Ghosh, and A. Majumdar, "Anharmonicity can enhance the performance of quantum refrigerators," *arXiv preprint arXiv:1902.10616*, 2019. [Cited on page 37.]

[47] F. L. Curzon and B. Ahlborn, "Efficiency of a carnot engine at maximum power output," *American Journal of Physics*, vol. 43, no. 1, pp. 22–24, 1975. [Cited on page 38.]

[48] P. D. Nation and J. Johansson, "Qutip: Quantum toolbox in python," *online at http://qutip. org*, 2011. [Cited on page 39.]

[49] L. Del Re, B. Rost, A. Kemper, and J. Freericks, "Driven-dissipative quantum mechanics on a lattice: Simulating a fermionic reservoir on a quantum computer," *Physical Review B*, vol. 102, no. 12, p. 125112, 2020. [Cited on page 39.]

[50] J. R. Johansson, P. D. Nation, and F. Nori, "Qutip: An open-source python framework for the dynamics of open quantum systems," *Computer Physics Communications*, vol. 183, no. 8, pp. 1760–1772, 2012. [Cited on page 39.]

[51] F. Plastina, A. Alecce, T. J. Apollaro, G. Falcone, G. Francica, F. Galve, N. L. Gullo, and R. Zambrini, "Irreversible work and inner friction in quantum thermodynamic processes," *Physical review letters*, vol. 113, no. 26, p. 260601, 2014. [Cited on pages 40, 41, and 48.]

[52] J. G. Muga, X. Chen, S. Ibáñez, I. Lizuain, and A. Ruschhaupt, "Transitionless quantum drivings for the harmonic oscillator," *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 43, no. 8, p. 085509, 2010. [Cited on page 44.]

[53] "Wikepedia page on probability generating functions." https://en.wikipedia.org/wiki/Probability-generating_function. Accessed: 2023-03-20. [Cited on page 54.]

[54] P. Morse and H. Feshbach, *Methods of Theoretical Physics*. No. pt. 1 in International series in pure and applied physics, McGraw-Hill, 1953. [Cited on page 54.]