Quantum thermodynamics of non-Hermitian Otto engines

A thesis

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by

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Certificate

This is to certify that this dissertation entitled *Quantum Thermodynamics of non-Hermitian Otto engines* towards the partial fulfilment of the BS-MS dual degree programme at the Indian Institute of Science Education and Research, Pune represents work carried out by Shivam Dosajh at Indian Institute of Science Education and Research (IISER) Pune and the University of Maryland, Baltimore County (UMBC) under the supervision of Dr. Sebastian Deffner (Associate Professor, Department of Physics, UMBC) and Dr. Juzar Thingna, along with Dr. Bijay K. Agarwalla (Associate Professor, Department of Physics, IISER Pune), during the academic year 2023-2024.

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This thesis is dedicated to the ones who persevere,
To the ones who try again,
To the ones who have the courage to follow their curiosities,
To the ones who remain hopeful,
And to the ones who live and love without the fear of judgement.

Declaration

I hereby declare that the matter embodied in the report entitled *Quantum Thermodynamics of non-Hermitian Otto engines* are the results of the work carried out by me at the Department of Physics, Indian Institute of Science Education and Research, Pune and the Department of Physics, University of Maryland Baltimore County, under the supervision of Dr. Sebastian Deffner, Dr. Juzar Thingna and Dr. Bijay K. Agarwalla and the same has not been submitted elsewhere for any other degree. Wherever others contribute, every effort is made to indicate this clearly, with due reference to the literature and acknowledgement of collaborative research and discussions.

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Abstract

One of the fundamental axioms of quantum mechanics is that observables are self-adjoint or Hermitian operators in a complex Hilbert space. What started as a mathematical curiosity in the late 90s, theoretical investigations into non-Hermitian $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians, which emulate open systems with balanced gain and loss while producing real eigenspectrums in certain parametric regimes have fledged into an active research field with various experimental realisations in classical as well as quantum setups. One of the most interesting applications of quantum $\mathscr{P}\mathscr{T}$-symmetric two-level systems or qubits is that they show suppressed decoherence when compared to their Hermitian counterparts. This motivates us to study the quantum thermodynamics of $\mathscr{P}\mathscr{T}$-symmetric qubits in simple processes to better understand their potential as building blocks for future quantum computers. In this thesis, we primarily study two popular mathematical approaches in literature used to analyze time-dependent $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians, which are called the canonical mapping approach and the non-canonical mapping approach. We then apply them separately to study two thermodynamic problems, namely, the proof of the Jarzynski equality using the non-canonical approach and the efficiency of the quantum Otto engine with a $\mathscr{P}\mathscr{T}$-symmetric qubit as the working medium using both approaches. Our findings suggest that it is possible to get higher efficiency and power outputs for these $\mathscr{P}\mathscr{T}$-symmetric qubit Otto engines as compared to their Hermitian counterparts.

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Chapter 1

Introduction

This chapter is divided into two sections. The first section is on the background and motivation underlining this thesis. This starts with a historical introduction to $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians. Several experimental confirmations and theoretical studies connecting $\mathscr{P}\mathscr{T}$-symmetric systems to open quantum systems with balanced gains and losses are subsequently discussed. We then emphasise the fact that $\mathscr{P}\mathscr{T}$-symmetric qubits show suppressed decoherence and hence, possess great potential to become building blocks of future quantum computers. This motivates us to study their thermodynamic properties like efficiency in simple processes like quantum heat engines, specifically in quantum Otto engines. The second section expands on the structure of the rest of the thesis.

Note: During this entire thesis, we set $\hbar = k_B = 1$

1.1 Background and Motivation

Any standard course on quantum mechanics often starts by listing out a set of axioms [1], called the Dirac-von Neumann axioms, that are essential to the mathematical foundation of the theory. They usually start by the supposition of a complex Hilbert space $\mathscr{H}$. Out of the three axioms, the first one is the most relevant to us. It states self-adjoint or Hermitian operators $\mathscr{O}(=\mathscr{O}^\dagger)$ in $\mathscr{H}$ are physical observables of the quantum system.

Hermiticity of observables is considered an important postulate in conventional quantum mechanics because of the mathematical properties that come along with it, namely real eigenvalues and orthogonal eigenstates [2]. This physically means that values obtained on measuring any observable are real numbers and that experimental outcomes are distinguishable, respectively. This makes the Hermiticity of observables a physically sensible and mathematically convenient axiom. However, in the late 90s [3] there was a revelation of non-Hermitian operators that had a real spectrum of eigenvalues in certain parametric regimes. The operators considered were of the following form:

$$H = p^2 + (ix)^N. \tag{1.1}$$

They showed that the eigenvalues are discrete, completely real, positive and infinitely many whenever $N \geq 2$. Note that the boundary case $N = 2$ is the simple harmonic oscillator. For the case $1 < N < 2$, there are infinitely many complex eigenvalues and only a finite number of real and positive eigenvalues. For $N \leq 1$, there are no real eigenvalues and all the eigenvalues are complex. The purely real part of the spectrum can be seen in the following figure:

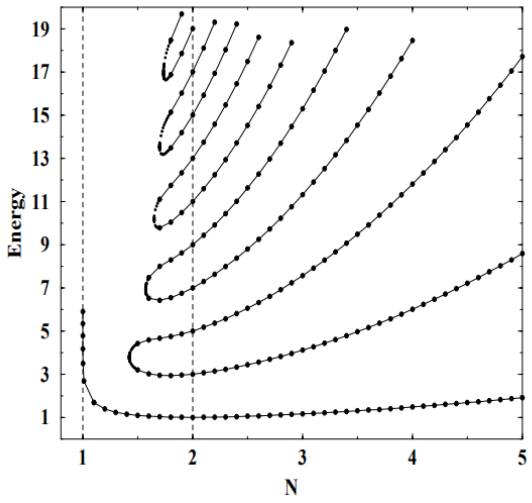

Figure 1.1: Purely real part of the spectrum of $H = p^2 + (ix)^N$ Ref. [3]

This curious behaviour of the spectrum was attributed to the operator H, henceforth called the Hamiltonian, having a parity-time ($\mathscr{P}\mathscr{T}$) symmetry. The parity or the space-reflection operator $\mathscr{P}$ defined by
$\mathscr{P}$: $x \to -x$ and $p \to -p$. Similarly, the time-reversal operator is an anti-linear operator defined by $\mathscr{T}$: $x \to x$, $p \to -p$, $i \to -i$. Note that the Hamiltonian above is not parity or time symmetric separately, but it is symmetric under the combined action of $\mathscr{P}\mathscr{T}$ [4] i.e.

$$[H, \mathscr{P}\mathscr{T}] = 0. \tag{1.2}$$

The spectrum is purely real when $N \geq 2$, and this parametric regime is said to be the $\mathscr{P}\mathscr{T}$-unbroken regime. For $N < 2$, the eigenvalues are either real or complex conjugates of each other. This is said to be the $\mathscr{P}\mathscr{T}$-broken regime. It is important to note that the Hamiltonian H is still $\mathscr{P}\mathscr{T}$-symmetric in all regimes. However, the eigenstates are no longer $\mathscr{P}\mathscr{T}$-symmetric in the $\mathscr{P}\mathscr{T}$-broken regime. The point in the parameter space separating the $\mathscr{P}\mathscr{T}$-unbroken and $\mathscr{P}\mathscr{T}$-broken regime is called the exceptional point.

Since then, $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians have found experimental confirmation in diverse settings like coupled optical waveguides [5], photonic circuits [6],

photonic lattices [7], LRC circuits [8], NMR [9], NV centres in diamond [10], semiconductor microcavities [11], ultracold atoms [12], trapped ions [13], circuit QED [14] and superconducting qubits [15] to state just a few. The reason $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians became so important was primarily their ability to model open-quantum systems with balanced gains and losses. To understand this better, consider the following illustration (inspired from [16]):

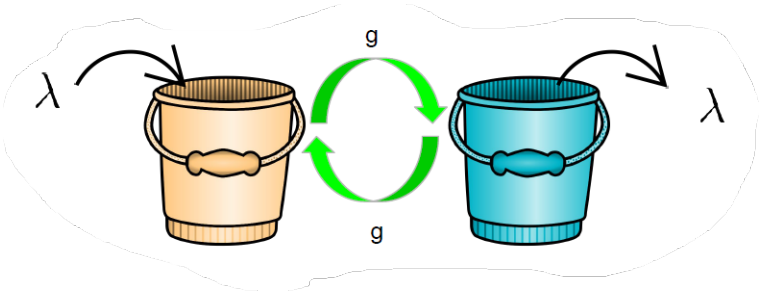

Figure 1.2: Illustration of $\mathscr{P}\mathscr{T}$-symmetric systems

The yellow bucket experiences a gain (of energy, particles or both) at a rate λ. The blue bucket experiences a loss at the same rate λ. The two buckets are also coupled via an interaction with strength g, exchanging energy and/or particles among each other. To see that this is a $\mathscr{P}\mathscr{T}$-symmetric system, consider the action of $\mathscr{P}$ and $\mathscr{T}$ one by one on this system. First, under the $\mathscr{P}$ operator, the yellow and blue buckets get exchanged, which would mean the blue bucket now undergoes gain while the yellow bucket undergoes loss. Next, applying the $\mathscr{T}$ operator to this system, the arrows reverse their direction, converting the gain into the loss and vice-versa. This brings us back to the original system we started with and hence, the system is $\mathscr{P}\mathscr{T}$-symmetric.

This simple idea served as the basis of many experiments already stated above, as well as many theoretical investigations, specifically in open-quantum systems exhibiting balanced gain and loss. It is well known that dropping the *jump terms* in the GKSL master equations [17] leads to time-evolution that is generated by a non-Hermitian Hamiltonian, which is viewed like a semi-classical limit to the

full quantum dynamics [18]. $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians have also been used in quantum systems to calculate mean-field dynamics for various open-quantum systems, like coupled harmonic oscillators [19], Bose-Einstein condensates [20], quantum dots [21], and XYZ-spin models [22] to state a few. Another interesting theoretical application of $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians is to give a phenomenological model of a quantum Otto engine with a conventional qubit as the working medium [23]. Although the chosen non-Hermitian Hamiltonian's physical origin is unclear, it can still model the effects of imposed reservoirs in the engine and produce the expected efficiency. Later in this thesis, we will use two mathematical approaches [24, 25] used to study time-dependent non-Hermitian Hamiltonians. Both these approaches will preserve unitarity in the sense that some modified definition of the inner product will be conserved in time. As a result, when the quantum adiabatic theorem is applied, we only get real values of the Berry phase for both approaches [24, 26]. However, the approach used in [23] to model the Otto engine relies on complex Berry phases that cause exponential decay or amplification of populations in the heat strokes.

Another extremely interesting application of non-Hermitian quantum mechanics is to design $\mathscr{P}\mathscr{T}$-symmetric qubits that could serve as building blocks for future quantum computers. This is because recent experimental investigations [15] with $\mathscr{P}\mathscr{T}$-symmetric qubits in superconducting transmon circuits has shown suppressed decoherence in the unbroken phase, which reduces further as the system approaches the exceptional point. This was done by measuring the decay rate of Rabi oscillations, which decreased as the system got closer to the exceptional point. Another experiment [27] found an enhanced violation of Leggett-Garg inequalities in the $\mathscr{P}\mathscr{T}$-symmetric trapped ion qubits indicating slower coherence damping as the exceptional point was approached. There is also experimental evidence [28] for perfect coherence at the exceptional point for $\mathscr{P}\mathscr{T}$-symmetric single-ion systems. Even theoretical investigations [29] have shown a slowing of

the pure decoherence or dephasing in $\mathscr{P}\mathscr{T}$-symmetric qubits as the exceptional point is approached.

Achieving higher coherence times for qubits will be incredibly important for building useful quantum computers, and $\mathscr{P}\mathscr{T}$-symmetric qubits show great potential here. Thus, studying the properties of these qubits in simple processes like quantum heat engines [30] could tell us whether it is beneficial to use $\mathscr{P}\mathscr{T}$-symmetric qubits as building blocks for quantum computers from a thermodynamic perspective. Analysing their efficiencies in such simple cyclic processes could help us answer if non-Hermitian working mediums provide any thermodynamic performance advantage over conventional working mediums. We note that it has already been shown [31] that the Carnot bound can be achieved for $\mathscr{P}\mathscr{T}$-symmetric systems in the quasi-static limit. However, another popular and interesting type of engine is the quantum Otto engine [30]. In this thesis, we primarily study two different mathematical approaches to analyze quantum Otto engines with $\mathscr{P}\mathscr{T}$-symmetric qubits as their working medium. In addition, we also study the application of these mathematical approaches to prove the Jaryznski equality [32, 33, 34, 31].

1.2 Structure of the thesis

The rest of this thesis is divided into three more chapters:

Chapter 2 - Mathematical Background and Approaches - All the necessary mathematical and physical preliminaries required to understand the rest of the thesis will be covered here. The first section, which is on standard quantum thermodynamics, will discuss several simple and fundamental results in the field. The second section, which is primarily on pseudo-Hermitian Hamiltonians provides a compendium of all the mathematics that will be used in the rest of the thesis to do calculations and perform derivations. Primarily, two mathematical approaches popular in literature [24, 25] for time-dependent metrics will be studied in detail.

Chapter 3 - Results - Both the approaches discussed in detail in the last chapter are applied here to solve two different problems - namely, the derivation of Jarzynski equality for non-Hermitian systems and constructing a quantum Otto engine with a $\mathscr{PT}$-symmetric qubit as the working medium. We will discuss pre-existing results for these problems [34, 31] and also provide original results. Furthermore, we restrict ourselves mostly to analytically tractable models for $\mathscr{PT}$-symmetric qubit Hamiltonians, but use numerics wherever necessary to do computations.

Chapter 4 - Discussion and Future Results - Here, we will summarise our findings and discuss their implications. We also discuss possible limitations of our methods and provide future research directions that could help solve some of those limitations. We also provide future research directions to conclude.

Chapter 2

Mathematical Background and Approaches

In this chapter, we will cover the theoretical preliminaries needed to understand this thesis. The first section of this chapter will discuss the mathematical and physical basics of conventional quantum thermodynamics [35, 36]. This will include a simple worked-out example of the quantum Otto engine [30, 35], as well as a discussion on the two-time measurement approach [37] and its application in calculating the efficiency of an Otto cycle with a Landau-Zener drive [38, 39]. The second part of this chapter includes a mathematical discussion on $\mathscr{P}\mathscr{T}$-symmetric [3, 40] and pseudo-Hermitian Hamiltonians [41]. The time-independent metric operator case is discussed first in detail. The two popular approaches for understanding non-Hermitian Hamiltonians with time-dependent metric operators [24, 25] are subsequently discussed in detail. In the next chapter, both these approaches will be used to do thermodynamic calculations for different models.

2.1 Hermitian Quantum Thermodynamics

The first law in classical thermodynamics is the statement of conservation of energy and also defines the meaning of work and heat [42, 43] (for an elucidating analogy explaining the first law using ponds and streams, please refer to [42]). The growing research field of quantum thermodynamics [44] has been able to extend a lot of these concepts and married them to quantum mechanics [35, 36]. Even though quantum thermodynamics is vast and diverse, for the thesis we only focus on the quantum version of the first law when the equilibrium state ρ_{eq} is given by the Gibbs state, which can be justified under the assumption of the quantum system having much lesser degrees of freedom than the thermal reservoir and extremely weak coupling between the quantum system and the reservoir [43]. This will involve defining the meaning of quantum heat and quantum work, and also restating the first law for quantum systems. Suppose the Hamiltonian of the system is given by H. The expectation value of the energy of the quantum system in this equilibrium state is obviously:

$$\langle E \rangle = \mathrm{Tr}\{\rho_{eq} H\}, \tag{2.1}$$

The infinitesimal change in the energy is formally given by:

$$d\langle E \rangle = \mathrm{Tr}\{d\rho_{eq} H\} + \mathrm{Tr}\{\rho_{eq} dH\}, \tag{2.2}$$

which indicates the breakup of the change in energy into two parts analogous to what is seen in the classical first law. To investigate further, note that as per the assumptions above, the equilibrium state of the system connected to a reservoir at temperature $T = 1/\beta$ is given by the Gibbs state [43]:

$$\rho_{eq} = \frac{e^{-\beta H}}{Z}, \tag{2.3}$$

where $Z = \mathrm{Tr}\left\{\left(e^{-\beta H}\right)\right\}$ is the partition function. In order to identify one of the terms in (2.2) as heat or work, we need to invoke the quantum definition of entropy, often called the von-Neumann entropy [1], given by $S = -\mathrm{Tr}\{\rho_{eq} \ln \rho_{eq}\}$. On calculating the infinitesimal change in the von-Neumann entropy dS for an isothermal process where the equilibrium state is given by (2.3), it is found:

$$dS = \beta \,\mathrm{Tr}\{d\rho_{eq} H\}. \tag{2.4}$$

When combined with the classical thermodynamic change in entropy for an isothermal quasi-static process $dS = \beta dQ$, we can identify the heat exchange in the process as $dQ = \mathrm{Tr}\{d\rho_{eq} H\}$ i.e. we were can identify one of the terms in (2.2) as the heat exchange and hence, the second term can be identified as the work in the process i.e. $dW = \mathrm{Tr}\{\rho_{eq} dH\}$. It now becomes possible to discuss the physical meaning of quantum heat and work under the assumptions we have chosen. The heat exchange is associated with the change solely in the state of the system i.e. the energy level populations specifically in the case of Gibbs states (which don't have coherences) while the Hamiltonian or the energy eigenvalues themselves don't change. The work in the process is related to changes in the Hamiltonian or the energy eigenvalues while the state of the system or the energy level populations are held constant. The changes in the Hamiltonian are often controlled by an extensive external parameter, which is naturally called the work parameter. With this knowledge, we emphasise that (2.2) acts as the operational definition of the first law of quantum thermodynamics for this thesis given the assumptions we have chosen. As a side note, for a discussion on the first law of quantum thermodynamics for non-Gibbs equilibrium states, see [35].

We also note that the definition of quantum work given above only holds for quasi-static processes. However, for finite-time processes, the definition changes a bit. For an isolated quantum system undergoing unitary dynamics, the change in the energy is attributed to work [39]. This makes sense because of the absence of any

external heat sources or sinks. We will expand on this in more detail when discussing a quantum Otto engine with analytically tractable finite-time driving. For a more general discussion on quantum work, refer to [37, 45].

2.1.1 Quantum Otto Engine

Instead of directly jumping to the quantum Otto engine, let's first briefly discuss the classical Otto engine [42]. Two of the four strokes are isentropic or adiabatic, which means no heat exchange takes place in these strokes and all the energy change is attributed to the work. The other two strokes are isochoric i.e. no work exchange and all the energy change is attributed to heat. This thermodynamic division, in which every stroke in the cycle is either pure heat exchange or pure work exchange, is the hallmark feature of the Otto engine. Other engines like the Carnot engine or the Stirling engine consist of isothermal strokes which invariably means a non-zero contribution of both heat and work, making the subsequent analysis more complicated. The quantum Otto engine serves as an elegant way to study quantum heat and quantum work and is one of the most theoretically [30, 46, 39, 47, 48, 49, 50] and experimentally [51, 52, 53, 54, 55] well-studied examples of a quantum heat engine.

Quantum adiabatic stroke - The quantum adiabatic theorem [2] tells us that the energy level populations of a quantum system do not change if the Hamiltonian of the system is driven or perturbed slowly enough such that no excitations are generated. Thus, a purely adiabatic stroke where no excitations are generated due to a thermal bath must preserve the energy level populations while the energy levels are changed quasistatically. As a result, no heat is exchanged in this process. If there are n energy levels with respective populations p_n, then $dE_n \neq 0, \quad dp_n = 0$ for quantum adiabatic strokes.

Quantum isochoric stroke - Here, the energy levels are kept constant while the energy level populations change as the system thermalises with the attached heat

bath. Thus, there is only heat exchange and no work is done. If there are n energy levels with respective populations p_n, then $dE_n = 0, \quad dp_n \neq 0$ for quantum isochoric strokes.

As an example, we will calculate the efficiency of a quantum Otto engine with quasi-static strokes and a qubit as the working medium [30, 35]. We consider a two-level system whose ground state energy has been set as 0. The energy splitting is given by Δ, which will also serve as the work parameter discussed before. Thus, Hamiltonian is given by:

$$H(\Delta) = \Delta |\Psi_1\rangle \langle\Psi_1|, \tag{2.5}$$

where $\{|\Psi_0\rangle, |\Psi_1\rangle\}$ are the lower and higher energy eigenstates respectively. There are 4 stages of the cycle, labelled as "A", "B", "C", "D" in Figure 2.1.

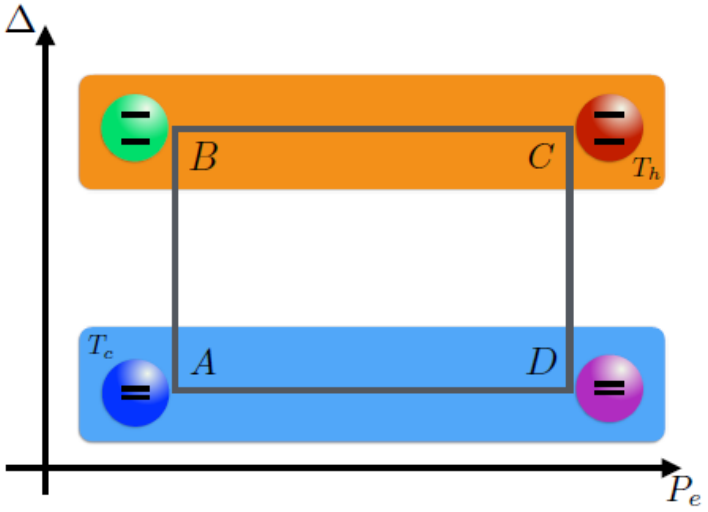

Figure 2.1: Schematic diagram for a standard quantum Otto engine. The x-axis denotes the excited energy level population. The y-axis denotes the energy splitting. Ref. [35]

At A, the value of the energy splitting is given by $\Delta = \Delta_i$. The qubit is attached to a thermal reservoir at a temperature $T_c = 1/\beta_c$ i.e. the state of the system at A is given by the Gibbs state (2.3). Then the reservoir is detached and the stroke $A \to B$

is performed. The value of the energy splitting is increased quasi-statically from Δ_i to $\Delta_f > \Delta_i$. Since this is a quantum adiabatic stroke, the energy level populations don't change and only the energy eigenvalues change. Thus, all the energy change is attributed to work and no heat exchange takes place.
The next stroke is $B \to C$. A thermal reservoir at a hot temperature $T_h = 1/\beta_h$ is attached to the qubit and the system is allowed to thermalise while keeping the Hamiltonian constant. All the energy change is attributed to the heat exchange and the work is zero since this is a quantum isochoric stroke.
The third stroke is $C \to D$ where the thermal reservoir is detached and the energy level splitting is brought back to Δ_i quasi-statically.
The fourth stroke is $D \to A$. The qubit is allowed to thermalise with the first thermal reservoir keeping the Hamiltonian constant and completing the cycle.

We have all the ingredients to calculate the excited state populations and hence, the expectation value of the energy at each stage. The results have been summarised in Figure 2.2. Note that the populations remain constant during the isentropic strokes $A \to B$ and $C \to D$ while the work parameter Δ remains constant during the isochoric strokes $B \to C$ and $D \to A$.

Stage	P_e	Δ	$\langle E \rangle$
A	$\frac{1}{2}\left(1-\tanh\frac{\beta_c\Delta_i}{2}\right)$	Δ_i	$\frac{\Delta_i}{2}\left(1-\tanh\frac{\beta_c\Delta_i}{2}\right)$
B	$\frac{1}{2}\left(1-\tanh\frac{\beta_c\Delta_i}{2}\right)$	Δ_f	$\frac{\Delta_f}{2}\left(1-\tanh\frac{\beta_c\Delta_i}{2}\right)$
C	$\frac{1}{2}\left(1-\tanh\frac{\beta_h\Delta_f}{2}\right)$	Δ_f	$\frac{\Delta_f}{2}\left(1-\tanh\frac{\beta_h\Delta_f}{2}\right)$
D	$\frac{1}{2}\left(1-\tanh\frac{\beta_h\Delta_f}{2}\right)$	Δ_i	$\frac{\Delta_i}{2}\left(1-\tanh\frac{\beta_h\Delta_f}{2}\right)$

Figure 2.2: The excited state population P_e, work parameter Δ, and energy at each stage of the Otto engine [35]

We can also calculate the work and heat exchange in each stroke:

Stroke	Net energy change	Work	Heat
A $\to$ B	$\frac{\Delta_f-\Delta_i}{2}\left(1-\tanh\frac{\beta_c\Delta_i}{2}\right)$	$\frac{\Delta_f-\Delta_i}{2}\left(1-\tanh\frac{\beta_c\Delta_i}{2}\right)$	0
B $\to$ C	$\frac{\Delta_f}{2}\left(\tanh\frac{\beta_c\Delta_i}{2}-\tanh\frac{\beta_h\Delta_f}{2}\right)$	0	$\frac{\Delta_f}{2}\left(\tanh\frac{\beta_c\Delta_i}{2}-\tanh\frac{\beta_h\Delta_f}{2}\right)$
C $\to$ D	$\frac{\Delta_i-\Delta_f}{2}\left(1-\tanh\frac{\beta_h\Delta_f}{2}\right)$	$\frac{\Delta_i-\Delta_f}{2}\left(1-\tanh\frac{\beta_h\Delta_f}{2}\right)$	0
D $\to$ A	$\frac{\Delta_i}{2}\left(\tanh\frac{\beta_h\Delta_f}{2}-\tanh\frac{\beta_c\Delta_i}{2}\right)$	0	$\frac{\Delta_i}{2}\left(\tanh\frac{\beta_h\Delta_f}{2}-\tanh\frac{\beta_c\Delta_i}{2}\right)$

Figure 2.3: Work and heat exchange in each stroke [35]

The net-work output is given by:

$$W_{out} = -(W_{A\to B} + W_{C\to D}) = \frac{\Delta_f - \Delta_i}{2}\left(\tanh\frac{\beta_c\Delta_i}{2} - \tanh\frac{\beta_h\Delta_f}{2}\right), \tag{2.6}$$

and the heat input is given by $Q_{in} = Q_{B\to C}$. The quantum Otto engine efficiency for this two-level system is hence given by:

$$\eta_O = \frac{W_{out}}{Q_{in}} = 1 - \frac{\Delta_i}{\Delta_f}, \tag{2.7}$$

which will always be less than the Carnot efficiency
($\eta_C = 1 - \frac{T_c}{T_h}$), since for W_{out} to be positive:

$$\beta_c\Delta_i > \beta_h\Delta_f \Longrightarrow \frac{\Delta_i}{\Delta_f} > \frac{T_c}{T_h} \Longrightarrow \eta_O < \eta_C. \tag{2.8}$$

2.1.2 Two-Time Measurement Approach

In the previous discussion, we only focussed on adiabatic work strokes. Here, the external parameter (Δ in the two-level system example) changes quasi-statically and the energy level populations do not change at all. Thus, we argued that no heat exchange takes place. Now, we will take the case of finite-time unitary work strokes [37, 39]. Suppose the Hamiltonian of an isolated quantum system is given by $H(\alpha(t))$ where $\alpha(t)$ is an external parameter that varies with time. It is as-

sumed that $H(\alpha(t))$ has a discrete non-degenerate spectrum. Also suppose that the duration of the whole work-stroke is Γ.

At $t = 0$, the system's energy is found after performing a projective measurement. Then, the system, isolated from the environment evolves unitarily for the duration Γ according to the time-dependent Schrödinger equation. Finally, at $t = \Gamma$, the system's energy is measured again by performing a projective measurement. If we consider many such copies of finite-time processes starting from the same initial conditions, we can construct a probability distribution for the work performed in these processes [31, 37, 45]:

$$\mathbb{P}(w) = \sum_{nm} \delta(w - w_{nm}) p_{nm}, \tag{2.9}$$

where p_{nm} is the specific probability of transition from the energy eigenstate $|\Psi_n(\alpha(0))\rangle$ to the energy eigenstate $|\Psi_m(\alpha(\tau))\rangle$ and $w_{nm} = E_m(\alpha(\tau)) - E_n(\alpha(0))$ is the work for the corresponding transition. Suppose the operator governing the dynamics is $U(0,t)$. Also, suppose that initially, at $t = 0$, the state is $\rho(0)$. Then the state of the system at $t = \Gamma$ is given by $\rho(\Gamma) = U(0,\Gamma)\rho(0)U^\dagger(0,\Gamma)$. The average work is found to be:

$$\langle w \rangle = \int dw \mathbb{P}(w) w = \sum_{nm} w_{nm} p_{nm} = \mathrm{Tr}\{\rho(\Gamma) H(\alpha(\Gamma))\} - \mathrm{Tr}\{\rho(0) H(\alpha(0))\}. \tag{2.10}$$

This clearly makes intuitive sense. However, the idea of a work distribution $\mathbb{P}(w)$ will play a key role later in the results chapter.

2.1.3 Otto Engine with a Landau-Zener Drive in work strokes

In this subsection, we will discuss an Otto engine with non-quasistatic work strokes. During the work strokes, the system is again assumed to be isolated such that no heat exchange with a bath takes place. However, since the work strokes occur in finite time now, the quantum adiabatic theorem does not hold any longer and we

will have general unitary time evolution depending on the drive. To keep things analytically tractable, we will assume a Landau-Zener [38, 39, 47] or linear drive for the work strokes. We assume "perfect and instantaneous thermalisation" [39]. Let the duration of each work stroke be equal to τ. We have the concept of a 'forward' drive and the 'reverse' or 'backward' drive [47]. The energy splitting increases during the 'forward' drive in the first work stroke and reduces back to the initial value in the 'reverse' drive in the second work stroke.
During the first work stroke:

$$H_1(t) = \Theta\sigma_x + vt\sigma_z; \qquad 0 \leq t \leq \tau, \tag{2.11}$$

where Θ is the tunneling constant and v is the 'speed' of the linear drive. The time-evolution operator is denoted by U_{LZ} for this work stroke. During the second work stroke:

$$H_2(t) = H_1(2\tau - t); \qquad \tau \leq t \leq 2\tau \tag{2.12}$$

The time-evolution operator is $\tilde{U}_{LZ}$. The stages A, B, C, D are defined in the same way as before. The state of the system at A and C after thermalisation is just the Gibbs state as we saw in the quasi-static Otto engine case. The states $B(D)$ is obtained by the action of $U_{LZ}(\tilde{U}_{LZ})$ on the states at $A(C)$. The altered schematic for this engine is given by:

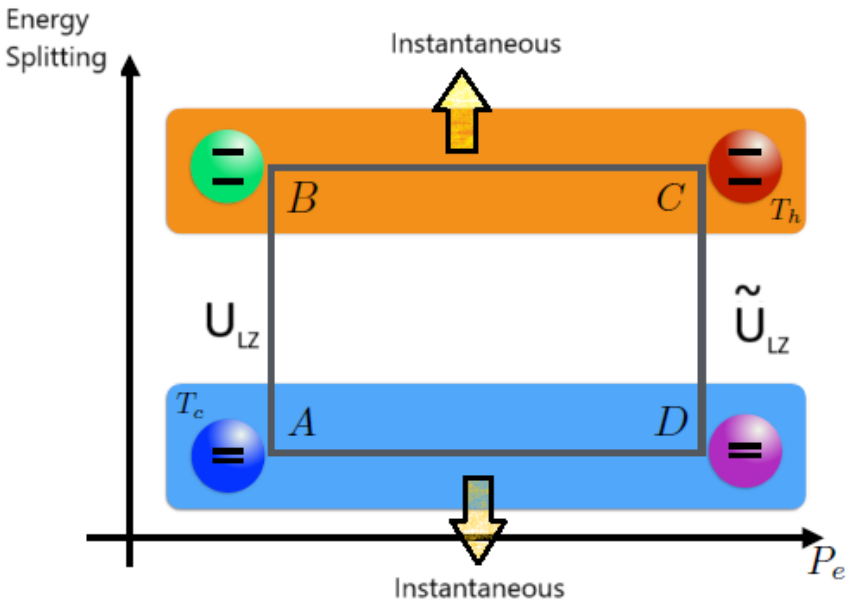

Figure 2.4: Altered schematic from [35] for LZ work strokes

The exact details on calculating U_{LZ} and $\tilde{U}_{LZ}$ can be found in [38, 47] and the work and heat exchange in each stroke can be found in [47, 39]. The results can be summarised as:

Stroke	Work	Heat
A $\rightarrow$ B	$-\Delta_f(1-2P)\tanh\beta_c\Delta_i + \Delta_i\tanh\beta_c\Delta_i$	0
B $\rightarrow$ C	0	$\Delta_f\left[(1-2P)\tanh\beta_c\Delta_i - \tanh\beta_h\Delta_f\right]$
C $\rightarrow$ D	$-\Delta_i(1-2P)\tanh\beta_h\Delta_f + \Delta_f\tanh\beta_h\Delta_f$	0
D $\rightarrow$ A	0	$\Delta_i\left[(1-2P)\tanh\beta_h\Delta_f - \tanh\beta_c\Delta_i\right]$

Figure 2.5: Work and heat exchange for the LZ Otto engine [47, 39]

Here, P is the diabatic transition probability given by $P = e^{-\pi\frac{\Theta^2}{v}}$ and Δ_i is the initial energy splitting given by $\Delta_i = \Theta$ and the Δ_f is the energy splitting at the end of the first work stroke given by $\Delta_f = \sqrt{\Theta^2 + v^2\tau^2}$.
To operate as an engine, we must have
$\langle W\rangle = \langle W_{A\rightarrow B}\rangle + \langle W_{C\rightarrow D}\rangle < 0$, $\langle Q_{B\rightarrow C}\rangle > 0$, $\langle Q_{D\rightarrow A}\rangle < 0$, which imply the fol-

lowing condition [39]:

$$P < \frac{1}{2}\left(1 - \frac{1+r\zeta}{r+\zeta}\right), \tag{2.13}$$

where $r = \frac{\Delta_f}{\Delta_i}$ and $\zeta = \frac{\tanh\beta_h\Delta_f}{\tanh\beta_c\Delta_i}$.
The efficiency of this Otto engine is found to be:

$$\eta_O^{LZ} = \frac{\langle W\rangle}{\langle Q_{in}\rangle} = 1 - \frac{\Delta_i}{\Delta_f}\left[\frac{\tanh\beta_c\Delta_i - (1-2P)\tanh\beta_h\Delta_f}{(1-2P)\tanh\beta_c\Delta_i - \tanh\beta_h\Delta_f}\right] \tag{2.14}$$

In the adiabatic limit ($P \to 0$), we get back the adiabatic Otto engine efficiency. This concludes our discussion on conventional quantum thermodynamics.

2.2 Mathematical Background

Now, we will discuss the mathematics of non-Hermitian Hamiltonians that will be used throughout this thesis to perform calculations. More specifically, first we will discuss the mathematical properties of pseudo-Hermitian Hamiltonians, which are more general than $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians. This discussion will assume time-independence of the metric operator (whose definition will be provided in this section). Mapping of such pseudo-Hermitian Hamiltonians to Hermitian Hamiltonians is also described in detail. An example to illustrate several important concepts is then presented. Next, two mathematical approaches - called the canonical transformation and non-canonical transformations - that are used to study pseudo-Hermitian Hamiltonians with time-dependent metrics are considered.

2.2.1 Pseudo-Hermitian Hamiltonians - The basics

A majority of these results and proofs come from Ali Mostafazadeh's work on Pseudo-Hermitian Hamiltonians[41]. Let's start with the definition of Pseudo-Hermitian operators.

Definition 1 [41] : "Suppose $\mathscr{O}$ is an operator in the Hilbert space $\mathscr{H}$. Then $\mathscr{O}$ is said to be $\mathscr{M}$-pseudo-Hermitian if there exists a Hermitian linear automorphism $\mathscr{M}$ in $\mathscr{H}$ such that $\mathscr{O}^\dagger = \mathscr{M}\mathscr{O}\mathscr{M}^{-1}$". In literature [41, 56], this linear Hermitian automorphism $\mathscr{M}$ is often called the metric operator. For the purposes of this section, we are assuming that $\mathscr{M}$ is time-independent.
We can now consider H in $\mathscr{H}$ that is $\mathscr{M}$-pseudo-Hermitian. Consider a modified definition of the inner-product, which is subsequently shown to be conserved in time.

Definition 2 [41]: "The modified inner-product $\langle\cdot|\cdot\rangle_{\mathscr{M}}$ is defined by:

$$\langle\Psi_1|\Psi_2\rangle_{\mathscr{M}} = \langle\Psi_1|\mathscr{M}|\Psi_2\rangle; \qquad |\Psi_1\rangle, |\Psi_2\rangle \in \mathscr{H} \quad " \tag{2.15}$$

This inner-product definition is indefinite i.e. there are some states that will have zero norm. We will show this subsequently. To see that $\langle\Psi_1|\Psi_2\rangle_{\mathscr{M}}$ is conserved in time, we note that $H^\dagger = \mathscr{M}H\mathscr{M}^{-1}$ and that the Schrödinger equation would imply

$$i\frac{d}{dt}\langle\Psi_1|\Psi_2\rangle_{\mathscr{M}} = \langle\Psi_1|\mathscr{M}H - H^\dagger\mathscr{M}|\Psi_2\rangle = 0. \tag{2.16}$$

If $|\lambda_i\rangle$ and $|\lambda_j\rangle$ are two energy eigenstates of H with energy eigenvalues λ_i and λ_j i.e. $H|\lambda_{i/j}\rangle = \lambda_{i/j}|\lambda_{i/j}\rangle$, then it can be easily shown that

$$\left(\lambda_i^* - \lambda_j\right)\langle\lambda_i|\mathscr{M}|\lambda_j\rangle = 0, \tag{2.17}$$

which immediately means (i) If the energy eigenvalues of two states are purely real, then those energy eigenstates are $\mathscr{M}$-orthogonal. (ii) If the energy eigenvalue of a state is a complex number, then the $\mathscr{M}$-semi-norm of the corresponding energy eigenstate must be zero. This is why the modified inner-product is indefinite.

We will now define the notion of a complete biorthonormal eigenbasis for pseudo-Hermitian Hamiltonians.

Definition 3 [41]: "An $\mathscr{M}$-pseudo-Hermitian Hamiltonian H is said to have a complete biorthonormal eigenbasis $\{|\Psi_n\rangle, |\Phi_n\rangle\}$ if the following conditions are satisfied:

(i) $H|\Psi_n\rangle = E\lambda_n|\Psi_n\rangle, \quad H^\dagger|\Phi_n\rangle = \lambda_n^*|\Phi_n\rangle,$

(ii) $\langle\Phi_m|\Psi_n\rangle = \delta_{mn}$,

(iii) $\sum_n |\Psi_n\rangle\langle\Phi_n| = \sum_n |\Phi_n\rangle\langle\Psi_n| = \mathbb{I}$. "

Here $\{|\Psi_n\rangle\}$ and $\{|\Phi_n\rangle\}$ are called the right and left eigenstates of H respec-

tivey. If H satisfies the above properties, then the eigenvalues are real or occur in complex conjugate pairs as:

$$\begin{aligned} H^{\dagger}\left|\Phi_n\right\rangle = \lambda_n^{*}\left|\Phi_n\right\rangle &\Longrightarrow \mathscr{M}H\mathscr{M}^{-1}\left|\Phi_n\right\rangle = \lambda_n^{*}\left|\Phi_n\right\rangle \\ &\Longrightarrow H\left(\mathscr{M}^{-1}\left|\Phi_n\right\rangle\right) = \lambda_n^{*}\left(\mathscr{M}^{-1}\left|\Phi_n\right\rangle\right). \end{aligned} \tag{2.18}$$

This means $\mathscr{M}^{-1}\left|\Phi_n\right\rangle$ is a right eigenstate of H but with eigenvalue λ_n^{*}. Thus, all the complex eigenvalues occur in complex conjugate pairs. From the above equation, we can also say that if n_0 denotes the eigenstates with a real eigenvalue and n_+, n_- denote eigenstates with positive and negative imaginary parts respectively, then:

$$\left|\Phi_{n_0}\right\rangle = \mathscr{M}\left|\Psi_{n_0}\right\rangle; \qquad \left|\Phi_{n_\pm}\right\rangle = \mathscr{M}\left|\Psi_{n_\mp}\right\rangle. \tag{2.19}$$

The following $\mathscr{M}$-orthonormality conditions also hold:

$$\left\langle\Psi_{n_0}|\Psi_{m_0}\right\rangle_{\mathscr{M}} = \delta_{m_0 n_0}; \qquad \left\langle\Psi_{n_+}|\Psi_{m_-}\right\rangle_{\mathscr{M}} = \delta_{m_+ n_-}. \tag{2.20}$$

Since we have the completeness relation

$$\mathbb{I} = \sum_{n_0}\left|\Psi_{n_0}\right\rangle\left\langle\Phi_{n_0}\right| + \sum_{n_+}\left(\left|\Psi_{n_+}\right\rangle\left\langle\Phi_{n_+}\right| + \left|\Psi_{n_-}\right\rangle\left\langle\Phi_{n_-}\right|\right), \tag{2.21}$$

on multiplying both sides by $\mathscr{M}$ and using (2.19), we can express the metric operator in terms of the left eigenvectors

$$\mathscr{M} = \sum_{n_0}\left|\Phi_{n_0}\right\rangle\left\langle\Phi_{n_0}\right| + \sum_{n_+}\left(\left|\Phi_{n_-}\right\rangle\left\langle\Phi_{n_+}\right| + \left|\Phi_{n_+}\right\rangle\left\langle\Phi_{n_-}\right|\right). \tag{2.22}$$

We now state a theorem of immense importance that will help us connect pseudo-Hermitian Hamiltonians to $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians. The detailed proof is not given here but can be found in [41].

Theorem [41]: "Suppose H is a general non-Hermitian Hamiltonian in $\mathscr{H}$ (not necessarily pseudo-Hermitian). Also suppose that H has a complete set of biorthonormal eigenbasis vectors $\{\left|\Psi_n\right\rangle, \left|\Phi_n\right\rangle\}$. Then H is pseudo-Hermitian only if one of

the following two statements holds true:

(1)H has a completely real eigenspectrum

(2)H has some complex eigenvalues in its spectrum but they all occur in complex conjugate pairs and have the same multiplicity."

An immediate corollary to this theorem shows that $\mathscr{P}\mathscr{T}$-symmetric operators are indeed pseudo-Hermitian.

Corollary [41]: "A $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian H having a complete biorthonormal eigenbasis is pseudo-Hermitian."

Proof [41]: To prove this theorem, we only need to prove that the eigenvalues of a $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian are real or occur in complex conjugate pairs. We are given $[H,\mathscr{P}\mathscr{T}]=0$. Suppose $|\lambda\rangle$ is an eigenstate of H with eigenvalue λ i.e. $H|\lambda\rangle=\lambda|\lambda\rangle$ Then we can define $|\lambda\rangle'=\mathscr{P}\mathscr{T}|\lambda\rangle$. It can be shown that $|\lambda\rangle'$ is also an eigenstate of H as follows:

$$H|\lambda\rangle'=H\mathscr{P}\mathscr{T}|\lambda\rangle=\mathscr{P}\mathscr{T}H|\lambda\rangle=\mathscr{P}\mathscr{T}\lambda|\lambda\rangle=\lambda^*|\lambda\rangle', \tag{2.23}$$

where the linearity of $\mathscr{P}$ and anti-linearity of $\mathscr{T}$ has been invoked in the final step.

Thus, we can equivalently study pseudo-Hermitian Hamiltonians in a variety of situations instead of studying $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians, under the assumption that a complete biorthonormal eigenbasis exists.

2.2.2 Mapping of time-independent $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians to Hermitian Hamiltonians

Suppose that H is a time-independent $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian with a discrete and complete biorthonormal basis $\{|\Psi_n\rangle,|\Phi_n\rangle\}$. Then from the above corollary, H is also pseudo-Hermitian. Thus, H will have a metric operator $\mathscr{M}$ associated to it such that $\mathscr{M}H=H^\dagger\mathscr{M}$. For this discussion, we will restrict to the $\mathscr{P}\mathscr{T}$-unbroken regime of H. In this regime, $\mathscr{M}$ is a positive-definite Hermitian

operator. Hence, it can be expressed as:

$$\mathscr{M} = V^\dagger V, \tag{2.24}$$

where V is some invertible operator. Then, the claim is that the operator $h \equiv VHV^{-1}$ is a Hermitian operator. This was first argued by Mostafazadeh in [57]. To see that h is indeed Hermitian:

$$\mathscr{M}H = H^\dagger \mathscr{M} \Longrightarrow V^\dagger V H = H^\dagger V^\dagger V \Longrightarrow VHV^{-1} = \left(VHV^{-1}\right)^\dagger. \tag{2.25}$$

However, it is important to note that the mapping V is not unique. This is because we can define $V' = UV$ where U satisfies $U^\dagger = U^{-1}$. Then $V'^\dagger V = V^\dagger V = \mathscr{M}$. The resulting Hermitian Hamiltonian obtained from V' is given by $h' = V'HV'^{-1} = UhU^\dagger$. Thus, the resulting Hamiltonians are unitary equivalent and describe the same system in two different bases.
The eigenstates and eigenvalue of h can also be found easily:

$$H\left|\Psi_n\right\rangle = \lambda_n \left|\Psi_n\right\rangle \Longrightarrow h\left(V\left|\Psi_n\right\rangle\right) = \lambda_n \left(V\left|\Psi_n\right\rangle\right). \tag{2.26}$$

Hence, the eigenstates of h are $\left|\psi_n\right\rangle \equiv V\left|\Psi_n\right\rangle$ with eigenvalue λ_n. In general, the relationship between any arbitrary state $\left|\Psi\right\rangle$ in the $\mathscr{P}\mathscr{T}$-symmetric picture and the corresponding state $\left|\psi\right\rangle$ in the Hermitian picture is given by [57] :

$$\left|\psi\right\rangle = V\left|\Psi\right\rangle. \tag{2.27}$$

The eigenstates of h are orthonormal under the Dirac inner product:

$$\left\langle\psi_m|\psi_n\right\rangle = \left\langle\Psi_m\right|\mathscr{M}\left|\Psi_n\right\rangle = \left\langle\Psi_m|\Psi_n\right\rangle_{\mathscr{M}} = \delta_{mn}. \tag{2.28}$$

We can define density operators in the $\mathscr{P}\mathscr{T}$-symmetric picture using (2.27). Since $\rho = \sum_n p_n |\psi_n\rangle \langle\psi_n|$ in the Hermitian picture, we can define [57, 29]:

$$\rho_{\mathscr{P}\mathscr{T}} = V^{-1}\rho V = \sum_n p_n |\Psi_n\rangle \langle\Psi_n| \mathscr{M}, \tag{2.29}$$

as the density operator in the $\mathscr{P}\mathscr{T}$-symmetric picture. This definition also ensures that the trace is unity i.e.

$$\mathrm{Tr}\{\rho_{\mathscr{P}\mathscr{T}}\} = \sum_k \langle\Phi_k| \left(\sum_n p_n |\Psi_n\rangle \langle\Psi_n| \mathscr{M} \right) |\Psi_k\rangle = 1, \tag{2.30}$$

where it's important to note that the trace has been taken with respect to the biorthonormal basis since that is the complete basis in this picture. Now that we studied the mathematical equivalence between the "$\mathscr{P}\mathscr{T}$-symmetric picture" and the "conventional Hermitian picture", let's study the physical equivalence [57, 58]. To calculate the expectation value of H when the system is in state $|\Psi\rangle$, we must use the modified inner product i.e.

$$\langle H\rangle = \langle\Psi|H\Psi\rangle_{\mathscr{M}}, \tag{2.31}$$

we expect this to be equal to the expectation value of h in the corresponding state $|\psi\rangle = V|\Psi\rangle$. This is indeed true:

$$\langle h\rangle = \langle\psi|h|\psi\rangle = \langle\Psi|\mathscr{M}H|\Psi\rangle = \langle H\rangle. \tag{2.32}$$

This also gives us a way to think about general observables $\mathscr{O}$ in the $\mathscr{P}\mathscr{T}$-symmetric picture. We know that observables o in the conventional Hermitian picture are Hermitian operators. Since the two pictures are equivalent, we can set the expectation values to be equal. This will give us a condition on the observables in the

$\mathscr{P}\mathscr{T}$-symmetric picture [57, 29]:

$$\begin{aligned} & \langle\psi|\, o\,|\psi\rangle = \langle\Psi|\mathscr{O}\Psi\rangle_{\mathscr{M}}, \\ \Longrightarrow \quad & \langle\Psi|\, V^{\dagger} o V\,|\Psi\rangle = \langle\Psi|\,\mathscr{M}\mathscr{O}\,|\Psi\rangle \Longrightarrow \quad o = V\mathscr{O}V^{-1}, \\ \Longrightarrow \quad & \mathscr{O}^{\dagger} = \mathscr{M}\mathscr{O}\mathscr{M}^{-1}. \end{aligned} \tag{2.33}$$

Hence, the observables in the $\mathscr{P}\mathscr{T}$-symmetric picture are also $\mathscr{M}$-pseudo-Hermitian. Let's also calculate the expectation values using the density operator method:

$$\langle o\rangle = \mathrm{Tr}\{\rho o\} = \mathrm{Tr}\Big\{\Big(V\rho_{\mathscr{P}\mathscr{T}}V^{-1}\Big)\Big(V\mathscr{O}V^{-1}\Big)\Big\} = \mathrm{Tr}\{\rho_{\mathscr{P}\mathscr{T}}\mathscr{O}\} = \langle O\rangle. \tag{2.34}$$

This serves as another consistency check for all the definitions and the physical equivalence between the two pictures. Let's now consider an example to put the above-discussed formalism to a test.

2.2.3 Example of a time-independent $\mathscr{P}\mathscr{T}$-symmetric qubit

Let us now consider a simple example to understand the utility of the formalism discussed in the previous subsection. This example was first considered in [59], but not from a pseudo-Hermitian standpoint. Consider the experimentally relevant Hamiltonian of a non-Hermitian qubit [5, 11, 12, 10] :

$$H = \begin{pmatrix} i\gamma & \kappa \\ \kappa & -i\gamma \end{pmatrix} = i\gamma\sigma_z + \kappa\sigma_x. \tag{2.35}$$

The $\mathscr{P}$ operator for a two-level system is simply given by σ_x operator while the $\mathscr{T}$ operator is given by the complex-conjugation operation. We find that $[H, \mathscr{P}\mathscr{T}]$ = 0. The eigenvalues are found to be $E_{\pm} = \pm\sqrt{\kappa^2 - \gamma^2}$. Thus, for $|\gamma| < |\kappa|$, we are in the $\mathscr{P}\mathscr{T}$-unbroken regime. Here, the eigenstates will be shown to be $\mathscr{P}\mathscr{T}$-symmetric. For $|\gamma| > |\kappa|$, we are in the $\mathscr{P}\mathscr{T}$-broken regime. Here, we will show the eigenstates are not $\mathscr{P}\mathscr{T}$-symmetric. At $|\gamma| = |\kappa|$, H becomes non-diagonalizable since its determinant becomes zero. This point, separating the sym-

metric and broken phases, is called the exceptional point (EP).

In the $\mathscr{P}\mathscr{T}$-symmetric regime, we first define ς such that $\sin\varsigma = \frac{\gamma}{\kappa}$. The right eigenstates are given by [59, 58]

$$|\Psi_+\rangle = \frac{1}{\sqrt{2\cos\varsigma}}\begin{pmatrix} e^{i\frac{\varsigma}{2}} \\ e^{-i\frac{\varsigma}{2}} \end{pmatrix}; \qquad |\Psi_-\rangle = \frac{i}{\sqrt{2\cos\varsigma}}\begin{pmatrix} e^{-i\frac{\varsigma}{2}} \\ -e^{i\frac{\varsigma}{2}} \end{pmatrix}, \tag{2.36}$$

with eigenvalues $\pm\kappa\cos\varsigma$ respectively. The left eigenstates are given by:

$$|\Phi_+\rangle = \frac{1}{\sqrt{2\cos\varsigma}}\begin{pmatrix} e^{-i\frac{\varsigma}{2}} \\ e^{i\frac{\varsigma}{2}} \end{pmatrix}; \qquad |\Phi_-\rangle = \frac{i}{\sqrt{2\cos\varsigma}}\begin{pmatrix} e^{i\frac{\varsigma}{2}} \\ -e^{-i\frac{\varsigma}{2}} \end{pmatrix}. \tag{2.37}$$

The biorthonormality and completeness relations can be easily verified. We can also easily verify that these eigenstates are $\mathscr{P}\mathscr{T}$-symmetric since $\mathscr{P}\mathscr{T}|\Psi_\pm\rangle = |\Psi_\pm\rangle$ and $\mathscr{P}\mathscr{T}|\Phi_\pm\rangle = |\Phi_\pm\rangle$. The metric operator can be found using (2.22):

$$\mathscr{M} = \begin{pmatrix} \sec\varsigma & -i\tan\varsigma \\ i\tan\varsigma & \sec\varsigma \end{pmatrix}. \tag{2.38}$$

Note that $\langle\Psi_n|\Psi_m\rangle_{\mathscr{M}} = \delta_{mn}$ where $m,n = \pm$. In the Hermitian limit ($\gamma = 0$), we get $|\Psi_+\rangle = |\Phi_+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \end{pmatrix}^T$, $|\Psi_-\rangle = |\Phi_-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \end{pmatrix}^T$ (apart from a global phase) and $\mathscr{M} = \mathbb{I}$ as expected.

Now, let's analyze what happens in the $\mathscr{P}\mathscr{T}$-broken regime ($\gamma > \kappa$). Here, we define the quantity $\cosh\alpha = \frac{\gamma}{\kappa}$ and the eigenvalues are $\pm i\kappa\sinh\alpha$. The right eigenstates are given by:

$$|\Psi_+\rangle_{broken} = \frac{1}{\sqrt{2\sinh\theta}}\begin{pmatrix} e^{\frac{\alpha}{2}} \\ -ie^{-\frac{\alpha}{2}} \end{pmatrix}; \qquad |\Psi_-\rangle_{broken} = \frac{i}{\sqrt{2\sinh\alpha}}\begin{pmatrix} e^{-\frac{\alpha}{2}} \\ -ie^{\frac{\alpha}{2}} \end{pmatrix}. \tag{2.39}$$

The left eigenstates are given by:

$$|\Phi_+\rangle_{broken} = \frac{1}{\sqrt{2\sinh\alpha}}\begin{pmatrix} e^{\frac{\alpha}{2}} \\ ie^{-\frac{\alpha}{2}} \end{pmatrix}; \qquad |\Phi_-\rangle_{broken} = \frac{-i}{\sqrt{2\sinh\alpha}}\begin{pmatrix} e^{-\frac{\alpha}{2}} \\ ie^{\frac{\alpha}{2}} \end{pmatrix}. \tag{2.40}$$

A straightforward calculation shows that $\mathscr{P}\mathscr{T}\,|\Psi_{\pm}\rangle_{broken} \neq |\Psi_{\pm}\rangle_{broken}$ and $\mathscr{P}\mathscr{T}\,|\Phi_{\pm}\rangle_{broken} \neq |\Phi_{\pm}\rangle_{broken}$. Again using (2.22) to find the metric operator in the $\mathscr{P}\mathscr{T}$-broken domain, we find that:

$$\mathscr{M}_{broken} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x. \tag{2.41}$$

As pointed out before, when the eigenvalues are complex, the modified inner-product is indefinite. For example, consider the state $|\xi\rangle = \begin{pmatrix} 1 & 0 \end{pmatrix}^T$. Then if we want to find the norm of this state with the inner product given by $\mathscr{M}_{broken}$:

$$\langle \xi | \xi \rangle_{\mathscr{M}_{broken}} = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0, \tag{2.42}$$

clearly showing that the inner product is indefinite in the $\mathscr{P}\mathscr{T}$-broken regime [58].

2.2.4 Canonical Transformation of time-dependent $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians

We will now discuss the first mathematical approach used to study non-Hermitian Hamiltonians $H(t)$ with a complete biorthonormal basis and time-dependent metric operators $\mathscr{M}(t)$. This was first proposed in [24]. By the Theorem's corollary, $H(t)$ is also pseudo-Hermitian. In this approach [24] "$H(t)$ is assumed to have an extended $\mathscr{P}\mathscr{T}$-symmetry such that at any time t, we have:

$$\mathscr{M}(t)H(t) = H^{\dagger}(t)\mathscr{M}(t)." \tag{2.43}$$

Just like before, in the $\mathscr{P}\mathscr{T}$-unbroken regime, we can express $\mathscr{M}(t)$ as:

$$\mathscr{M}(t) = V^{\dagger}(t)V(t), \tag{2.44}$$

such that $V(t)$ is invertible (note here that $V(t)$ isn't unique). There are a great number of similarities between the time-dependent canonical mapping approach

and the time-independent approach that we discussed earlier. However, there are a few key differences as well. We first provide a compendium of all the similarities. [24, 60]:

	Time-independent approach	Canonical approach
Quasi-Hermiticity relation	$\mathscr{M}H = H^\dagger \mathscr{M}$	$\mathscr{M}(t)H(t) = H^\dagger(t)\mathscr{M}(t)$
Modified Inner Product	$\langle\Psi_1(t)\|\mathscr{M}\|\Psi_2(t)\rangle$	$\langle\Psi_1(t)\|\mathscr{M}(t)\|\Psi_2(t)\rangle$
Hamiltonian mapping	$h = VHV^{-1}$	$h(t) = V(t)H(t)V^{-1}(t)$
State mapping	$\|\psi(t)\rangle = V\|\Psi(t)\rangle$	$\|\psi(t)\rangle = V(t)\|\Psi(t)\rangle$
Condition on observables	$\mathscr{O}^\dagger = \mathscr{M}\mathscr{O}\mathscr{M}^{-1}$	$\mathscr{O}^\dagger(t) = \mathscr{M}(t)\mathscr{O}(t)\mathscr{M}^{-1}(t)$
Density operator defintion	$\rho_{\mathscr{P}\mathscr{T}}(t) = V^{-1}\rho(t)V$	$\rho_{\mathscr{P}\mathscr{T}}(t) = V(t)^{-1}\rho(t)V(t)$

Figure 2.6: Similarities between the two approaches [57, 24]

This approach has been called the canonical mapping approach since it is possible to map the non-Hermitian Hamiltonian (or in fact, any observable) to a a Hermitian operator (observable) using a canonical time-dependent transformation. This automatically ensures that the expectation value of any observable is the same in both pictures. We are following consistent notation where $|\Psi(t)\rangle$ denotes states in the "non-Hermitian picture" and $|\psi(t)\rangle$ denotes states in the "Hermitian picture". We again emphasise that this mapping can only be successfully performed in the $\mathscr{P}\mathscr{T}$-unbroken regime [24, 31] For the remainder of this discussion, we will restrict to the $\mathscr{P}\mathscr{T}$-unbroken regime.

In the time-independent case, we saw that the modified inner product was preserved if the dynamics of the states was governed by the standard TDSE (Time-Dependent Schrödinger Equation). It was shown in [24] that if the modified inner product in the canonical approach is preserved (i.e. 'unitarity' is imposed), then the dynamics isn't given by the TDSE. Thus, if it is demanded:

$$\frac{d}{dt}\langle\Psi_1(t)|\Psi_2(t)\rangle_{\mathscr{M}(t)} = \frac{d}{dt}\langle\Psi_1(t)|\mathscr{M}(t)|\Psi_2(t)\rangle = 0, \tag{2.45}$$

then dynamics of any arbitrary state $|\Psi(t)\rangle$ is determined by [24]:

$$i\frac{d}{dt}|\Psi(t)\rangle = \left(H(t) - \frac{i}{2}\mathscr{M}^{-1}(t)\frac{d}{dt}\mathscr{M}(t)\right)|\Psi(t)\rangle\,. \tag{2.46}$$

This serves as a key difference between the time-independent metric case and the canonical mapping approach.

ain the "Hermitian picture", we get [24]:

$$i\frac{d}{dt}|\psi(t)\rangle = \left[h(t) + \frac{i}{2}\left(\dot{V}(t)V^{-1}(t) - \left(\dot{V}(t)V^{-1}(t)\right)^{\dagger}\right)\right]|\psi(t)\rangle\,, \tag{2.47}$$

Among all the infinite choices for the mapping $V(t)$ satisfying $V^{\dagger}(t)V(t) = \mathscr{M}(t)$, we can define a "proper mapping" [24] $V_p(t)$ such that $\dot{V}_p(t)V_p^{-1}(t) = \left(\dot{V}_p(t)V_p^{-1}(t)\right)^{\dagger}$. Then we have:

$$i\frac{d}{dt}|\psi(t)\rangle = h(t)\,|\psi(t)\rangle\,. \tag{2.48}$$

This allows us to form a stronger mapping between the "$\mathscr{P}\mathscr{T}$-symmetric picture" and the "conventional Hermitian picture" since now $h(t)$ also generates the dynamics. In fact, under this "proper mapping" [24], certain problems in the "$\mathscr{P}\mathscr{T}$-symmetric picture" can be reduced to Hermitian problems. This will also serve as a very useful calculation tool while solving thermodynamic engine efficiency problems in the $\mathscr{P}\mathscr{T}$-symmetric regime.

Since we can canonically transform $H(t)$ in the unbroken regime into $h(t)$ that has real eigenvalues and also generates the time dynamics via the standard Schrödinger equation (2.48), this strongly indicates that the eigenvalues of $h(t)$ and $H(t)$ (they are equal) are indeed the energy eigenvalues. Hence, we can identify the eigenvalues $\lambda_n(t)$ with the eigenenergies $E_n(t)$.

As argued before, we can't make any sense of the $\mathscr{P}\mathscr{T}$-broken regime using this approach. Also note that $H(t)$ does not generate the time-dynamics via the standard time-dependent Schrödinger equation. This is in contrast to what is seen in

several experiments [5, 11]. In the next section, we will see another approach that offers a way to circumvent both these problems.

2.2.5 Non-Canonical Transformation of time-dependent $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians

In this section, an alternative approach to studying time-dependent $\mathscr{P}\mathscr{T}$-Hamiltonians with time-dependent metrics is discussed. This was first put forward in [25]. This approach differs from the earlier approach in terms of the equations governing the dynamics of the states. Moreover, it allows us to study systems even in the $\mathscr{P}\mathscr{T}$-broken regime [61].

This approach assumed [25] that "the dynamics for the non-Hermitian $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians and the conventional Hermitian Hamiltonians is governed by the time-dependent Schrödinger equation:

$$i\frac{d}{dt}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle\,, \quad i\frac{d}{dt}|\psi(t)\rangle = h(t)|\psi(t)\rangle\,. \tag{2.49}$$

Here $H(t) \neq H^{\dagger}(t)$ and $h(t) = h^{\dagger}(t)$." Note that for this approach, the word 'Hamiltonian' is used for operators that generate the dynamics via the TDSE, and not necessarily operators that give the energy eigenvalues. It is further assumed that the states in the two pictures have the following relationship [25] :

$$|\psi(t)\rangle = W(t)|\Psi(t)\rangle\,, \tag{2.50}$$

where $W(t)$ is a time-dependent invertible operator. To keep things clear, a separate energy operator $\mathscr{E}(t)$ will be defined and studied later in this approach. Let's contrast the canonical and non-canonical approach [24, 25]:

	Canonical approach	Non-canonical approach
State mapping	$\|\psi(t)\rangle = V(t)\|\Psi(t)\rangle$	$\|\psi(t)\rangle = W(t)\|\Psi(t)\rangle$
Metric definition	$\mathscr{M}(t) = V^\dagger(t)V(t)$	$\mathscr{W}(t) = W^\dagger(t)W(t)$
Modified Inner Product	$\langle\Psi_1(t)\|\mathscr{M}(t)\|\Psi_2(t)\rangle$	$\langle\Psi_1(t)\|\mathscr{W}(t)\|\Psi_2(t)\rangle$
Quasi-Hermiticity relation	$\mathscr{M}(t)H(t) = H^\dagger(t)\mathscr{M}(t)$	$H^\dagger(t)\mathscr{W}(t) - \mathscr{W}(t)H(t) = i\frac{d}{dt}\mathscr{W}(t)$
Hamiltonian mapping	$h(t) = V(t)H(t)V^{-1}(t)$	$h(t) = W(t)H(t)W^{-1}(t) + i\frac{dW(t)}{dt}W^{-1}(t)$
Condition on observables	$\mathscr{O}^\dagger(t) = \mathscr{M}(t)\mathscr{O}(t)\mathscr{M}(t)$	$\tilde{\mathscr{O}}^\dagger(t) = \mathscr{W}(t)\tilde{\mathscr{O}}(t)\mathscr{W}(t)$
Mapping of observables	$\mathscr{O}(t) = V^{-1}(t)o(t)V(t)$	$\tilde{\mathscr{O}}(t) = W^{-1}(t)o(t)W(t)$
Density operator definition	$\rho_{\mathscr{P}\mathscr{T}}(t) = V^{-1}(t)\rho(t)V(t)$	$\tilde{\rho}_{\mathscr{P}\mathscr{T}}(t) = W^{-1}(t)\rho(t)W(t)$
Energy operator definition	$H(t)$	$\mathscr{E}(t) = W^{-1}(t)h(t)W(t)$

Figure 2.7: Contrasting the canonical and non-canonical approach [24, 25]

Let's note a few things about this approach. The modified inner product defined here is preserved time and thus, we get 'unitary' dynamics. The definition of the observables along with the state mapping and the density operator definition are all mathematically consistent to ensure that expectation values are equal in the non-canonical "non-Hermitian picture" and the "Hermitian picture".

From the above equations, it becomes clear that $H(t)$ is a "non-observable" [25] in this approach. Thus, its eigenvalues do not give the energies. However, a closely related energy operator has been defined in the last row of Figure 2.7. We further find [25]:

$$\mathscr{E}(t) = H(t) + iW^{-1}(t)\dot{W}(t) \neq H(t) \tag{2.51}$$

Note that this is different from the Hamiltonian of the system since it does not generate the time evolution. In direct contrast to the previous approach, this approach treats the non-Hermitian Hamiltonian $H(t)$ as a non-observable i.e. its eigenvalues are not the eigenenergies of the system [25]. This is not an issue since there is no underlying physical reason to believe that the non-Hermitian Hamiltonian should be an observable quantity. Having a separate energy operator in this approach also offers the advantage of 'mending' the $\mathscr{P}\mathscr{T}$-broken [61] and making more sense

of it. Thus, on performing projective energy measurements in the two-time measurement approach, the system collapses into one of the eigenstates of $\mathscr{E}(t)$ and not $H(t)$.

Chapter 3

Results

In this chapter, we present the results of applying both these approaches to two thermodynamic problems, namely the Jarzynski equality [32] and the Otto engine efficiency. In the first section, we use the canonical approach to find the efficiency of a $\mathscr{PT}$-symmetric qubit undergoing an Otto cycle. The second section will discuss results related to the proof of the Jarzynski equality in the non-canonical approach, specifically in the $\widetilde{\mathscr{PT}}$-unbroken regime, whose meaning is also explained here. Next, the non-canonical approach is used to find the efficiency of an analytically tractable model of a $\mathscr{PT}$-symmetric qubit [61] undergoing an Otto cycle.

3.1 Results from canonical approach

3.1.1 $\mathscr{P}\mathscr{T}$-symmetric qubit Otto Engine

In this section, we will present our results on attempting to use the canonical approach to run an Otto engine for a $\mathscr{P}\mathscr{T}$-symmetric qubit. The model we will be using is:

$$H(t) = \begin{pmatrix} i\lambda(t) & 1 \\ 1 & -i\lambda(t) \end{pmatrix} = i\lambda(t)\sigma_z + \sigma_x, \tag{3.1}$$

where $\lambda(t)$ is an externally controlled time-dependent drive. This simple model has been investigated in various experimental [11, 12, 10, 62, 63] and theoretical [31, 29, 34, 64] studies. Since we are using the canonical approach, the energy eigenvalues are given by the eigenvalues of the Hamiltonian:

$$E_{\pm}(t) = \pm\sqrt{1-\lambda^2(t)}. \tag{3.2}$$

As we will restrict ourselves to the $\mathscr{P}\mathscr{T}$-unbroken regime, we will always have $|\lambda(t)| < 1$ at all instants of time. The work strokes of the Otto engine will be 'unitary' in the sense the modified inner product will be preserved. We also assume perfect thermalisation with the bath. But now, the concept of a Gibbs state needs to be thought about more carefully. When discussing the canonical transformation approach for systems with a time-dependent metric, results related to a "proper transformation" [24] were discussed, which said that there exists a "proper transformation" $V_p(t)$ such that the canonically transformed $h_p(t) = V_p(t)H(t)V_p^{-1}(t)$ also generates the time-dynamics of the states via (2.48). It was argued that this "proper transformation" established a stronger physical correspondence between the two pictures. Thus, to define the Gibbs state for the $\mathscr{P}\mathscr{T}$-symmetric picture at some inverse temperature β, we assume that the correspondingly mapped density operator in the Hermitian picture is given by:

$$\rho^{eq} = \frac{e^{-\beta h_p}}{Z}, \tag{3.3}$$

which means by

$$\rho^{eq}_{\mathscr{P}\mathscr{T}} = V_p^{-1}\rho^{eq}V_p = \frac{e^{-\beta H}}{Z}, \tag{3.4}$$

where h_p is the properly mapped Hermitian Hamiltonian at some appropriate instant of time. Furthermore, it is also assumed that thermalisation happens perfectly and instantaneously. The immediate task at hand then becomes calculating the metric $\mathscr{M}(t)$ and "proper transformation" $V_p(t)$ for the model considered in (3.1). The metric can be calculated quite easily following similar steps that led us to (2.38) in the example discussed in the previous chapter. We find:

$$\mathscr{M}(t) = \begin{pmatrix} \sec\Upsilon(t) & -i\tan\Upsilon(t) \\ i\tan\Upsilon(t) & \sec\Upsilon(t) \end{pmatrix}, \tag{3.5}$$

where $\sin\Upsilon(t) = \lambda(t)$. The "proper mapping" [24] $V_p(t)$ is found to be:

$$V_p(t) = \frac{1}{\sqrt{\cos(\Upsilon(t))}} \begin{pmatrix} i\sin\frac{\Upsilon(t)}{2} & \cos\frac{\Upsilon(t)}{2} \\ \cos\frac{\Upsilon(t)}{2} & -i\sin\frac{\Upsilon(t)}{2} \end{pmatrix}, \tag{3.6}$$

and the properly mapped Hermitian Hamiltonian $h_p(t)$ is found to be:

$$h_p(t) = V_p(t)H(t)V_p^{-1}(t) = \cos\Upsilon(t)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sqrt{1-\lambda^2(t)}\sigma_x. \tag{3.7}$$

Since the properly mapped Hermitian Hamiltonian takes such a simple form, we can do all our calculations in the Hermitian picture. We can do this as we have already shown the equivalence of dynamics and the expectation value of observables in both pictures. The time-evolution operator in the "Hermitian picture" is given by:

$$U(t_1,t_2) = e^{-i\int_{t_1}^{t_2} h_p(s)ds} = \begin{pmatrix} \cos\varphi(t_1,t_2) & -i\sin\varphi(t_1,t_2) \\ -i\sin\varphi(t_1,t_2) & \cos\varphi(t_1,t_2) \end{pmatrix}, \tag{3.8}$$

where $\varphi(t_1,t_2)=\int_{t_1}^{t_2}\sqrt{1-\lambda^2(s)}ds$. Now, we have all the ingredients to construct an Otto engine. Suppose that at $t=0$, the system is connected to a cold thermal bath at temperature $T_c=1/\beta_c$. Also, $\lambda(0)=\lambda_i$. Let's call this stage of the engine A. The density operator in the Hermitian picture is given by (3.3):

$$\rho^A=\frac{e^{-\beta_c h_p(0)}}{Z_c}=\frac{e^{-\beta_c\sqrt{1-\lambda_i^2}}}{Z_c}\left|\psi_+\right\rangle\left\langle\psi_+\right|+\frac{e^{\beta_c\sqrt{1-\lambda_i^2}}}{Z_c}\left|\psi_-\right\rangle\left\langle\psi_-\right|, \tag{3.9}$$

where $Z_c=\mathrm{Tr}\left\{e^{-\beta_c h_p(0)}\right\}=2\cosh\sqrt{1-\lambda_i^2}$ and $\left|\psi_\pm\right\rangle$ are the eigenstates of $h_p(0)$, which are given by:

$$\left|\psi_\pm\right\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \pm1\end{pmatrix}. \tag{3.10}$$

Note that these are independent of time. The energy of this state can be calculated as:

$$\langle E_A\rangle=\mathrm{Tr}\left\{\rho^A h_p(0)\right\}=-\sqrt{1-\lambda_i^2}\tanh\beta_c\sqrt{1-\lambda_i^2}. \tag{3.11}$$

Then the first stroke ($A\to B$) of the Otto engine is the compression stroke. Suppose that the duration of this stroke is τ. Let $\lambda(\tau)=\lambda_f$ where $\lambda_f>\lambda_i$. Unitary dynamics is assumed in the work strokes just like the Landau-Zener Otto engine example considered in the previous chapter. This is because the system is considered to be isolated from the external reservoirs. As a result, the density operator at the end of the work stroke is found to be:

$$\rho^B=U(0,\tau)\rho^A U^\dagger(0,\tau)=\frac{e^{-\beta_c\sqrt{1-\lambda_i^2}}}{Z_c}\left|\psi_+\right\rangle\left\langle\psi_+\right|+\frac{e^{\beta_c\sqrt{1-\lambda_i^2}}}{Z_c}\left|\psi_-\right\rangle\left\langle\psi_-\right|, \tag{3.12}$$

which is in fact equal to ρ_A. Due to the simple form of the properly mapped $h_p(t)$ (3.7), the populations do not change even for arbitrary time-dependent drives $\lambda(t)$. When the time evolution operator (3.8) acts on the eigenstates $\left|\psi_\pm\right\rangle$, they only develop a global phase which gets cancelled while writing the density operator.

The energy of this state can be calculated as:

$$\langle E_B \rangle = \mathrm{Tr}\{\rho^B h_p(\tau)\} = -\sqrt{1-\lambda_f^2}\tanh\beta_c\sqrt{1-\lambda_i^2}. \tag{3.13}$$

In the process $B \to C$, the system is connected to a hot thermal reservoir at temperature $T_h = 1/\beta_h$ while the Hamiltonian is kept fixed. We emphasise again that the duration of this thermalising stroke is assumed to be negligible. We get:

$$\rho^C = \frac{e^{-\beta_h h_p(\tau)}}{Z_h} = \frac{e^{-\beta_h\sqrt{1-\lambda_f^2}}}{Z_h}|\psi_+\rangle\langle\psi_+| + \frac{e^{\beta_h\sqrt{1-\lambda_f^2}}}{Z_h}|\psi_-\rangle\langle\psi_-|, \tag{3.14}$$

where $Z_h = 2\cosh\beta_h\sqrt{1-\lambda_f^2}$. The energy of this state is:

$$\langle E_C \rangle = \mathrm{Tr}\Big\{\rho^C h_p(\tau)\Big\} = -\sqrt{1-\lambda_f^2}\tanh\beta_h\sqrt{1-\lambda_f^2}. \tag{3.15}$$

The third stroke ($C \to D$) is the expansion stroke. Again, unitary dynamics take place in this stroke and the duration is τ again. By the end of this work stroke, the value of the drive parameter is brought back to the initial value i.e. $\lambda(2\tau) = \lambda_i$. This also means that the Hamiltonian is reset by the end of this stroke:
$h_p(2\tau) = h_p(0)$. We finally get:

$$\rho^D = U(\tau,2\tau)\rho^C U^\dagger(\tau,2\tau) = \frac{e^{-\beta_h\sqrt{1-\lambda_f^2}}}{Z_h}|\psi_+\rangle\langle\psi_+| + \frac{e^{\beta_h\sqrt{1-\lambda_f^2}}}{Z_h}|\psi_-\rangle\langle\psi_-|, \tag{3.16}$$

which is in fact equal to ρ^C. The energy of this state is:

$$\langle E_D \rangle = \mathrm{Tr}\{\rho^D h_p(2\tau)\} = -\sqrt{1-\lambda_i^2}\tanh\beta_h\sqrt{1-\lambda_f^2}. \tag{3.17}$$

In the final stroke $D \to A$, the cycle is completed by connecting the system to the initial thermal reservoir while the Hamiltonian is kept fixed. This returns the system to the initial state ρ_A.

The work in the compression stroke is:

$$\begin{aligned}\langle W_1\rangle &= \langle E_B\rangle - \langle E_A\rangle, \\ &= \tanh\beta_c\sqrt{1-\lambda_i^2}\left(\sqrt{1-\lambda_i^2}-\sqrt{1-\lambda_f^2}\right).\end{aligned} \tag{3.18}$$

The heat exchange in the isochoric heating stroke is:

$$\begin{aligned}\langle Q_h\rangle &= \langle E_C\rangle - \langle E_B\rangle, \\ &= -\sqrt{1-\lambda_f^2}\left(\tanh\beta_h\sqrt{1-\lambda_f^2}-\tanh\beta_c\sqrt{1-\lambda_i^2}\right).\end{aligned} \tag{3.19}$$

The work in the expansion stroke is:

$$\begin{aligned}\langle W_2\rangle &= \langle E_D\rangle - \langle E_C\rangle, \\ &= \tanh\beta_h\sqrt{1-\lambda_f^2}\left(\sqrt{1-\lambda_f^2}-\sqrt{1-\lambda_i^2}\right).\end{aligned} \tag{3.20}$$

The heat exchange in the isochoric cooling stroke is:

$$\begin{aligned}\langle Q_c\rangle &= \langle E_A\rangle - \langle E_D\rangle, \\ &= -\sqrt{1-\lambda_i^2}\left(\tanh\beta_c\sqrt{1-\lambda_i^2}-\tanh\beta_h\sqrt{1-\lambda_f^2}\right).\end{aligned} \tag{3.21}$$

The net work output is given by:

$$\begin{aligned}\langle W_{out}\rangle &= -\left(\langle W_1\rangle + \langle W_2\rangle\right) \\ &= \left(\sqrt{1-\lambda_i^2}-\sqrt{1-\lambda_f^2}\right)\times\left(\tanh\beta_c\sqrt{1-\lambda_i^2}-\tanh\beta_h\sqrt{1-\lambda_f^2}\right)\end{aligned} \tag{3.22}$$

We demand $\langle W_{out}\rangle > 0$ for engine operation implying:

$$\sqrt{\frac{1-\lambda_i^2}{1-\lambda_f^2}} > \frac{T_c}{T_h}. \tag{3.23}$$

We can now calculate the efficiency:

$$\eta = \frac{\langle W_{out} \rangle}{\langle Q_h \rangle} = 1 - \sqrt{\frac{1-\lambda_i^2}{1-\lambda_f^2}}. \tag{3.24}$$

The result we have obtained is very similar to the result (2.7) for the adiabatic Otto engine discussed for a standard Hermitian qubit. However, a key difference is that the external drive is not varied quasi-statically in this case. Thus, using the canonical transformation approach, we have found that for the $\mathscr{P}\mathscr{T}$-symmetric qubit model (3.1) considered here in the unbroken phase, the efficiency for an Otto engine with arbitrary time-dependent drives $\lambda(t)$ is just equal to the adiabatic Otto engine efficiency. Thus, the details of the drive in the work strokes do not matter at all. However, we believe that this is a result of the simple model that we have chosen and is not going to hold true for other more complicated $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians. Anyhow, using (3.23), it is straightforward to see that this Otto engine efficiency will always be less than the Carnot efficiency.

An obvious limitation of the canonical approach is that we are completely restricted to the $\mathscr{P}\mathscr{T}$-unbroken regime. Moreover, using this approach, it is theoretically impossible to explore what happens when some of the strokes happen across the exceptional point in the $\mathscr{P}\mathscr{T}$-broken to get any advantage in efficiency, as it has been investigated in experiments [65]. This motivates the study of the non-canonical approach in which it is possible to access parts of $\mathscr{P}\mathscr{T}$-broken regime.

3.2 Results from non-canonical approach

3.2.1 Jarzynski equality in the $\widetilde{\mathscr{P}\mathscr{T}}$-unbroken regime

The Jarzynski equality is one of the most fundamental results in non-equilibrium thermodynamics. It says that for an isothermal process happening at inverse temperature β, the non-equilibrium work W (which is a fluctuating quantity) done in

finite time is related via an *equality* with the free energy difference ΔF (i.e. work done quasi-statically) as follows:

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}, \tag{3.25}$$

where "the average $\langle \cdot \rangle$ is over an ensemble of finite-time non-equilibrium realisations of the process" [31]. Analogues of the Jarzynski equality also hold for closed quantum systems undergoing unitary dynamics where the work is defined using the two-time measurement approach [33]. Moreover, the Jarzynski equality also holds for $\mathscr{P}\mathscr{T}$-symmetric [34] and pseudo-Hermitian systems [31] using the canonical approach as long as the spectrum is purely real.

In this subsection, we will present results related to the proof of the Jarzynski equality in non-Hermitian systems using the non-canonical approach in *certain* parametric regimes. In the last section, we discussed the result that the Jaryznski equality holds in the $\mathscr{P}\mathscr{T}$-unbroken phase and this followed the canonical approach. However, using the non-canonical approach, it becomes possible to extend the validity of the Jaryznski equality even to certain parts of the $\mathscr{P}\mathscr{T}$-broken regime.

Let's now elaborate on what we mean by this. In the non-canonical approach, $H(t)$ only determines the time evolution via (2.49), while the energy operator $\mathscr{E}(t)$ determines the energy eigenvalues and energy eigenstates. As usual, we suppose that $H(t)$ is $\mathscr{P}\mathscr{T}$-symmetric, and some parameters control whether the eigenvalues of $H(t)$ are real or not. However, since the energy operator has completely different eigenvalues, there are situations possible in which the system is in the $\mathscr{P}\mathscr{T}$-broken regime but the energy eigenvalues are real. Conversely, it is also possible that the system is in the $\mathscr{P}\mathscr{T}$-unbroken regime but the energy eigenvalues are complex.

To identify whether the eigenvalues of $\mathscr{E}(t)$ are real or complex, another symme-

try, called the $\widetilde{\mathscr{P}\mathscr{T}}$-symmetry is introduced [61] such that:

$$\left[\mathscr{E}(t), \widetilde{\mathscr{P}\mathscr{T}}\right] = 0 \tag{3.26}$$

Note that $\widetilde{\mathscr{P}\mathscr{T}}$ does not have the same nice physical interpretation of space-reflection and time-reversal. However, it is still an anti-linear symmetry of the energy operator. In general, we have $\left[H(t), \widetilde{\mathscr{P}\mathscr{T}}\right] \neq 0$ and $[\mathscr{E}(t), \mathscr{P}\mathscr{T}] \neq 0$. For a detailed discussion on how to calculate $\widetilde{\mathscr{P}\mathscr{T}}$, refer to [61].

The remainder of this subsection is dedicated to proving the validity of the Jarynzki equality in the $\widetilde{\mathscr{P}\mathscr{T}}$-unbroken regime. The Hamiltonians in the non-canonical approach are given by $H(\alpha(t))$ and $h(\alpha(t))$ in accordance with the notational convention of (2.49). We will assume that the system is in the $\widetilde{\mathscr{P}\mathscr{T}}$-unbroken regime which implies that the energy eigenvalues are real. The system is assumed to be isolated from the external environment resulting in 'unitary' work strokes. The duration of the entire process is Γ. The two-time measurement scheme is used. We can do this because, as mentioned before, the physical energies of the system are given by the eigenvalues of $h(\alpha(t))$ or equivalently $\mathscr{E}(t)$ (since they are related by a similarity transform). Thus, any projective measurement of the energy collapses the system into one of the eigenstates of the $\mathscr{E}(t)$ when viewed in the "non-Hermitian picture". Since the system is isolated from the environment, the time-evolution between two projective measurements is 'unitary' i.e. the modified inner product is conserved in the "non-Hermitian picture". Hence, we can use the two-time measurement approach even in the non-canonical case. The states in the "Hermitian picture" and the "non-Hermitian picture" are related by (2.50) i.e.

$$|\psi(t)\rangle = W(t)\,|\Psi(t)\rangle\,, \tag{3.27}$$

such that $\mathscr{W}(t) = W^{\dagger}(t)W(t)$. The time-evolution operator governing the dynamics of states in the "non-Hermitian picture" is formally given by:

$$\tilde{U}(t_f,t_i) = e^{-i\int_{t_i}^{t_f} H(\alpha(s))ds}; \quad \left|\Psi(t_f)\right\rangle = \tilde{U}(t_f,t_i)\left|\Psi(t_i)\right\rangle, \tag{3.28}$$

while the time-evolution operator governing the dynamics of the states in the "Hermitian picture" is given by:

$$u(t_f,t_i) = e^{-i\int_{t_i}^{t_f} h(\alpha(s))ds}; \quad \left|\psi(t_f)\right\rangle = u(t_f,t_i)\left|\psi(t_i)\right\rangle, \tag{3.29}$$

By combining equations (3.27), (3.28) and (3.29), we find:

$$\tilde{U}(t_f,t_i) = W^{-1}(t_f)u(t_f,t_i)W(t_i), \tag{3.30}$$

which has also been stated in [25]. Suppose that for $t < 0$, the system was connected to a thermal reservoir at temperature $T = 1/\beta$. The initial state in the "Hermitian picture" is given by:

$$\rho(0) = \frac{e^{-\beta h(\alpha(0))}}{Z_0} = \frac{1}{Z_0}\sum_n e^{-\beta E_n(0)}\left|\psi_n(0)\right\rangle\left\langle\psi_n(0)\right|, \tag{3.31}$$

where $Z_0 = \mathrm{Tr}\left\{e^{-\beta h(\alpha(0))}\right\}$. For simplicity, we assume that $h(\alpha(t))$ (and equivalently, the non-Hermitian energy operator $\mathscr{E}(t)$) have a discrete and non-degenerate spectrum with the energy eigenstates being $\{|\psi_n(t)\rangle\}$ and corresponding energy eigenvalues being $\{E_n(t)\}$. This means the partition function $Z_0 = \sum_n E_n(0)$. The density operator in the "non-Hermitian picture" is given by:

$$\tilde{\rho}(0) = W^{-1}(0)\rho(0)W(0) = \frac{1}{Z_0}\sum_n \left|\Psi_n(0)\right\rangle\left\langle\Psi_n(0)\right|\mathscr{W}(0), \tag{3.32}$$

where $|\Psi_n(t)\rangle$ are the eigenstates of $\mathscr{E}(t)$. To calculate the average of the exponential work, we first need to find the transition probability p_{nm}, which is the probability of the specific transition $|\Psi_n(0)\rangle \to |\Psi_m(\Gamma)\rangle$. Note that p_{nm} can be

expressed as the product of finding the system in state $|\Psi_n(0)\rangle$ at $t=0$, multiplied by the probability of finding the system in state $|\Psi_m(\Gamma)\rangle$ at $t=\Gamma$ given the state at the initial time was $|\Psi_n(0)\rangle$. This can be mathematically expressed as:

$$\begin{aligned} p_{nm} &= \frac{e^{-\beta E_n(0)}}{Z_0} \times |\langle \Psi_m(\Gamma)| \tilde{U}(\Gamma,0) |\Psi_n(0)\rangle_{\mathscr{W}(\Gamma)}|^2, \\ &= \frac{e^{-\beta E_n(0)}}{Z_0} \times |\langle \Psi_m(\Gamma)| \mathscr{W}(\Gamma) \tilde{U}(\Gamma,0) |\Psi_n(0)\rangle|^2. \end{aligned} \tag{3.33}$$

Using equations (3.27) and (3.30), we can substitute $|\Psi_n(0)\rangle = W^{-1}(0)|\psi_n(0)\rangle$, $|\Psi_m(\Gamma)\rangle = W^{-1}(\Gamma)|\psi_m(\Gamma)\rangle$ and $\tilde{U}(\Gamma,0) = W^{-1}(\Gamma)u(\Gamma,0)W(0)$ to obtain:

$$p_{nm} = \frac{e^{-\beta E_n(0)}}{Z_0} \times |\langle \psi_m(\Gamma)| u(\Gamma,0) |\psi_n(0)\rangle|^2. \tag{3.34}$$

Now we can calculate the average of the exponentiated work $\langle e^{-\beta w}\rangle$:

$$\langle e^{-\beta w}\rangle = \sum_{n,m} e^{-\beta w_{nm}} p_{nm}, \tag{3.35}$$

where we are summing over all possible transitions and the energy change in a particular transition is given by $w_{nm} = E_m(\Gamma) - E_n(0)$. On substituting (3.34) in (3.35), we find:

$$\begin{aligned} \langle e^{-\beta w}\rangle &= \frac{1}{Z_0}\sum_{n,m} e^{-\beta E_m(\Gamma)} |\langle \psi_m(\Gamma)| u(\Gamma,0) |\psi_n(0)\rangle|^2, \\ &= \frac{1}{Z_0}\sum_{n,m} e^{-\beta E_m(\Gamma)} \langle \psi_m(\Gamma)| u(\Gamma,0) |\psi_n(0)\rangle \langle \psi_n(0)| u^\dagger(\Gamma,0) |\psi_m(\Gamma)\rangle, \\ &= \frac{1}{Z_0}\sum_{n,m} e^{-\beta E_m(\Gamma)} \langle \psi_m(\Gamma)| u(\Gamma,0)u^\dagger(\Gamma,0) |\psi_m(\Gamma)\rangle, \\ &= \frac{1}{Z_0}\sum_{m} e^{-\beta E_m(\Gamma)} = \frac{Z_\Gamma}{Z_0}, \\ &= e^{-\beta \Delta F}, \end{aligned} \tag{3.36}$$

where we have used the completeness of the energy eigenstates in the "Hermitian picture" and that $u^{\dagger}(\Gamma,0) = u^{-1}(\Gamma,0)$. As stated before, $F = -\frac{1}{\beta}\ln Z$. Thus, we have been able to show that the Jarzynski equality holds in the $\widetilde{\mathscr{P}\mathscr{T}}$-unbroken regime using the non-canonical approach. This allows us to extend the Jarzynski equality to certain parametric portions of the $\mathscr{P}\mathscr{T}$-broken regime. We note that there are some similarities in the above derivation with the example taken in [60].

3.2.2 Analytically tractable model

We will now consider an analytically tractable example that was first studied in [61] to verify the Jarzynski equality in the $\mathscr{P}\mathscr{T}$-broken regime. The Hamiltonian is:

$$H(t) = -\frac{1}{2}\left(\omega\mathbb{I} + \gamma\alpha(t)\sigma_z + i\alpha(t)\sigma_x\right), \tag{3.37}$$

with the eigenvalues of this Hamiltonian being:

$$\lambda_{\pm}(t) = -\frac{1}{2}\omega \pm \frac{1}{2}\alpha(t)\sqrt{\gamma^2 - 1}, \tag{3.38}$$

which are not the eigenenergies of the system. The system is in the $\mathscr{P}\mathscr{T}$-unbroken regime for $|\gamma| > 1$ and in the $\mathscr{P}\mathscr{T}$-broken regime for $|\gamma| < 1$.
As seen in [66, 61], it is easier to solve for $W(t)$ if some pre-selected form for $h(t)$ is chosen. For the purposes of this problem, the form of $h(t)$ was chosen to be:

$$h(t) = -\frac{1}{2}\left(\omega\mathbb{I} + \Lambda(t)\sigma_z\right), \tag{3.39}$$

where the function $\Lambda(t)$ needs to be determined by solving the non-canonical quasi-Hermiticity relation. On doing this calculation (detailed in [61]), it was found that:

$$\Lambda(t) = \frac{\alpha(t)}{\zeta(t)}, \tag{3.40}$$

where $\zeta(t) = c_1\cosh\Xi(t) + c_2\sinh\Xi(t) \pm \sqrt{c_1^2 - c_2^2 - 1/(1-\gamma^2)}$ and $\Xi(t) = \sqrt{1-\gamma^2}\int_0^t \alpha(s)ds$. Here the constants c_1, c_2 need to be determined from

the initial conditions like the initial energy eigenvalues. The operator $W(t)$, which is assumed to be Hermitian in this case, is found to be:

$$W(t) = \sqrt{\zeta(t)}\mathbb{I} + \frac{\tilde{\zeta}(t)\sqrt{1-\gamma^2}}{\sqrt{\zeta(t)}}\sigma_x + \frac{1-\gamma\zeta(t)}{\sqrt{\zeta(t)}}\sigma_y, \tag{3.41}$$

where $\tilde{\zeta}(t) = c_1 \sinh\Xi(t) + c_2 \cosh\Xi(t)$. Since $W(t)$ must be an invertible operator, we must $\det\{W(t)\} \equiv \pm 2\delta \neq 0$, which implies the condition:
$\delta = \gamma + (1-\gamma^2)\sqrt{c_1^2 - c_2^2 - 1/(1-\alpha^2)} \neq 0$. The energy operator $\mathscr{E}(t)$ is found to be:

$$\mathscr{E}(t) = -\frac{1}{2}\left[\omega\mathbb{I} + \frac{\alpha(t)}{\delta}\left(i(\gamma\zeta(t)-1)\sigma_x + i(\tilde{\zeta}(t)\sqrt{1-\gamma^2})\sigma_y + (\zeta(t)-\delta)\sigma_z\right)\right]. \tag{3.42}$$

The eigenvalues of this operator are the energy eigenvalues and as expected, they are found to be equal to the eigenvalues of $h(t)$ in (3.38):

$$E_{\pm}(t) = -\frac{1}{2}(\omega + \Lambda(t)) = -\frac{1}{2}\left(\omega + \frac{\alpha(t)}{\zeta(t)}\right). \tag{3.43}$$

To find the $\widetilde{\mathscr{P}\mathscr{T}}$-unbroken regime, we only need to find when the function $\Lambda(t) \in \mathbb{R}$. For $|\gamma| > 1$ ($\mathscr{P}\mathscr{T}$-unbroken regime), this happens when $c_1 \in \mathbb{R}, c_2 \in i\mathbb{R}$. For $|\gamma| < 1$ ($\mathscr{P}\mathscr{T}$-broken regime), this happens when $c_1, c_2 \in \mathbb{R}$ and $c_1^2 > c_2^2 + 1/(1-\gamma^2)$. The exact expressions for the $\widetilde{\mathscr{P}\mathscr{T}}$ operator, as well as the energy eigenstates in both Hermitian and non-Hermitian picture have also been calculated in [61], but these will not be required for our discussion.

We will now use this example to illustrate the validity of the Jarzynski equality in the $\widetilde{\mathscr{P}\mathscr{T}}$-unbroken regime. To do this, we choose a linear drive in $\alpha(t)$ with a total duration Γ. The expression of the drive is:

$$\alpha(t) = \alpha_i + \frac{\alpha_f - \alpha_i}{\Gamma}t. \tag{3.44}$$

For our example, we will set $\gamma = 0.5, \omega = 1, \alpha = 0.1, c_1 = 4, c_2 = 1, \Gamma = 1, \beta = 1$ and α_f is kept variable but always $\alpha_f > \alpha_i$. These set of parameters ensure the system is always in the $\mathscr{PT}$-broken regime but still in the $\widetilde{\mathscr{PT}}$-unbroken regime. For isothermal processes, we have according to the second law of thermodynamics:

$$\langle w \rangle \geq \Delta F, \tag{3.45}$$

Thus, one of the first checks we do is to investigate the quantity $\langle W_{irr} \rangle \equiv \langle w \rangle - \Delta F$ numerically, and check if it is greater than zero for different values of α_f. We find:

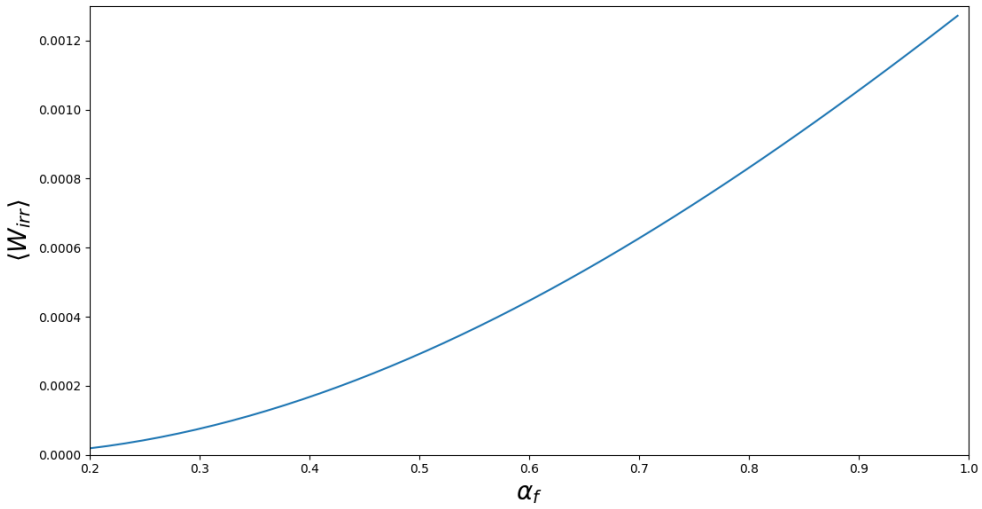

Figure 3.1: The quantity $\langle W_{irr} \rangle$ is always positive. Parameter values: $\gamma = 0.5, \omega = 1, \alpha = 0.1, c_1 = 4, c_2 = 1, \Gamma = 1, \beta = 1$

Here, $0.2 \leq \alpha_f \leq 0.99$. As expected, we indeed find that the quantity is always positive and in fact, $\langle W_{irr} \rangle$ increases as α_f increases. Finally, we can calculate the quantity $\langle e^{-\beta(w-\Delta F)} \rangle$ numerically. We obtain:

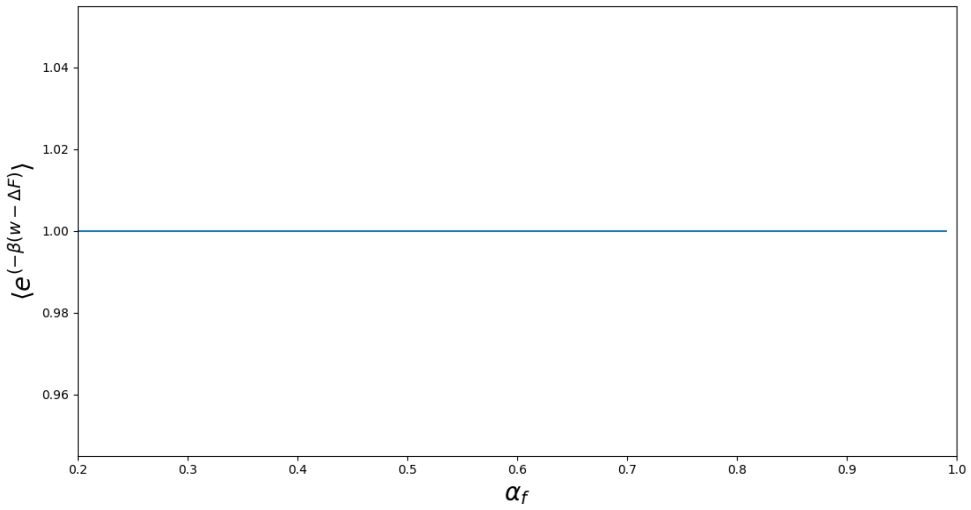

Figure 3.2: The Jarzynski equality is satisfied since $\langle e^{-\beta(w-\Delta F)} \rangle = 1$ for all values of α_f. Parameter values: $\gamma = 0.5, \omega = 1, \alpha = 0.1, c_1 = 4, c_2 = 1, \Gamma = 1, \beta = 1$

which gives a direct verification of the results we already derived in the previous subsection. Thus, we have explicitly shown the validity of the proof in the previous subsection using a numerical example.

3.2.3 Example of Otto Engine in the non-canonical approach

In this subsection, we will discuss results related to constructing an Otto engine using the non-canonical approach. We will use the same analytically tractable model of a two-level system that we had considered before as the working medium:

$$H(t) = -\frac{1}{2}\left(\omega\mathbb{I} + \gamma\alpha(t)\sigma_z + i\alpha(t)\sigma_x\right), \tag{3.46}$$

and the corresponding Hermitian Hamiltonian being:

$$h(t) = -\frac{1}{2}\left(\omega\mathbb{I} + \Lambda(t)\sigma_z\right) = -\frac{1}{2}\left(\omega\mathbb{I} + \frac{\alpha(t)}{\zeta(t)}\sigma_z\right), \tag{3.47}$$

with $\zeta(t)$ defined as before. We assume the system is in the $\widetilde{\mathscr{P}\mathscr{T}}$-unbroken phase so that the energy eigenvalues are purely real. The energy operator $\mathscr{E}(t)$ is given

by (3.42). Moreover, the energy eigenvalues are given by:

$$E_{\pm}(t) = -\frac{1}{2}\left(\omega + \frac{\alpha(t)}{\zeta(t)}\right) \tag{3.48}$$

Now let's talk about the drive $\alpha(t)$. We will start with the curious case of choosing $\alpha(t) = 1$ i.e. the Hamiltonian (3.46) $H(t) = H$ of the system is time-independent. However, this can lead to a time-dependent metric $\mathscr{W}(t)$ and a time-dependent Hermitian Hamiltonian $h(t)$ as seen in [66]. Also, we suppose that the system is in the $\mathscr{PT}$-unbroken phase i.e. $|\gamma| > 1$ and $c_1 \in \mathbb{R}, c_2 \in i\mathbb{R}$. Let's see how the energy eigenvalues vary with time for a specific set of parameters:

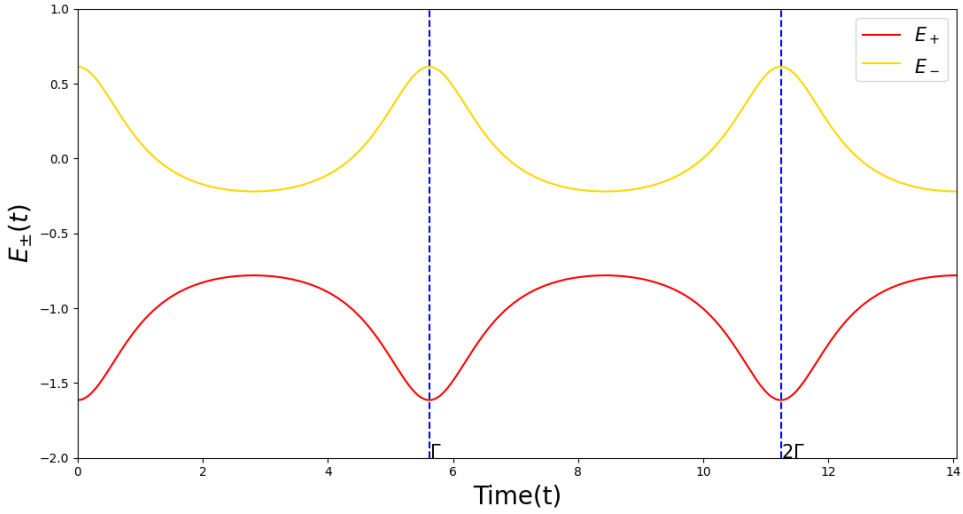

Figure 3.3: Variation of energy eigenvalues with time for the chosen parameters $\alpha(t) = 1, \gamma = 1.5, \omega = 1, c_1 = -\frac{2}{3}, c_2 = 0$. Blue dashed lines are drawn at $t = \Gamma$ and $t = 2\Gamma$

The choice of the parameters in Figure 3.3 is because the initial condition chosen for this example is $\mathscr{W}(0) = \mathbb{I}$. From the above figure, it's clear that the energy eigenvalues are periodic in time. The time-period Γ of oscillations is equal to the time-period of the function $\zeta(t)$ which, for $\alpha(t) = 1$ is easily found to be:

$$\Gamma(\gamma) = \frac{2\pi}{\sqrt{|1-\gamma^2|}} \tag{3.49}$$

For the set of parameters chosen in Figure 3.3, $\Gamma \approx 5.62$.

The construction for the Otto engine using the non-canonical approach will be similar in spirit to the construction of the Otto engine using the canonical approach. In particular, we will suppose that when the working medium is connected to a thermal bath at temperature $T = 1/\beta$, then the density operator in the "Hermitian picture" will be given by:

$$\rho_{eq} = \frac{e^{-\beta h}}{Z} = \frac{e^{-\beta E_+}}{Z} |\psi_+\rangle \langle\psi_+| + \frac{e^{-\beta E_-}}{Z} |\psi_-\rangle \langle\psi_-|, \tag{3.50}$$

with $Z = \mathrm{Tr}\left\{e^{-\beta h}\right\}$ and $|\psi_\pm\rangle$ being the eigenstates of h at some appropriate instant of time. The corresponding density operator in the "non-Hermitian picture" is found to be:

$$\tilde{\rho}_{eq} = W^{-1}\rho W = \frac{e^{-\beta E_+}}{Z} |\Psi_+\rangle \langle\Psi_+| \mathscr{W} + \frac{e^{-\beta E_-}}{Z} |\Psi_-\rangle \langle\Psi_-| \mathscr{W}, \tag{3.51}$$

where $|\Psi_\pm\rangle$ are the eigenstates of the energy operator $\mathscr{E}$, all at some appropriate instant of time. Again due to the simple form of the Hermitian Hamiltonian $h(t)$, it becomes mathematically simpler to run the entire cycle in the Hermitian picture. This means the time-evolution operator (for work strokes of the Otto cycle) for the states in the "Hermitian picture" is given by:

$$u(t_f, t_i) = \begin{pmatrix} e^{-i\int_{t_i}^{t_f} E_+(s)ds} & 0 \\ 0 & e^{-i\int_{t_i}^{t_f} E_-(s)ds} \end{pmatrix}. \tag{3.52}$$

Let's now discuss how the strokes of the Otto engine will be implemented, specifically when the temporal energy profile is given by 3.3 (however, this can be generalised very easily to different energy profiles coming from arbitrary initial conditions). Suppose that for $t < 0$, the system is connected to a hot thermal bath at temperature $T_h = 1/\beta_h$. Then the state of the system in the "Hermitian picture" at

$t = 0$ is given by:

$$\rho_A = \frac{e^{-\beta_h h(0)}}{Z}, \tag{3.53}$$

where $Z = e^{-\beta_h E_+(0)} + e^{-\beta_h E_-(0)}$. But the eigenstates $\{|\psi_\pm(t)\rangle\}$ of $h(t)$ are actually independent of time:

$$|\psi_+(t)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad |\psi_-(t)\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{3.54}$$

Thus, we can just say:

$$\rho_A = \frac{e^{-\beta_h h(0)}}{Z} = \frac{e^{-\beta_h E_+(0)}}{Z} |\psi_+\rangle \langle\psi_+| + \frac{e^{-\beta_h E_-(0)}}{Z} |\psi_-\rangle \langle\psi_-|, \tag{3.55}$$

The energy of this state is:

$$\langle E_A \rangle = \mathrm{Tr}\{\rho_A h(0)\} = E_+(0)\frac{e^{-\beta_h E_+(0)}}{Z} + E_-(0)\frac{e^{-\beta_h E_-(0)}}{Z}. \tag{3.56}$$

The first stroke of this Otto engine ($A \to B$)will be the unitary expansion stroke. The system is disconnected from the hot thermal bath and evolves unitary for a duration of $\tau_1 < \Gamma$ in this first stroke. From Figure 3.3, it is clear that the energy splitting decreases. For now, we can let τ_1 be variable. The state of the system in the "Hermitian picture" at the end of this stroke is:

$$\rho_B = u(\tau_1, 0)\rho_A u^\dagger(\tau_1, 0) = \frac{e^{-\beta_h h(0)}}{Z} = \frac{e^{-\beta_h E_+(0)}}{Z} |\psi_+\rangle \langle\psi_+| + \frac{e^{-\beta_h E_-(0)}}{Z} |\psi_-\rangle \langle\psi_-|, \tag{3.57}$$

which is indeed equal to ρ_A. The energy is:

$$\langle E_B \rangle = \mathrm{Tr}\{\rho_B h(\tau_1)\} = E_+(\tau_1)\frac{e^{-\beta_h E_+(0)}}{Z} + E_-(\tau_1)\frac{e^{-\beta_h E_-(0)}}{Z}. \tag{3.58}$$

The next stroke ($B \to C$) is the isochoric cooling stroke. The system is connected to a cold thermal reservoir at temperature $T_c = 1/\beta_c$. The time taken for this

thermalisation to happen is assumed to be negligible. We get:

$$\rho_C = \frac{e^{-\beta_c E_+(\tau_1)}}{Z'} |\psi_+\rangle \langle\psi_+| + \frac{e^{-\beta_c E_-(\tau_1)}}{Z'} |\psi_-\rangle \langle\psi_-|, \tag{3.59}$$

where $Z' = e^{-\beta_c E_+(\tau_1)} + e^{-\beta_c E_-(\tau_1)}$. The energy is:

$$\langle E_C \rangle = \mathrm{Tr}\{\rho_C h(\tau_1)\} = E_+(\tau_1)\frac{e^{-\beta_c E_+(\tau_1)}}{Z'} + E_-(\tau_1)\frac{e^{-\beta_c E_-(\tau_1)}}{Z'}. \tag{3.60}$$

The third stroke ($C \to D$)is the unitary compression stroke. The system is disconnected from the cold thermal bath and is allowed to evolve unitarily for a duration $\tau_2 = T - \tau_1$. Choosing this specific duration for the second unitary work stroke ensures that the energy eigenvalues are brought back to the initial value and the cycle is eventually completed. We get:

$$\begin{aligned} \rho_D &= u(\tau_2 + \tau_1, \tau_1)\rho_C u^\dagger(\tau_2 + \tau_1, \tau_1) = u(T, \tau_1)\rho_C u^\dagger(T, \tau_1), \\ &= \frac{e^{-\beta_c E_+(\tau_1)}}{Z'} |\psi_+\rangle \langle\psi_+| + \frac{e^{-\beta_c E_-(\tau_1)}}{Z'} |\psi_-\rangle \langle\psi_-|, \end{aligned} \tag{3.61}$$

which is indeed equal to ρ_C. Note that $h(T) = h(0)$. The energy of this state is found to be:

$$\langle E_D \rangle = \mathrm{Tr}\{\rho_D h(T)\} = \mathrm{Tr}\{\rho_D h(0)\} = E_+(0)\frac{e^{-\beta_c E_+(\tau_1)}}{Z'} + E_-(0)\frac{e^{-\beta_c E_-(\tau_1)}}{Z'}. \tag{3.62}$$

Finally, the last stroke ($D \to A$) is the isochoric heating stroke, where the system is connected to the initial thermal reservoir at temperature T_h thereby completing the cycle. The duration of this stroke is also assumed to be negligible compared to the work strokes. As before, the work and heat exchange for each stroke is found

to be:

$$\begin{aligned}\langle W_1\rangle &= \langle E_B\rangle - \langle E_A\rangle,\\ \langle Q_c\rangle &= \langle E_C\rangle - \langle E_B\rangle,\\ \langle W_2\rangle &= \langle E_D\rangle - \langle E_C\rangle,\\ \langle Q_h\rangle &= \langle E_A\rangle - \langle E_D\rangle.\end{aligned} \tag{3.63}$$

The net work output and heat injected is given by $\langle W_{out}\rangle = -(\langle W_1\rangle + \langle W_2\rangle)$ and $\langle Q_{in}\rangle = \langle Q_h\rangle$. For the system to function like an engine, we must have $\langle W_{out}\rangle > 0$ which would imply:

$$\frac{|E_+(\tau_1) - E_-(\tau_1)|}{|E_+(0) - E_-(0)|} > \frac{T_c}{T_h}. \tag{3.64}$$

The efficiency is finally given by:

$$\eta = \frac{\langle W_{out}\rangle}{\langle Q_{in}\rangle} = 1 - \frac{|E_+(\tau_1) - E_-(\tau_1)|}{|E_+(0) - E_-(0)|}. \tag{3.65}$$

Combining (3.64) and (3.65), we again find that this Otto engine efficiency will be less than the Carnot efficiency. It is possible to compute all the above quantities numerically since we have computed the temporal energy profiles numerically in Figure 3.3. The efficiency given above as a function of the duration of the first work stroke is given in the following figure.

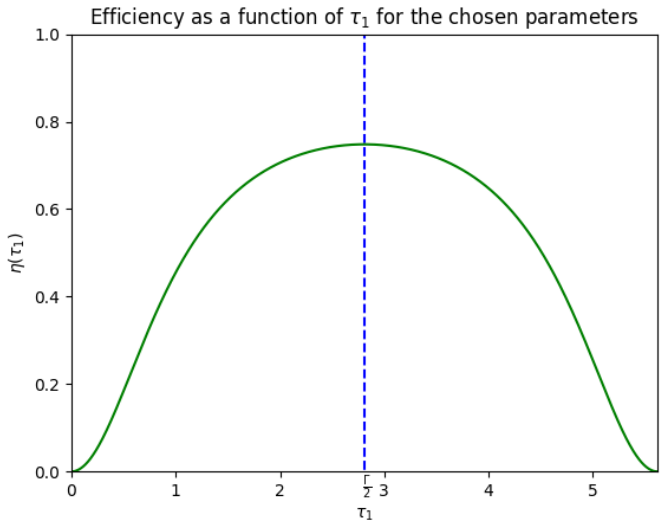

Figure 3.4: Efficiency η as a function of τ_1 for the specific Otto engine described above

It is clear from the above Figure 3.4 that the efficiency is maximum when the duration of the first and second work strokes are equal. The maximum efficiency obtained in this case is $\eta_{max} \approx 0.748$. Even for different values of γ, the maximum efficiency is obtained when $\tau_1 = \tau_2 = \frac{\Gamma(\gamma)}{2}$. We can also plot how this maximum efficiency η_{max} depends on γ:

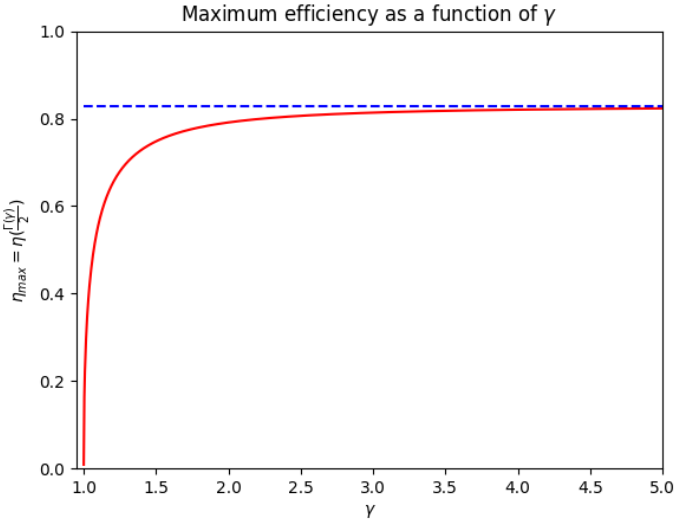

Figure 3.5: η_{max} is plotted against $\gamma \in (1,5]$. The red curve shows the maximum efficiency as a function of γ. The blue dashed line is the asymptotic efficiency for large γ.

From Figure 3.5, it is clear that the maximum efficiency increases with γ but then flattens out. The asymptotic efficiency for γ is numerically obtained to be

$$\lim_{\gamma\to\infty} \eta_{max}(\gamma) \approx 0.8284 \tag{3.66}$$

We need to do further work to explain these results analytically.

In summary, we were able to construct an Otto engine in the $\widetilde{\mathscr{PT}}$-unbroken and $\mathscr{PT}$-unbroken regime using the non-canonical approach. The non-Hermitian Hamiltonian was time-independent for the specific drive ($\alpha(t) = 1$) that we chose to construct this engine. We showed that under suitable initial conditions, the maximum efficiency is obtained when the duration of both the work strokes is equal, and we can get reasonably high values of efficiency for larger values of γ. Also, note that a larger value of γ means a smaller cycle duration Γ. Thus, it is possible to obtain higher power outputs in such engines. We also note that for other drives considered in [61, 67] like $\alpha(t) \sim \cos t$, we do get periodic temporal energy profiles. However, they always exhibit energy level crossings making it difficult to construct a useful Otto engine from such drives.

Chapter 4

Discussion and Future Directions

4.1 Discussion on the mathematical approaches and the Jarzynski equality

We learnt about two mathematical approaches used to study systems with time-dependent metrics. The canonical approach has been applied in various works like those on non-Hermitian topological phases [68], quantum work relations and response theory for $\mathscr{PT}$-symmetric systems [69], the Jarzynski equality for $\mathscr{PT}$-symmetric and pseudo-Hermitian systems [34, 31] and the Crook's fluctuation theorem for pseudo-Hermitian systems [70] to state just a few. Thus, under the assumption that the energy eigenvalues of the system are given by the eigenvalues of the Hamiltonian and we are restricted to the $\mathscr{PT}$-unbroken regime, the canonical approach works well. The obvious drawback is that the dynamics do not follow the standard TDSE.

The non-canonical approach is the second popular approach used to study systems with time-dependent metrics. We note that the non-canonical approach has been used in various theoretical studies like decoherence properties in anti-$\mathscr{PT}$-symmetric qubits [71], measurement-based heat engines [72], heat engines in the $\mathscr{PT}$-broken regime [73] and $\mathscr{PT}$-parametric amplifiers [74] to state just a few. Our proof of the Jarzynski equality in the $\widetilde{\mathscr{PT}}$-unbroken regime adds to these re-

sults. We were also able to numerically verify our results. The proof and the subsequent verifications also allowed us to extend the scope of the Jarzynski equality even to some parts of the $\mathscr{P}\mathscr{T}$-broken regime, something which the canonical approach could not do.

4.2 Discussion on the quantum Otto Engines results

Using the canonical approach, we studied the quantum Otto engine with the experimentally relevant two-level working medium (3.1). Of course, our analysis was only restricted to the $\mathscr{P}\mathscr{T}$-unbroken regime. During our analysis, we assumed perfectly thermalising strokes that also happen instantaneously. By finding the properly mapped Hermitian Hamiltonian, we were able to find the efficiency of this quantum Otto engine for any arbitrary drive. Due to the simple form of the properly mapped Hermitian Hamiltonian, we found that irrespective of the drive, the efficiency of this engine is given by:

$$\eta_O = 1 - \sqrt{\frac{1-\lambda_i^2}{1-\lambda_f^2}}, \tag{4.1}$$

implying that only the initial and final value of the externally controlled work parameter matters. In other words, only the initial and final energy splitting matters, which implies the work strokes can be performed in arbitrarily short durations without affecting the efficiency of the engine. Thus, it is possible to get very high (theoretically infinite) power outputs from such a quantum Otto engine. However, we still note that the efficiency η_O itself never becomes higher than the Carnot efficiency in accordance with the second law of thermodynamics. It is important to emphasise that the results obtained here are dependent on the model of the two-level system chosen since there is no reason the properly mapped Hermitian

Hamiltonian will take such a simple form for other models. Nevertheless, a quantum Otto engine with the $\mathscr{P}\mathscr{T}$-symmetric qubit model chosen in (3.1) can offer an advantage in terms of efficiency as well as power for finite-time quantum Otto engines with Hermitian working mediums. Let's now discuss the results derived for the quantum Otto engine with a $\mathscr{P}\mathscr{T}$-symmetric qubit model (3.46) using the non-canonical approach. In contrast to the previous case, here, the nature of the drives plays a crucial role. We considered the specific drive $\alpha(t) = 1$, which produced periodically oscillating energy eigenvalues with no energy level crossings. This made the whole analysis much more simpler. However, for other arbitrary time-dependent functions $\alpha(t)$, we may not necessarily get periodic temporal energy profiles and/or no energy level crossings. Thus, we have to be extremely careful about the external drive we choose in order to get a cyclic thermal engine. Again in contrast with the previous case, the duration of the entire cycle is not an arbitrary quantity here. The duration of the cycle is strictly determined by the value of the non-Hermiticity parameter γ. We had already seen earlier that even though it is possible to have the duration of the two work strokes unequal, but the efficiency is maximum when the durations are equal (see Figure 3.4). In accordance with the second law of thermodynamics, the efficiency is nevertheless always less than the Carnot efficiency. We also found that it is possible to increase the efficiency by increasing the value of γ (see Figure 3.5). Even using the non-canonical approach, we were unable to run a quantum Otto engine completely in the $\mathscr{P}\mathscr{T}$-broken regime since we could not find drives that created suitable energy profiles. We need to do more analysis to find if this engine gives any efficiency or power advantage over conventional finite-time quantum Otto engines.

4.3 Future directions

4.3.1 A more physical model

Till now, we have relied on mathematical approaches, namely canonical and non-canonical maps to calculate the efficiencies of quantum Otto engines with $\mathscr{P}\mathscr{T}$-symmetric qubits as the working medium. Admittedly, this approach is not the most physical in nature and in future works, we would like to work with systems more closely related to experiments. Here, we present an idea for such a future research direction. Even though the example is related to classical optics and not quantum mechanics, it provides an illustration of the limitations of our previous approaches.

We try to construct a cyclic heat engine using the classical $\mathscr{P}\mathscr{T}$-symmetric coupled optical waveguide structure presented in [5, 75, 76]. The system consists of two parallel coupled optical waveguides in a complex refractive index potential. Light propagates along z-axis. Transverse oscillations of electric field take place along y-axis. The complex refractive index $n(x)$ varies along x-axis. The system is $\mathscr{P}\mathscr{T}$-symmetric if:

$$n(x) = n^*(-x), \tag{4.2}$$

in other words, "the real part of the refractive index is an even function of x while the imaginary part of the refractive index is an odd function of x" [5]. This can be seen in the following figure:

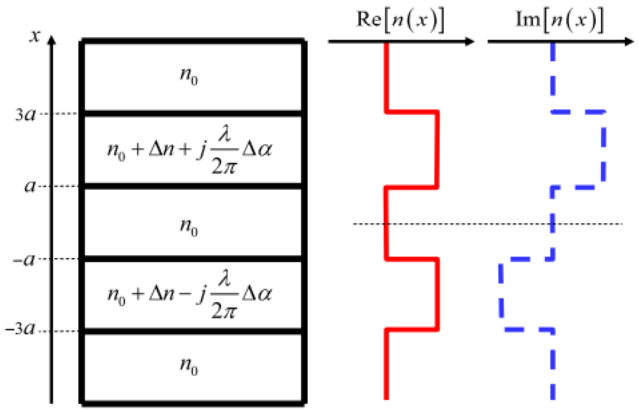

Figure 4.1: Refractive index potential in a $\mathscr{P}\mathscr{T}$-symmetric coupled optical waveguide structure. Ref. [75]

"The paraxial equation of diffraction determines the electric field $E = E(x,z)$:

$$i\frac{\partial E}{\partial z} + \frac{1}{2k}\frac{\partial^2 E}{\partial x^2} + k_0\left(\mathrm{Re}\{n(x)\} + i\,\mathrm{Im}\{n(x)\}\right)E = 0, \tag{4.3}$$

where $k_0 = 2\pi/\lambda, k = k_0 n_0$, with λ being the vacuum wavelength and n_0 being the substrate index" [5] as shown in figure above. On using the coupled mode approach [76], the electric fields $E_1(z)$ and $E_2(z)$ in the two waveguides follow the equation:

$$\begin{aligned} i\frac{dE_1}{dz} - i\frac{\gamma}{2}E_1 + \kappa E_2 = 0 \\ i\frac{dE_2}{dz} + i\frac{\gamma}{2}E_2 + \kappa E_1 = 0 \end{aligned} \tag{4.4}$$

Rewriting in matrix terms:

$$i\frac{d}{dz}\begin{pmatrix} E_1 \\ E_2 \end{pmatrix} = \begin{pmatrix} i\frac{\gamma}{2} & -\kappa \\ -\kappa & -i\frac{\gamma}{2} \end{pmatrix}\begin{pmatrix} E_1 \\ E_2 \end{pmatrix} = H\begin{pmatrix} E_1 \\ E_2 \end{pmatrix} \tag{4.5}$$

which is somewhat like the Schrödinger equation but with time replaced by the z-coordinate. The matrix H plays the role the role of the Hamiltonian. However, its eigenvalues no longer give the energies. The energy is given by the classical intensities in the two waveguides $I_1 \sim \int |E_1(z)|^2 dz$ and $I_2 \sim \int |E_2(z)|^2 dz$. Thus

we clearly cannot use the canonical or the non-canonical approach to solve this problem. However, we can still design a heat engine using this system.

First, we argue that it is not possible to construct a 'continuous' heat engine with the two coupled optical waveguides kept at different temperatures. Such a temperature gradient necessarily breaks the $\mathscr{P}\mathscr{T}$-symmetry. To see this, we first note that the refractive index in both waveguides must be a function of the temperature of the waveguides. However, $\mathrm{Re}\{n\}$ should be equal in both waveguides while the imaginary part of the refractive index in one waveguide is the negative of the imaginary part of the refractive index in the other waveguide to preserve the $\mathscr{P}\mathscr{T}$-symmetry of the system. Keeping the two waveguides at different temperatures will change the refractive index in such a manner that the condition for $\mathscr{P}\mathscr{T}$-symmetry will not be satisfied. In particular, $\mathrm{Re}\{n\}$ is no longer going to be the same in both waveguides even if it is assumed that the gain or loss determined by $\mathrm{Im}\{n\}$ is independent of temperature. Thus, it is not possible to construct a continuous heat engine using this system.

Let's now talk about our idea for a Stirling engine with the $\mathscr{P}\mathscr{T}$-symmetric coupled optical waveguide. We will assume that at any given instant, both the waveguides are at the same temperature T. This can be achieved by connecting both the waveguides to a thermal reservoir at temperature T. The distance between the two waveguides is denoted by D. The refractive index is given by $n(x) = n(x;T,D)$ i.e. it's dependent on the temperature as well as the distance. Using the methods detailed in [75, 76], it is possible to find γ and κ, and hence, $E_1(z;T,D)$ and $E_2(z;T,D)$ in (4.5) that take the dependence of the temperature and distance between waveguides into account. The bottom line is that it is possible to find the electric field amplitudes in both the waveguides as a function of the temperature and the distance between the waveguides. The total internal energy U at any moment is given by the sum of the intensities in both waveguides i.e.

$U(T,D) \sim I_1(T,D) + I_2(T,D)$. We can now think of two thermodynamic strokes immediately:
(1) Isochoric stroke - In this stroke D is kept constant while the temperature of the system is changed $T_i \to T_f$. The initial and final internal energy is given by $U_i \sim I_1(T_i,D) + I_2(T_i,D)$ and $U_f \sim I_1(T_f,D) + I_2(T_f,D)$. Note that no work is done in this process and all the internal energy change can be attributed to heat flowing into or out of the thermal reservoir whose temperature is being changed.
(2) Isothermal stroke - In this stroke, T is kept constant. However, the distance between the waveguides changes $D_i \to D_f$. The initial and final value of the internal energy is $U_i \sim I_1(T,D_i) + I_2(T,D_i)$ and $U_f \sim I_1(T,D_f) + I_2(T,D_f)$. However, this process is more complicated since there is going to be both work and heat exchange. Specifically, we need a physical model of the force between the two waveguides to calculate the work done to change the distance between the waveguides. This force is called the optical gradient force and this study [77] gives a detailed analysis of the optical gradient force between two $\mathscr{P}\mathscr{T}$-symmetric coupled optical waveguides. Thus, we intend to study the results of this study in more detail and use it to find the work done to change the distance between two waveguides. We can then also find the heat exchange in this process since we also know the total internal energy change.

By performing isochoric and isothermal strokes alternatively, with suitable initial and final values of the temperature and distance between waveguides, it is possible to construct a Stirling engine [42]. Thus, we intend to find the efficiency of such a classical $\mathscr{P}\mathscr{T}$-symmetric coupled optical waveguide Stirling engine in the future

4.3.2 More Quantum Otto engines

We calculated the efficiency of a quantum Otto engine in the non-canonical approach using the analytically tractable model (3.46). We aim to calculate the efficiency of the same model quantum Otto engine using the canonical approach to do

a direct comparison between the two approaches. To do this, we will need to find the "proper mapping" for this model. Our first attempts suggest that this could be difficult to do analytically and we might have to resort to a numerical analysis.

We also intend to calculate the efficiency of Otto engines using the non-canonical approach in the $\widetilde{\mathscr{P}\mathscr{T}}$-symmetric but $\mathscr{P}\mathscr{T}$-broken regime. This will involve finding specific drives that result in periodic temporal energy profiles but also do not have energy crossings.

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