Quantum state estimation and work extraction processes beyond IID

by

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A thesis submitted in satisfaction of the
requirements for the degree of

Doctor of Philosophy

University of Technology Sydney

Faculty of Engineering & Information Technology

August 2021

Certificate of original authorship

I, Maria Quadeer, declare that this thesis is submitted in fulfilment of the requirements for the award of the degree of Doctor of Philosophy in the Faculty of Engineering and Information Technology at the University of Technology Sydney.

This thesis is wholly my own work unless otherwise referenced or acknowledged. In addition, I certify that all information sources and literature used are indicated in the thesis. This document has not been submitted for qualifications at any other academic institution.

This research is supported by the Australian Government Research Training Program.

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Maria Quadeer

To ammu.

Abstract

This thesis explores two specific problems within the broad context of one-shot information theory.

In the first part of this thesis, we investigate Bayesian and minimax estimators for quantum state estimation under general Bregman divergences with single-shot measurements. We also study the problem of covariant state estimation and obtain optimal measurements for the same.

In the second part, we study work extraction processes mediated by finite-time interactions with an ambient bath—*partial thermalizations*—as continuous time Markov processes for two-level systems. We analyze the distribution of work for the case where the energy gap of a two-level system is driven at a constant rate. We also analyse work extraction cycles by modifying the Carnot cycle, incorporating processes involving partial thermalizations.

Acknowledgements

I will be, forever, indebted to Marco for his patience and time in helping me get so far. His democratic approach towards research and his readiness to discuss conceptual issues have made these past years sufferable. His encouragement when it came to doing things differently and his ever-timely feedback have enabled me to pursue things my own way. He has tolerated my digressions, sometimes with great enthusiasm, and which I have deeply enjoyed.

None of this would have been possible without Chris, who agreed to fund my PhD, and has been a pillar of great help and support throughout these years. His kindness, empathetic attitude, and a disposition to listen with care made life in Sydney bearable. His silent support is something that I will always cherish.

I would like to thank Kamil for his time and willingness to share his research ideas with me and for teaching me the shrewd skill that is to publish papers.

I have to thank: Desh, for setting a great example as an academic and a person—the time I spent with him and others at RRI in Bangalore has had a lasting impression; Sesh, for letting me do a project with him during my masters and his general help & guidance; Prof. Sibasish, who trusted and supported me during a challenging time, and Manik da for the many nights spent on the rooftop of the hostel at IMSc discussing physics and socialist ideas.

I could not have been who I am without abbu, who taught me some of the most important lessons in life, and who would have been very proud if he were alive today. Bereft of his presence, I wonder if this void can ever be filled. I am beholden to ammu, in perpetuity. She has taken care of me in the most distressing of times and has been a source of great strength

and determination. The family mentions would be heavily incomplete without my nani-ammi and nana-abba, who took care of me when I was little, and who's ideals far exceeded their times. Their memories are an eternal source of love and warmth in my life.

I must say a few words about my middle sister, Iram, who has always fed me amazing dishes and who's *coolness* I cannot mimic, and my little darling sister, Fatima, who has made a gazillion elaborate cards for me. I have missed them deeply over these years.

And now to mention the most current person who has been a constant throughout the highs and lows of life and who has kept me sane—Geet—he prefers not be spoken too much about.

I would also like to thank Lily, Robyn, and Camila for offering generous help with the university paperwork whenever needed.

I must also acknowledge the support of the Sydney Quantum Academy's top-up and extension scholarships that gave me a-much-needed extra time in the end.

Finally, I would like to thank the socialist policies around higher education in India that enabled a nobody.

Contents

1

Introduction

> And God said: let there be independent and identically prepared systems.
>
> a quantum physicist

One of the assumptions that is made but almost never justified in quantum physics is that there exists a preparation procedure that renders physical systems in *independent and identically distributed* (IID) quantum states, i.e. different physical systems that are independent of each other but have the same quantum description [Shankar (1994)]. To characterise a system in an unknown state we need to perform a *measurement* which requires infinitely many copies of the system that are in the same (unknown) state since the applicability of Born's probability rule rests on the correspondence between frequency and probability—that only holds asymptotically; imagine the many number of times one would have to flip a coin to ascertain its bias. Standard thermodynamics is another avenue where the *thermodynamic limit*, i.e. the limit of large number of particles, is assumed. In this limit, all higher moments about the mean for quan-

tities such as work become negligible in comparison to the mean itself. This is in the same vein as the issue of requiring IID quantum states for characterising physical systems. Consider a semi-classical two-level system that can be set-up as a Carnot engine [Quan *et al.* (2007)]. For each run of the cycle this engine would have a mean efficiency and variance (about mean). While the mean efficiency would be the Carnot efficiency, its variance would be a constant that would only vanish in the limit of many number of independent runs of the cycle (law of large numbers).

As we move beyond these IID settings, we study these problems using techniques of *one-shot information theory*, which allows one to systematically incorporate small size effects. In the one-shot setting, one is typically interested in performing tasks with small number of systems or small number of runs of an experiment. Such processes incur cost/error, and depending upon the specifics of the problem, we can either look for optimal processes that minimize, let us say the average cost, or accept an error if the probability of getting the desired outcome is sufficiently large.

In classical information theory, a first question is that of compressing messages [Shannon (1948)]. A message is a stream of letters of an alphabet imagined to be output by an ideal source that produces an IID stream of letters (i.e. independently drawn from the same probability that distribution) from the given alphabet. For a large stream of letters, the question is if we can compress it to a shorter string of letters without much loss of information. For example, if the alphabet is binary and the zeroes occur with probability p and ones with probability $1-p$ then, by the law of large numbers, we know that a typical string of n binary letters would have np number of zeroes and $n(1-p)$ number of ones for large n. Now, the total number of such typical strings is $\binom{n}{np}$ which, using the stirling approximation, is of order $2^{nH(p)}$, where $H(p)$ is the Shannon entropy for the binary distribution. The fact that out of all possibilities a partic-

ular message, i.e. a certain combination of zeroes and ones is observed is quantified in terms of the *surprisal* for individual events (occurrence of zero or one), which is simply the negative logarithm of the probability of occurrence of that particular bit value. This is because observing an event with a small probability of occurrence is highly surprising; surprisal is inversely proportional to probability, and the logarithm function captures the intuitive notion of information conveyed by the occurrence of joint events fairly well—we expect the information obtained by observing two independent events to be the sum of surprisals for each of those events. Thus, the information obtained on average is the expectation of the surprisal with respect to the underlying probability distribution, and is referred to as the *Shannon entropy*. To convey (essentially) all of the information in an n bit string it suffices to encode only the typical strings as the probability that a string is atypical vanishes in the limit of large n. More generally, for a source that produces an IID stream of symbols from any alphabet, the noiseless source coding theorem [Shannon (1948)] states that any compression of the output must be at least the Shannon entropy number of logical bits per symbol. Anything less than that threshold would, almost certainly, lead to information loss upon transmission.

In the quantum setting, one has a quantum signal source that encodes each message from a classical source (that produces a stream of IID symbols) into a corresponding stream of IID quantum states. Then, the task of source coding for transmission of such quantum messages is essentially the same, and in fact, it was shown that the *Von Neumann entropy* of the ensemble of quantum states at the source is the minimum number of *qubits* needed to encode each state in the ensemble [Schumacher (1995)].

One may think of an IID premise as ideal and ask what happens realistically. Such questions have been studied both in the classical and quantum cases and constitute the subject matter of one-shot information theory

[Tomamichel (2012)]. In fact, various problems in quantum information processing borrow from one-shot information theory and fall within the beyond IID project[1]. While the beyond IID program is itself multi-faceted, this thesis focuses on two specific areas that were introduced in the beginning.

In Part I, we study quantum state estimation within the one-shot measurements' framework. We do so by defining an estimator/estimate of an unknown quantum state as a function on the space of measurement outcomes to the set of density matrices. Furthermore, we work on a Bayesian estimation procedure which naturally accommodates the one-shot formalism and is optimal (minimizes average risk/error) for a class of loss functions (that quantify the overlap between an estimate and the true state) called Bregman divergences, e.g. relative entropy. This is due to the fact that the Bayesian estimate is an average with respect to the posterior distribution over the set of density matrices; we can represent our existing knowledge of the state in terms of a prior distribution over the set of density matrices which can be updated using the Bayes' rule after the measurement is made to obtain the posterior distribution. Furthermore, we obtain optimal measurements for the case when the quantum states lie in *orbits* generated by a group (*covariant* state estimation).

In Part II, we concentrate on the connection between one-shot information theory, statistical physics & the mathematical foundations of thermodynamics; one that is fairly old [Jaynes (1957)]. Questions of equilibriation and thermalization for closed quantum systems have been a topic of interest for a long time, dating back to the 1929 article on the Quantum Ergodic theorem [Goldstein *et al.* (2010)]. It has been shown that thermalization can be seen as a generic property that arises due to entangle-

[1]The annual workshop, Beyond IID, provides an ever expanding list of topics that belong to this overarching scheme.

ment between a system and its environment and that almost all systems equilibriate [Popescu *et al.* (2006); Linden *et al.* (2009); Gogolin and Eisert (2016)]. Quantum information theoretic tools have been central to such analyses and to the formulation of quantum thermodynamics as a *resource theory* [Chitambar and Gour (2019)].

Resource theories are operational theories that allow us to analyze physical properties of a system mathematically and employ information theoretic tools. Imagine a scenario in which you can only perform a certain set of operations, like *LOCC—local operations and classical communication*. Clearly, having an *entangled* state can be of use as it may allow you to perform operations that lie outside the set of LOCC operations; an entangled state is thus a *resource*. Naturally, there are some states that come for *free*—the *separable* states, as they can always be created via free operations (LOCC operations) and do not have any resource value (not entangled). Moreover, the set of separable states is invariant under LOCC operations. Thus, one can formulate this scenario as a resource theory of entanglement where entangled states are *resource states*, separable states are *free states* and LOCC operations are *allowed operations*. Then one can then ask how much resource is needed to perform a task using only the allowed operations. In the context of thermodynamics [Gour *et al.* (2015)], the set of allowed operations are *thermal* operations that model the physical process of thermalisation, in which a system is brought in contact with a bath at some fixed temperature and then allowed to evolve and then separated from it such that the combined energy of the system and the bath is conserved [Korzekwa (2016)]. Thus, the states that are *athermal* at that particular temperature become a resource for thermal operations while the state that is thermal at that temperature, the *Gibbs state*, is a free state. The main question then is how much resource (work) can be extracted while converting a given state to another via thermal operations.

Regime	Description	(Ir)reversibility
single-shot ($n = 1$)	Given: ρ & σ Ask: Is the transformation $\rho \mapsto \sigma$ possible under a thermal operation?	irreversible [Horodecki and Oppenheim (2013)]
asymptotic ($n \to \infty, \epsilon \to 0$)	Given: n copies of ρ Ask: What is the maximal rate of transformation R^* at which one can generate R^*n copies of the state σ under thermal operations with asymptotically vanishing error?	reversible [Brandão *et al.* (2013)]
finite-size - small deviation ($n < \infty, \epsilon > 0$)	Given: n copies of ρ Ask: What is the correction to R^* when allowing for a constant error? Can one still recover the maximal rate in the asymptotic regime?	approximately reversible asymptotically [Chubb *et al.* (2018)]
finite-size - moderate deviation ($n < \infty, \epsilon \to 0$)	Given: n copies of ρ Ask: What is the correction to R^* when allowing for an error that vanishes asymptotically? Can one still recover the maximal rate in the asymptotic regime?	approximately reversible if resonance condition holds [Chubb *et al.* (2019)]

Table 1.1: n is the number of copies of the state that needs to transformed, namely ρ while ϵ is the error associated with the transformation, i.e., the final state might not be *exactly* σ but could be 'ϵ' away from σ under a chosen distance-measure such as infidelity.

The question posed above is fairly general—one that asks for resource interconversion—posed naturally in the single-shot setting. Resource theories of *Coherence*, *Entanglement* and thermodynamics are known to be reversible in the asymptotic regime, i.e. when one has access to infinitely many copies of the system the interconversions are reversible. As the interconversion problems in resource theories are posed in the single-shot regime one can explore questions of irreversibility and finite-size effects rigorously. This question was first looked at in Ref. [Kumagai and Hayashi (2013)] in the context of entanglement concentration and recently in Ref. [Chubb *et al.* (2018)] for thermodynamics. While the latter references studied finite-size effects, analysis in the intermediate-size regime has been been done in Ref. [Kumagai and Hayashi (2017)] in the context of entanglement and was extended to thermodynamics in Refs. [Chubb *et al.* (2019); Korzekwa *et al.* (2019)]. Table 1.1 summarizes the various regimes under which the resource interconversion problem has been studied in the context of thermodynamics. These results are on resource inter-convertibility, but the link between thermodynamics and information theory constitutes other themes. Here, we study fluctuations of work done during finite-time (out-of-equilibrium) processes in line with the one-shot statistical physics framework [Garner (2018)].

One-shot work extraction processes have been studied earlier [Åberg (2013); Egloff *et al.* (2015)] and it has been shown that the more traditional approach towards out-of-equilibrium phenomena, i.e. fluctuation theorems [Jarzynski (1997); Crooks (1999)] are equivalent to such approaches [Halpern *et al.* (2015)]. To give a brief overview of the basic idea, let us consider two work extraction processes, each with different distributions but the same mean work value. Then, imagine we are interested in a minimum threshold to be overcome, e.g. the activation energy of some chemical reaction. The question is how *good* are these two protocols. Let us further assume that the mean values for the two exceed the required threshold

but since their distributions are not alike, this threshold might be exceeded with a high probability in one case but almost never in the other. Thus, if we could guarantee a fixed amount of work with high probability, then that *guaranteed work* provides a better measure of how good the two distributions are in comparison to average work as considered in Ref. [Egloff *et al.* (2015)]. There is another notion of one-shot work called (ϵ, δ)-deterministic work, which means that the work would fall within an interval of width 2δ around the said value with probability $1 - \epsilon$ [Åberg (2013)]. The difference between the former and latter can be seen by thinking about the case where both ϵ and δ are zero; while deterministic work would imply a distribution with no spread at all, guaranteed work simply implies that the spread must lie above the given threshold. This makes it amply clear that the distribution of work is equally important.

Here, we consider finite-time work extraction in two-level systems and study the distribution of work when the system is driven at a constant rate. Finite-time processes are relevant to modern experiments done with small systems driven over timescales shorter than the thermalization time of the respective systems.

The thesis is organised as follows, where chapters 2, 3, 4, and 5 form the basis of our first publication [1] while chapters 6, 7 (sections 7.1 and 7.2), and 9 constitute our second published work [2]. We looked at some unpublished directions in section 7.3 of chapter 7 and chapter 8 which we have described below.

In Chapter 2, we give an overview of the problem of state estimation and formalise it within the decision-theoretic framework defining general quantities such as quantum measurements, estimators, loss functions, risk, and Bregman divergence for density matrices. More specific definitions are made along the way.

In Chapter 3, we take a closer look at Bayesian state estimation. In Sec-

tion 3.1, we prove that it is almost generic in the sense that for any given estimator there is always a sequence of Bayes estimators that in the limit are just as good or better. We establish a relation between Bayesian and minimax estimation in Section 3.2; a minimax estimator is one that minimizes the risk in the worst case.

In Chapter 4, we introduce covariant state estimation and covariant measurements. We show that for covariant estimation, there exists a covariant measurement that is minimax.

In Chapter 5, we work out the complete minimax estimation problem for the case of a qubit.

In Chapter 6, we give a short introduction to thermalization processes in two-level systems discussing related works and give the model under which we analyse our problem.

In Chapter 7, we obtain an analytical expression for average work output for a partially thermalizing two-level system which is driven at a constant rate. In Section 7.1, we obtain a lower bound for variance as a function of the time duration. In Section 7.2, we present our numerical results obtained from Monte-Carlo simulations of the Markov process describing the work extraction protocol to obtain estimates for variance. In Section 7.3, we attempt to obtain the distribution of work analytically.

In Chapter 8, we consider optimal work extraction processes within our model as a constrained optimization problem but find a few roadblocks which we discuss.

In Chapter 9, we define work extraction cycles that involve partial thermalization processes using two-level systems and obtain optimal cycles under different sets of constraints.

Finally, I summarise our work in Chapter 10.

Part I

Quantum state estimation

2

Overview & formalism

In this chapter, we review some of the results on quantum state estimation and outline our results in Section 2.1. We then lay out the mathematical formalism used throughout Part I in Section 2.2.

2.1 Background

Quantum state tomography [Fano (1957); Pauli (1958)] refers to the process of determining an unknown quantum state of a physical system by performing quantum measurements. Any information processing task necessarily involves verifying the output of a quantum channel which mandates the study of quantum state tomography, apart from the unavoidable theoretical necessity. With recent developments leading to a transition of quantum computation from theory to practice, the verification of quantum systems and processes is of particular importance.

Given an unknown quantum state with no prior knowledge, it is clear that the measurement must be *informationally complete*, i.e. a measurement with outcome statistics sufficient to fully specify the quantum state

[Watrous (2018)]. Conventional data-processing techniques such as *direct inversion* and *maximum likelihood estimation*, thus, implicitly assume that the measurement statistics are informationally complete.

In direct inversion, given a fixed informationally complete measurement, one identifies the frequencies of each outcome with the corresponding probabilities. Then, by inverting Born's rule one obtains a unique *estimator* for the density operator that reproduces the measurement statistics; an estimator is defined as a map on the set of measurement outcomes $\mathcal{X}$, $\hat{\rho} : \mathcal{X} \mapsto \mathcal{S}(\mathcal{H})$, where $\mathcal{S}(\mathcal{H})$ is the set of density operators on the underlying Hilbert space $\mathcal{H}$ that describes the physical system. However, this strategy suffers from the drawback that such an estimator might not be a *physical* state and would yield negative eigenvalues.

Example 1. *Suppose one measures an unknown quantum state in* $\mathbb{C}^2$ *along the* x*,* y *and* z *directions. Assuming that each of the measurements are performed only once, let us suppose that each of the outcome is 'up'. Thus,* $n_x = n_y = n_z = 1$ *and* $N_x = N_y = N_z = 1$*, so that* $p_x = n_x/N_x = 1$*, etc. Now, an estimator that would yield the same probabilities would be the one with the Bloch vector:* $(2p_x - 1, 2p_y - 1, 2p_z - 1) = (1, 1, 1)$*. This is an invalid quantum state as it lies outside the Bloch ball, and thus necessarily has negative eigenvalues.*

Ref. [Hradil (1997)] referred to such a shortcoming of direct inversion and proposed an alternative that enforces positivity on the estimator, called *maximum likelihood estimation*.

A likelihood functional $\mathcal{L}[\rho] : \mathcal{S}(\mathcal{H}) \mapsto [0, 1]$ is the probability of observing a data set $\mathbb{D}$ given that the system is in the state ρ :

$$\mathcal{L}[\rho] = p(\mathbb{D}|\rho) \tag{2.1}$$

The data set $\mathbb{D}$ is characterized by the outcome set of the given measurement $\{E_1, ..., E_N | E_i \geq 0, \sum_{i=1}^{N} E_i = \mathbb{I}\}$. Thus, $p(\mathbb{D}|\rho) = \prod_{i=1}^{N} (\mathrm{Tr}[E_i \rho])^{n_i}$

where n_i is the number of times the i-th outcome is recorded in $\mathbb{D}$. Maximum likelihood estimation involves maximizing Equation (2.1) over the space of density operators $\mathcal{S}(\mathcal{H})$, and thus obtaining as the estimator the state that maximizes the likelihood functional.

The problem with MLE is that the estimator $\hat{\rho}_{MLE}$ can be rank-deficient. A rank-deficient estimator is not good, as it would mean that by performing only finite number of measurements we are absolutely certain to rule out many possibilities. This kind of certainty must be bogus, suggesting that there has to be a better estimator. Let us look at Example 1 once again to illustrate this point.

Example 1 (continued). *Given the choice of measurement and the corresponding outcomes, the likelihood functional is* $\mathcal{L}[\rho] = (1 + r_x)(1 + r_y)(1 + r_z)/6^3$, *which needs to be maximized under the constraint* $\|\vec{r}\| \leq 1$*—that characterizes the physical set of states in* $\mathbb{C}^2$. *This implies that* $r_x = r_y = r_z = 1/\sqrt{3}$, *which corresponds to an estimator that is a pure state.*

This shows that state estimators that are unphysical in direct inversion get mapped to the closest physical states in MLE, that lie on the state space boundary, and are thus rank-deficient. In fact, it can be shown [Blume-Kohout (2010)] that if there exists a ρ_{DI} obtained via direct inversion over a data set $\mathbb{D}$ which is physical, then, it also maximizes the likelihood functional, i.e. $\hat{\rho}_{DI} = \hat{\rho}_{MLE}$. Although, Example 1 is an instance of an extreme case where probabilities are approximated by frequencies of a single measurement, it suffices to illustrate that in direct inversion as well as MLE, all that one cares about is to obtain an estimate of the true state that reproduces the observed measurement statistics, regardless of the fact that in the light of new data the state's estimate might change completely. Ref. [Blume-Kohout (2010)] gives a detailed critique of both direct inversion and MLE, proposing *Bayesian Mean Estimation* (BME) to be a more plausible estimation technique. Moreover, it has been shown

that such an estimation technique is quantitatively better in Ref. [Ferrie and Blume-Kohout (2018)].

Generally speaking, in estimation theory [Lehmann and Casella (1998)], the average measure of closeness of an estimator to the actual state is defined as the *risk*,

$$R(\rho, \hat{\rho}) = \mathbb{E}_{X|\rho}[L(\rho, \hat{\rho}(X))], \tag{2.2}$$

where X is the random variable corresponding to the measurement outcomes and L is a distance-measure between the true state and the estimator. One way of choosing an optimal estimator is to look at the *average risk*—defined as the expectation of risk with respect to a *prior* distribution over $\mathcal{S}(\mathcal{H})$. Then, by minimizing the average risk over the set of all probability distributions over $\mathcal{S}(\mathcal{H})$, one obtains what is called a *Bayes estimator*, $\hat{\rho}_B$ [(Lehmann and Casella, 1998, pg. 228)]. In fact, it has been shown that the Bayes estimator is the mean if the loss function is the relative entropy [Tanaka and Komaki (2005)], while in Ref. [Banerjee *et al.* (2005)] the same was proved for a more general class of distance-measures called *Bregman divergence* (see Definition 3), which generalizes two important distance-measures—relative entropy and Hilbert-Schmidt distance, but in the classical setting. We provide a proof for the quantum setting in Section A.1 for completion.

Now, the Bayesian mean estimator for a prior distribution $\pi(\rho)$ is given by

$$\hat{\rho}_B(\mathbb{D}) = \int_{\mathcal{S}(\mathcal{H})} p(\rho|\mathbb{D})\rho \, \mathrm{d}\rho, \tag{2.3}$$

where $p(\rho|\mathbb{D})$ is the posterior probability density given by the Bayes rule:

$$p(\rho|\mathbb{D}) = \frac{p(\mathbb{D}|\rho)\pi(\rho)}{p(\mathbb{D})}, \tag{2.4}$$

and $p(\mathbb{D}) = \int_{\mathcal{S}(\mathcal{H})} \mathrm{d}\pi(\rho) p(\mathbb{D}|\rho)$. However, BME can yield nonsensical estimators if one starts with a *bad* prior, as the following example illustrates.

Example 2. *Consider a σ_X measurement on an unknown quantum state ρ in $\mathbb{C}^2$. Suppose there exists a prior $\pi(\rho)$ such that it assigns zero measure to all states in $\mathbb{C}^2$ but $|-\rangle\langle -|$. A single measurement outcome of '+' rules out the outcome '$-$' and thus annihilates the prior!*

In fact, it should be clear from the above example that some priors can be annihilated by a finite number of (independent) measurements. Thus, in general, one needs a *robust* [Blume-Kohout (2010)] prior that cannot be annihilated in order to prevent rank-deficient estimates. However, the estimator's knowledge of the true state can *still* be jeopardized in the presence of an adversary who provides her with a wrong prior. Therefore, although BME seems to be the best bet, it remains inherently ambiguous due to its dependence on the choice of priors. A systematic approach towards deriving *optimality* criteria for priors is thus a compelling problem.

The *minimax* approach, complementary to BME, seems to be doing just that. In *classical statistics*, the problem of estimating probability distributions (analogous to state estimation) has been studied using the minimax approach [Clarke and Barron (1994); Merhav and Feder (1998); Xie and Barron (2000); Komaki (2011)], that offers an alternative characterization of optimality of estimators. In the minimax approach, one looks at the space of all possible estimators defined on $\mathcal{X}$ and, for each estimator $\hat{\rho}$, picks the state ρ for which it has the worst performance or *risk* (quantified in terms of a suitably chosen distance-measure between the estimator and the true state). Then, the *minimax estimator* is the one that has the *best* worst-case risk. Such an estimator necessarily works for all states $\rho \in \mathcal{S}(\mathcal{H})$. It can be shown [Clarke and Barron (1994)] that such a minimax estimator is a Bayes estimator given a particular choice of 'non-

informative' prior. Thus, the solution to the minimax problem leads to a natural identification of a prior.

However, as pointed out in Ref. [Blume-Kohout (2010)], no such rigorous statements were known for the quantum analogue of the problem until then. Recently, the authors of Ref. [Koyama *et al.* (2017)] have studied the quantum minimax estimation problem in analogy to the classical problem [Komaki (2011)], quantifying the estimator's risk in terms of relative entropy. To summarize, they find that given an unknown quantum state ρ and some estimator $\hat{\rho}$ of it, there always exists a sequence of Bayes estimators that perform at least as well as $\hat{\rho}$ in the limiting case. Moreover, they show that there always exists a class of priors, called *latent information priors* (although, conventionally, such priors are called *least favourable*, and we shall follow the convention!) for which there is a corresponding sequence of Bayes estimators whose limit is *minimax*. Finally, they define a *minimax POVM* as a POVM that minimizes the minimax risk, see Definition 4, and study the qubit ($\mathbb{C}^2$) case in detail, obtaining the class of the least favourable priors as well as the minimax POVM for $\mathbb{C}^2$.

We extend the work done in Ref. [Koyama *et al.* (2017)] on minimax analysis (as discussed earlier) to a more general class of distance-measures called the *Bregman divergence*, see Definition 3, that generalizes both relative entropy and Hilbert-Schmidt distance. We also generalize the minimax POVM for $\mathbb{C}^2$ to Hilbert-Schmidt distance, finding that such a minimax POVM is a spherical 2-design. Moreover, by re-formulating Holevo's theorem [(Holevo, 1982, pg. 171)] for the *covariant state estimation problem* in terms of estimators, we find that a *covariant* POVM is minimax with Bregman divergence as the distance-measure. In fact, we show that a unitary 2-design arising out of a subgroup of the covariant group would also form a minimax POVM.

2.2 Mathematical preliminaries

Consider a quantum system $\mathcal{S}$ described by a finite-dimensional Hilbert space $\mathcal{H}$ with $\mathcal{S}(\mathcal{H})$ as the set of density operators on $\mathcal{H}$. Then, consider a quantum measurement to be an experiment in which the quantum system $\mathcal{S}$ is measured and let $\mathcal{X}$ be the corresponding outcome space of the measurement outcomes. Each possible event of the experiment can be identified with a subset B $\subseteq \mathcal{X}$, the event being 'the measurement outcome x lies in B'. The probability distribution of the events is thus defined over a Σ-algebra of the measurable subsets B $\subseteq \mathcal{X}$. To be in touch with physical reality, we choose the outcome space to be a Haursdorff space, i.e. a topological space where for any $x_1, x_2 \in \mathcal{X}$ there exist two disjoint open sets $X_1, X_2 \subset \mathcal{X}$ such that $x_1 \in X_1$ and $x_2 \in X_2$. This ensures that the Σ-algebra is a Borel Σ-algebra generated by countable intersections, countable unions and relative complements of open subsets of $\mathcal{X}$. Let $\mathcal{P}(\mathcal{H})$ be the set of positive operators on $\mathcal{H}$.

Definition 1 (Quantum measurement)**.** *A Positive Operator-Valued Measure (POVM) is a map $P : \Sigma \mapsto \mathcal{P}(\mathcal{H})$, where Σ is the Σ-algebra of all measurable subsets of $\mathcal{X}$. Thus, a POVM associates an operator P(B) to each $B \in \Sigma$ satisfying the following:*

1. $P(B) \geq 0, \quad \forall B \in \Sigma.$
2. $P(\mathcal{X}) = \mathbb{I}.$
3. $P\Big(\bigcup_{i=1}^{\infty} B_i\Big) = \sum_{i=1}^{\infty} P(B_i), \qquad$ *where* $\forall B_i, B_j$ *s.t.* $B_i \cap B_j = \emptyset$.

The set of all POVMs on Σ forms a convex set denoted by $\mathcal{P}$. A POVM is *informationally complete* [Watrous (2018)] if the operators $\{P(B)\}$ span $L(\mathcal{H})$, the space of linear operators on $\mathcal{H}$. The measurement statistics of such an IC-POVM is sufficient to determine, uniquely, all possible states that the quantum system could be in, in the limit when an infinite number

of measurements are performed. Optimization of data-processing deals with the practical aspect of not having infinite resources and minimizing the corresponding statistical error. Ref. [Bisio *et al.* (2009)] reviews the theoretical development of optimization techniques in quantum tomography based on informationally complete measurements. However, in this paper, we make no assumptions on the POVM. In fact, we look at an alternative definition for an optimal POVM—to be discussed later in this section.

The following lemma (see Section A.2 for proof) provides a convenient way of representing a POVM as an operator-valued density.

Lemma 1 (Existence of a POVM density)**.** *Every $P \in \mathcal{P}$ admits a density, i.e. for any POVM P there exists a finite measure $\mu(dx)$ over $\mathcal{X}$ such that $\mu(\mathcal{X}) = 1$ and*

$$P(B) = \int_B d\mu(x) M(x), \tag{2.5}$$

with $M(x) \geq 0$, and $\mathrm{tr}[M(x)] = d$ μ-almost everywhere.

The conditional probability of the event 'the measurement outcome x' lies in B given that the system is in a state ρ' is given by Born's rule as

$$\Pr[x' \in B|\ \rho] = \mathrm{tr}\, P(B)\rho = \int_B \mathrm{d}\mu(x)\, \mathrm{tr}\, M(x)\rho, \tag{2.6}$$

or, in the differential form as

$$\mathrm{d}p(x|\rho) = \mathrm{d}\mu(x)\, \mathrm{tr}\, M(x)\rho \tag{2.7}$$

which will come in handy later. Now that we have defined a quantum measurement, we proceed with the formulation.

In estimation theory [Lehmann and Casella (1998)], one typically parametrizes the system $\mathcal{S}$ by a parameter θ. The data set of the measurement outcomes is represented by a *random variable* X. Using this data set one estimates the

parameter θ or more generally ρ_θ—the *estimand*. Succinctly, this involves two random variables Θ and X defined as below:

- In the Bayesian model, the quantity θ that parametrizes the system $\mathcal{S}$ is treated as a random variable Θ. This random variable is defined over the parameter space Ω_Θ[1] and is distributed according to an a-priori probability distribution $\pi_\Theta \in \mathcal{P}(\Theta)$ (where $\mathcal{P}(\Theta)$ is the set of all probability distributions on Θ).
- X is the random variable associated with the outcomes of the measurement performed on the system $\mathcal{S}$, defined over the sample space $\mathcal{X}$. The outcomes of the measurement are conditioned on the random variable Θ. Thus, X is distributed according to the conditional probability $p_X(x|\theta)$, given by Equation (2.6).

The parameter space Θ is chosen to be a compact metric space. The set of all bounded continuous real-valued function on Θ is denoted by $\mathcal{C}(\Theta, \mathbb{R})$. The set of probability distributions $\mathcal{P}(\Theta)$ on Θ is endowed with a weak topology, which essentially defines the notion of *weak convergence*.

Definition 2. *A sequence of probability measures $\pi_n \in \mathcal{P}(\Theta)$ weak converges to μ if for every $f \in \mathcal{C}(\Theta, \mathbb{R})$,*

$$\int f d\pi_n \to \int f d\mu, \quad \text{as } n \to \infty. \tag{2.8}$$

Then, as Θ is a compact metric space and $\mathcal{P}(\Theta)$ is endowed with a weak topology, by [(Parthasarathy, 1967, Theorem 6.4)], it implies that $\mathcal{P}(\Theta)$ is also a compact metric space.

The central problem in quantum state estimation is to obtain an *estimator* of ρ_θ. We define an *estimator* as the map

$$\hat{\rho} : \mathcal{X} \mapsto \mathcal{S}(\mathcal{H}). \tag{2.9}$$

[1]However, we will abuse notation and refer to the parameter space as Θ from now onwards.

The value of $\hat{\rho}$(x) is the estimate of ρ_θ when the measurement outcome is $X = x$. We want $\hat{\rho}$(X) to be close to ρ_θ, but $\hat{\rho}$(X) is a random variable. One way of defining a meaningful measure of closeness is by defining an expectation over the conditional distribution of X, Equation (2.6). Let $L(\rho_\theta, \hat{\rho}(x))$ be the *loss function* that quantifies the closeness of an estimated state $\hat{\rho}$(x) to the true state ρ_θ. We assume two things about L:

1. $L(\rho_\theta, \hat{\rho}(x)) \geq 0, \forall\theta \in \Theta,\ \hat{\rho}$, with equality if and only if $\rho_\theta = \hat{\rho}(x)$.
2. $L(\rho_\theta, \rho_\theta) = 0, \quad \forall\theta \in \Theta$.

The average measure of closeness of $\hat{\rho}$(X) to ρ_θ is defined as the *risk function*

$$R(\rho_\theta, \hat{\rho}) = \mathbb{E}_{X|\theta}[L(\rho_\theta, \hat{\rho}(X))]. \tag{2.10}$$

One would like to obtain an estimator that minimizes the risk for all values of θ. Obviously, this problem does not have a solution, i.e. there does not exist an estimator that uniformly minimizes the risk for all values of θ except for the case when ρ_θ is a constant. Instead, one can look at the following two quantities that are a good measure of the risk in a global sense:

1. Average risk:

$$r(\pi, \hat{\rho}) = \int_\Theta \mathrm{d}\pi(\theta) R(\rho_\theta, \hat{\rho}), \tag{2.11}$$

   where $\pi(\theta)$ is an a-priori distribution over the parameter space Θ.

2. Worst-case/minimax risk:

$$\inf_{\hat{\rho}} \sup_{\theta} R(\rho_\theta, \hat{\rho}). \tag{2.12}$$

The estimator that minimizes the average risk is the Bayes estimator $\hat{\rho}_B$ [(Lehmann and Casella, 1998, pg.228)]. In Ref. [Tanaka and Komaki

(2005)] it was shown that the Bayes estimator is the mean if the loss function is the relative entropy $D(\rho_\theta||\hat{\rho}(x))$, i.e.,

$$\hat{\rho}_B = x \mapsto \int_\Theta \mathrm{d}\pi(\theta|x)\rho_\theta, \tag{2.13}$$

where $\mathrm{d}\pi(\theta|x)$ is the posterior probability distribution obtained via the Bayes rule,

$$\mathrm{d}\pi(\theta|x) = \frac{\mathrm{d}p(x|\theta)}{\mathrm{d}p_\pi(x)}\mathrm{d}\pi(\theta),$$

where $p_\pi(B) = \int_B \int_\Theta \mathrm{d}p(x|\theta)\mathrm{d}\pi(\theta)$. Note that in the continuous case, the likelihood ratio $\frac{p(x|\theta)}{p_\pi(x)}$ is replaced by the corresponding Radon-Nikodym derivative, which is defined uniquely upto the null set of p_π. In fact, the same was proved [Banerjee *et al.* (2005)] for a more general class of distance-measures called *Bregman divergence* which is the measure we will use in our analysis, but only in the classical setting. We provide a proof for the quantum setting in Section A.1 for completion. Let us now define Bregman divergence.

Definition 3 (Bregman divergence for density matrices)**.** *Let $f : [0,1] \mapsto \mathbb{R}$ be a strictly convex continuously-differentiable real-valued function. Then, the Bregman divergence between density matrices ρ, σ is defined as*

$$D_f(\rho,\sigma) = \mathrm{tr}\left(f(\rho) - f(\sigma) - f'(\sigma)(\rho-\sigma)\right).$$

Bregman divergence generalizes two important classes of distance-measures: the relative entropy obtained by choosing $f : x \mapsto x\log x$ and the Hilbert-Schmidt distance (Schatten 2-norm) obtained by choosing $f : x \mapsto x^2$.

Let us now look at a few of its important properties. First, Bregman divergence is invariant under unitary transformations of its arguments, i.e. $D_f(U\rho U^\dagger, U\sigma U^\dagger) = D_f(\rho,\sigma)$. Second, it is not a metric, as it is neither symmetric nor satisfies the triangle inequality, but by the strict

convexity of f, $D_f(\rho,\sigma) \geq 0$, with equality if and only if $\rho = \sigma$. Third, the convexity of f implies that $D_f(.,.)$ is convex in its first argument; it is jointly convex if f'' is operator convex and numerically non-increasing [Pitrik and Virosztek (2015)]. Moreover, by generalizing the proof of lower semi-continuity of relative entropy as in Ref. [Wehrl (1978)], we obtain the lower semi-continuity of Bregman divergence (see Section A.3 for the proof).

3

Bayesian state estimation

3.1 Existence of a Bayesian estimator for any estimator

Theorem 1. *Let $\hat{\rho} : \mathcal{X} \mapsto \mathcal{S}(\mathcal{H})$ be an estimator. Then, there exists a convergent sequence of priors such that the corresponding sequence of Bayes estimators $(\hat{\rho}_B^{\pi_n})_n$ converges, with*

$$R(\rho_\theta, \hat{\rho}) \geq R\Big(\rho_\theta, \lim_{n\to\infty} \hat{\rho}_B^{\pi_n}\Big), \quad \forall \theta \in \Theta. \tag{3.1}$$

Proof. Consider the average distance between the Bayes estimator and a given estimator $\hat{\rho}$ for some prior $\pi \in \mathcal{P}(\Theta)$ as the map

$$g : \pi \mapsto D_{\hat{\rho}}^f(\pi) = \int_{\mathcal{X}} \mathrm{d}p_\pi(x)\; D_f(\hat{\rho}_B^\pi(x), \hat{\rho}(x)).$$

Now, the Bayes estimator is uniquely defined up to the null set of p_π. In fact, it is discontinuous on $\mathcal{X}$, see Section A.4, and the points of discontinuity belong to the null set of p_π. So, unless the null set of p_π is empty, the Bayes estimator cannot be defined continuously since there can exist different sequences that converge to the same prior, but the limit of

the corresponding sequences of Bayes estimators may not coincide on the null set of p_π. To deal with the discontinuity of the Bayes estimator, we consider closed subsets of $\mathcal{P}(\Theta)$ with the defining property that every element of these subsets renders the corresponding Bayes estimator continuous on $\mathcal{X}$. Then, g is lower semi-continuous on each closed subset as Bregman divergence is lower-semi continuous (Section A.3). Thus, there exists a prior π_n in every subset that minimizes it on that subset. So, we look at the sequence of such priors $(\pi_n)_n$ and find that the corresponding sequence of Bayes estimators $(\hat{\rho}_B^{\pi_n})_n$ converges to a limit that has a risk lower than or equal to that of the given estimator. Let us now proceed with the proof.

We define the closed subsets of $\mathcal{P}(\Theta)$ as

$$\mathcal{P}_{\mu/n} = \left\{ \frac{\mu}{n} + \left(1 - \frac{1}{n}\right) \pi \middle| \pi \in \mathcal{P}(\Theta) \right\}, \tag{3.2}$$

where μ is a measure such that $p_\mu(x) > 0$, for all $x \in \mathcal{X}$. The latter condition ensures that the Bayes estimator for a prior that lies in $\mathcal{P}_{\mu/n}$ is continuous on $\mathcal{P}_{\mu/n}$. Then, as a closed subset of a compact set is compact, there exists a prior $\pi_n \in \mathcal{P}_{\mu/n}$ such that $D^f_{\hat{\rho}}(\pi_n) = \inf_{\pi \in \mathcal{P}_{\mu/n}} D^f_{\hat{\rho}}(\pi)$. In fact, as $\mathcal{P}(\Theta)$ is a compact metric space, the sequence of priors $(\pi_n)_n$ has a convergent subsequence. Let us denote this subsequence as $(\pi^{'}_m)_m$. Let n_m be such that $\pi_{n_m} = \pi^{'}_m$.

Then, the idea is to use the fact that each $\pi^{'}_m$ minimizes $D^f_{\hat{\rho}}$ on the corresponding closed subset $\mathcal{P}_{\mu/n_m}$ to obtain a suitable condition. To begin with, we define a prior in the neighbourhood of $\pi^{'}_{m+1} \in \mathcal{P}_{\mu/n_{m+1}}$ by taking a convex sum of it with another element in $\mathcal{P}_{\mu/n_{m+1}}$. Observe that $\left(\frac{n_m}{n_{m+1}}\pi^{'}_{m+1} + (1 - \frac{n_m}{n_{m+1}})\delta(\theta - \theta_0)\right)$ lies in $\mathcal{P}_{\mu/n_{m+1}}$, for any $\theta_0 \in \Theta$. So, we define a prior

$$\pi(\theta) = u\left(\frac{n_m}{n_{m+1}}\pi^{'}_m + \left(1 - \frac{n_m}{n_{m+1}}\right)\delta(\theta - \theta_0)\right) + (1-u)\pi^{'}_{m+1}, \tag{3.3}$$

with $0 \leq u \leq 1$. This is like considering a perturbation in the neighbourhood of π'_{m+1} and noting that the derivative of $D^f_{\hat{\rho}}(\pi)$ is positive as one approaches π'_{m+1} as it minimizes $D^f_{\hat{\rho}}(\pi)$ on the set $\mathcal{P}_{\mu/n_{m+1}}$. Thus, we have

$$\begin{aligned} 0 \leq \frac{\mathrm{d}}{\mathrm{d}u} D^f_{\hat{\rho}}(\pi)\Big|_{u=0} &= \frac{\mathrm{d}}{\mathrm{d}u} \int_{\mathcal{X}} \mathrm{d}p_\pi(x)\; D_f(\hat{\rho}^\pi_B(x), \hat{\rho}(x))\Big|_{u=0} \\ &= \int_{\mathcal{X}} \frac{\mathrm{d}p_\pi(x)}{\mathrm{d}u}\Big|_{u=0} D_f(\hat{\rho}^{\pi'_{m+1}}_B(x), \hat{\rho}(x)) + \\ &\quad \int_{\mathcal{X}} \mathrm{d}p_{\pi'_{m+1}}(x) \frac{\mathrm{d}}{\mathrm{d}u} D_f(\hat{\rho}^\pi_B(x), \hat{\rho}(x))\Big|_{u=0}. \end{aligned} \tag{3.4}$$

Let $k = \frac{n_m}{n_{m+1}}$. Then,

$$\begin{aligned} \mathrm{d}p_\pi(x) &= \int \mathrm{d}p(x|\theta) \Big(u\Big(k\pi'_m(\theta) + (1-k)\delta(\theta - \theta_0)\Big) + \\ &\qquad (1-u)\pi'_{m+1}(\theta) \Big) \mathrm{d}\theta. \end{aligned}$$

$$\implies \frac{\mathrm{d}p_\pi(x)}{\mathrm{d}u}\Big|_{u=0} = k\mathrm{d}p_{\pi'_m}(x) + (1-k)\mathrm{d}p(x|\theta_0) - \mathrm{d}p_{\pi'_{m+1}}(x). \tag{3.5}$$

So, the first term in (3.4) is

$$\int_{\mathcal{X}} \Big(k\mathrm{d}p_{\pi'_m}(x) + (1-k)\mathrm{d}p(x|\theta_0) - \mathrm{d}p_{\pi'_{m+1}}(x)\Big) D_f\big(\hat{\rho}^{\pi'_{m+1}}_B(x), \hat{\rho}(x)\big),$$

while the second term, using Lemma 16, is

$$\begin{aligned} &= \int_{\mathcal{X}} \mathrm{d}p_{\pi'_{m+1}}(x) \frac{\mathrm{d}}{\mathrm{d}u} \operatorname{tr} f\big(\hat{\rho}^\pi_B(x)\big) - f'\big(\hat{\rho}(x)\big)\big(\hat{\rho}^\pi_B(x) - \hat{\rho}(x)\big)\Big|_{u=0} \\ &= \int_{\mathcal{X}} \mathrm{d}p_{\pi'_{m+1}}(x) \operatorname{tr}\Big(f'\big(\hat{\rho}^{\pi'_{m+1}}_B(x)\big) - f'\big(\hat{\rho}(x)\big)\Big) \frac{\mathrm{d}}{\mathrm{d}u} \hat{\rho}^\pi_B(x)\Big|_{u=0}. \end{aligned} \tag{3.6}$$

Let us now calculate the derivative of the Bayes estimator.

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}u}\hat{\rho}_B^{\pi}(x)\Big|_{u=0} &= \frac{\mathrm{d}}{\mathrm{d}u}\int_{\Theta}\frac{\mathrm{d}p(x|\theta)}{\mathrm{d}p_{\pi}(x)}\rho_{\theta}\mathrm{d}\pi(\theta)\Big|_{u=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}u}\int_{\Theta}\frac{1}{\frac{\mathrm{d}p_{\pi}(x)}{\mathrm{d}p(x|\theta)}}\rho_{\theta}\mathrm{d}\pi(\theta)\Big|_{u=0} \\
&= \int_{\Theta}\frac{\rho_{\theta}\Big(k\mathrm{d}\pi_m^{'}(\theta)+(1-k)\delta(\theta-\theta_0)\mathrm{d}\theta-\mathrm{d}\pi_{m+1}^{'}(\theta)\Big)}{\frac{\mathrm{d}p_{\pi_{m+1}^{'}}}{\mathrm{d}p(x|\theta)}}- \\
&\int_{\Theta}\frac{\rho_{\theta}\mathrm{d}\pi_{m+1}^{'}(\theta)}{\left(\frac{\mathrm{d}p_{\pi_{m+1}^{'}}}{\mathrm{d}p(x|\theta)}\right)^2}\frac{\mathrm{d}}{\mathrm{d}u}\left(\frac{\mathrm{d}p_{\pi}(x)}{\mathrm{d}p(x|\theta)}\right)\Big|_{u=0}. \qquad (3.7)
\end{aligned}$$

Now, the derivative with respect to u in the second term can be calculated by exchanging the order of differentiation as $p(x|\theta)$ is independent of u. So, we have

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}u}\left(\frac{\mathrm{d}p_{\pi}(x)}{\mathrm{d}p(x|\theta)}\right)\Big|_{u=0} &= \frac{\mathrm{d}}{\mathrm{d}p(x|\theta)}\left(\frac{\mathrm{d}p_{\pi}(x)}{\mathrm{d}u}\right)\Big|_{u=0} \\
&= k\frac{\mathrm{d}p_{\pi_m^{'}}(x)}{\mathrm{d}p(x|\theta)}+(1-k)\frac{\mathrm{d}p(x|\theta_0)}{\mathrm{d}p(x|\theta)}-\frac{\mathrm{d}p_{\pi_{m+1}^{'}}}{\mathrm{d}p(x|\theta)}(x).
\end{aligned}$$

Plugging in (3.7) we obtain,

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}u}\hat{\rho}_B^{\pi}(x)\Big|_{u=0} &= \int_{\Theta}\frac{\rho_{\theta}\Big(k\mathrm{d}\pi_m^{'}(\theta)+(1-k)\delta(\theta-\theta_0)\mathrm{d}\theta-\mathrm{d}\pi_{m+1}^{'}(\theta)\Big)}{\frac{\mathrm{d}p_{\pi_{m+1}^{'}}}{\mathrm{d}p(x|\theta)}}- \\
&\int_{\Theta}\frac{\rho_{\theta}\mathrm{d}\pi_{m+1}^{'}(\theta)}{\left(\frac{\mathrm{d}p_{\pi_{m+1}^{'}}}{\mathrm{d}p(x|\theta)}\right)^2}\left(k\frac{\mathrm{d}p_{\pi_m^{'}}(x)}{\mathrm{d}p(x|\theta)}+(1-k)\frac{\mathrm{d}p(x|\theta_0)}{\mathrm{d}p(x|\theta)}-\frac{\mathrm{d}p_{\pi_{m+1}^{'}}(x)}{\mathrm{d}p(x|\theta)}\right).
\end{aligned}$$

Now, in the limit $m \to \infty$, the coefficient of k vanishes in the expression above due to weak convergence, while the last term of the first integral cancels with the last term of the second integral. So, we have

$$\lim_{m\to\infty} \frac{\mathrm{d}}{\mathrm{d}u}\hat{\rho}_B^{\pi}(x)\Big|_{u=0} = \lim_{m\to\infty}(1-k)\frac{\mathrm{d}p(x|\theta_0)}{\mathrm{d}p_{\pi'_{m+1}}(x)}\Big(\rho_{\theta_0} - \hat{\rho_B}^{\pi'_{m+1}}(x)\Big). \quad (3.8)$$

Applying the limit and plugging (3.8) in (3.6), we find that the second term in (3.4) is

$$\begin{aligned} &= \lim_{m\to\infty}\int_{\mathcal{X}} \mathrm{d}p_{\pi'_{m+1}}(x)\,\mathrm{tr}\left(f'\big(\hat{\rho}_B^{\pi'_{m+1}}(x)\big) - f'\big(\hat{\rho}(x)\big)\right)(1-k)\frac{\mathrm{d}p(x|\theta_0)}{\mathrm{d}p_{\pi'_{m+1}}(x)}\Big(\rho_{\theta_0} - \hat{\rho}_B^{\pi'_{m+1}}(x)\Big) \\ &= \lim_{m\to\infty}(1-k)\int_{\mathcal{X}} \mathrm{d}p(x|\theta_0)\,\mathrm{tr}\left(f'\big(\hat{\rho}_B^{\pi'_{m+1}}(x)\big) - f'\big(\hat{\rho}(x)\big)\right)\Big(\rho_{\theta_0} - \hat{\rho}_B^{\pi'_{m+1}}(x)\Big). \end{aligned}$$

Finally, combining both the terms of (3.4) and applying the limit, we find that

$$\begin{aligned} 0 \;\leq\; & \lim_{m\to\infty}\frac{\mathrm{d}}{\mathrm{d}u}D_{\hat{\rho}}^{f}(\pi)\Big|_{u=0} \\ = \; & \lim_{m\to\infty}\int_{\mathcal{X}}\Big(k\mathrm{d}p_{\pi'_{m+1}}(x) + (1-k)\mathrm{d}p(x|\theta_0) - \mathrm{d}p_{\pi'_{m+1}}(x)\Big)D_f\big(\hat{\rho}_B^{\pi'_{m+1}}(x), \hat{\rho}(x)\big) + \\ & (1-k)\int_{\mathcal{X}}\mathrm{d}p(x|\theta_0)\,\mathrm{tr}\left(f'\big(\hat{\rho}_B^{\pi'_{m+1}}(x)\big) - f'\big(\hat{\rho}(x)\big)\right)\Big(\rho_{\theta_0} - \hat{\rho}_B^{\pi'_{m+1}}(x)\Big). \quad (3.9) \end{aligned}$$

This implies that

$$\begin{aligned} \lim_{m\to\infty}(1-k)\int_{\mathcal{X}}\mathrm{d}p_{\pi'_{m+1}}(x)\Big)D_f\big(\hat{\rho}_B^{\pi'_{m+1}}(x), \hat{\rho}(x)\big) \leq \\ \lim_{m\to\infty}(1-k)\int_{\mathcal{X}}\mathrm{d}p(x|\theta_0)\,\mathrm{tr}\left(f'\big(\hat{\rho}_B^{\pi'_{m+1}}(x)\big) - \right. \\ \left. f'\big(\hat{\rho}(x)\big)\right)\Big(\rho_{\theta_0} - \hat{\rho}_B^{\pi'_{m+1}}(x)\Big) + \\ \int_{\mathcal{X}}\mathrm{d}p(x|\theta_0)D_f\big(\hat{\rho}_B^{\pi'_{m+1}}(x), \hat{\rho}(x)\big). \quad (3.10) \end{aligned}$$

The right-hand side of the inequality above can be rearranged to obtain

$$\lim_{m\to\infty} \underbrace{\int_{\mathcal{X}} \mathrm{d}p_{\pi'_{m+1}}(x)\Big) D_f\big(\hat{\rho}_B^{\pi'_{m+1}}(x), \hat{\rho}(x)\big)}_{\geq 0, \text{ due to non-negativity of Bregman divergence.}} \leq \lim_{m\to\infty} \int_{\mathcal{X}} \mathrm{d}p(x|\theta_0) D_f\big(\rho_{\theta_0}, \hat{\rho}(x)\big) - D_f\big(\rho_{\theta_0}, \hat{\rho}_B^{\pi'_{m+1}}(x)\big).$$

This implies that

$$\lim_{m\to\infty} R(\rho_{\theta_0}, \hat{\rho}_B^{\pi'_{m+1}}) \leq R(\rho_{\theta_0}, \hat{\rho}), \qquad \forall \theta_0 \in \Theta.$$

But, as Bregman divergence is lower semi-continuous (Section A.3), we have

$$R(\rho_{\theta_0}, \lim_{m\to\infty} \hat{\rho}_B^{\pi'_{m+1}}) \leq \lim_{m\to\infty} R(\rho_{\theta_0}, \hat{\rho}_B^{\pi'_{m+1}}).$$

Therefore, we arrive at our result, i.e.

$$R(\rho_{\theta_0}, \lim_{m\to\infty} \hat{\rho}_B^{\pi'_{m+1}}) \leq R(\rho_{\theta_0}, \hat{\rho}), \qquad \forall \theta_0 \in \Theta.$$

□

3.2 A Bayesian method for minimax state estimation

Theorem 2. *There exists a convergent sequence of priors $(\pi_n)_n$ such that the limit of the sequence maximizes the average risk, Equation* (2.11)*, of the Bayes estimator. The limit of such a sequence is referred to as a least favourable prior. Moreover, the sequence of Bayes estimators $(\hat{\rho}_B^{\pi_n})_n$ converges such that the limit of the sequence is minimax, i.e*

$$\inf_{\hat{\rho}} \sup_{\theta} R(\rho_\theta, \hat{\rho}) = \sup_{\theta} R(\rho_\theta, \lim_{n\to\infty} \hat{\rho}_B^{\pi_n}).$$

Proof. Consider the average risk of the Bayes estimator for a prior $\pi \in \mathcal{P}(\Theta)$ as the map

$$h : \pi \mapsto r(\pi, \hat{\rho}_B^\pi) = \int_\Theta \mathrm{d}\pi(\theta) \int_\mathcal{X} \mathrm{d}p(x|\theta) D_f\big(\rho_\theta, \hat{\rho}_B^\pi(x)\big).$$

Due to the discontinuity of the Bayes estimator, we follow the same regularization arguments as made earlier and define closed subsets of $\mathcal{P}(\Theta)$, Equation (3.2), such that the Bayes estimator is continuous on each of these subsets. The map $h : \pi \mapsto r(\pi, \hat{\rho}_B^\pi)$ is then continuous on each of the subsets. Since these subsets are closed subsets of a compact set they are themselves compact. Therefore, h attains a maximum on each of the subsets. Then, denoting the maxima in each subset $\mathcal{P}_{\mu/n_{m+1}}$ as π'_{m+1}, we define a prior as done earlier in Equation (3.3) as a convex sum of π'_{m+1} and another element in $\mathcal{P}_{\mu/n_{m+1}}$. Since the average risk is maximized on $\mathcal{P}_{\mu/n_{m+1}}$, the derivative of $r(\pi, \hat{\rho}_B^\pi)$ is negative as one approaches π'_{m+1}, i.e.

$$\begin{aligned} 0 \geq \frac{\mathrm{d}}{\mathrm{d}u} r(\pi, \hat{\rho}_B^\pi)\bigg|_{u=0} &= \frac{\mathrm{d}}{\mathrm{d}u} \int_\Theta \mathrm{d}\pi(\theta) \int_\mathcal{X} \mathrm{d}p(x|\theta) D_f\big(\rho_\theta, \hat{\rho}_B^\pi(x)\big)\bigg|_{u=0} \\ &= \int_\Theta \frac{\mathrm{d}\pi(\theta)}{\mathrm{d}u}\bigg|_{u=0} \int_\mathcal{X} \mathrm{d}p(x|\theta) D_f\big(\rho_\theta, \hat{\rho}_B^{\pi'_{m+1}}(x)\big) + \\ &\quad \int_\Theta \mathrm{d}\pi'_{m+1}(\theta) \int_\mathcal{X} \mathrm{d}p(x|\theta) \frac{\mathrm{d}}{\mathrm{d}u} D_f\big(\rho_\theta, \hat{\rho}_B^\pi(x)\big)\bigg|_{u=0}. \end{aligned} \tag{3.11}$$

Evaluating the derivatives using Lemma 16, the first term in (3.11) is

$$\int_\mathcal{X} \mathrm{d}p(x|\theta_0) D_f\big(\rho_{\theta_0}, \hat{\rho}_B^{\pi'_{m+1}}(x)\big) - \int_\Theta \mathrm{d}\pi'_{m+1}(\theta) \int_\mathcal{X} \mathrm{d}p(x|\theta) D_f\big(\rho_\theta, \hat{\rho}_B^{\pi'_{m+1}}(x)\big),$$

while the derivative in the second term of (3.11) is

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}u}D_f\big(\rho_\theta,\hat{\rho}_B^{\pi}(x)\big)\Big|_{u=0} &= \frac{\mathrm{d}}{\mathrm{d}u}\,\mathrm{tr}\left[f(\rho_\theta)-f(\hat{\rho}_B^{\pi}(x))-f'(\hat{\rho}_B^{\pi}(x))\big(\rho_\theta-\hat{\rho}_B^{\pi}(x)\big)\right]\Big|_{u=0}\\ &= \mathrm{tr}\Big[-f'(\hat{\rho}_B^{\pi'_{m+1}}(x))\frac{\mathrm{d}}{\mathrm{d}u}\hat{\rho}_B^{\pi}(x)\Big|_{u=0}+f'(\hat{\rho}_B^{\pi'_{m+1}}(x))\frac{\mathrm{d}}{\mathrm{d}u}\hat{\rho}_B^{\pi}(x)\Big|_{u=0}\\ &\quad -\big(\rho_\theta-\hat{\rho}_B^{\pi'_{m+1}}(x)\big)\frac{\mathrm{d}}{\mathrm{d}u}f'(\hat{\rho}_B^{\pi}(x))\Big|_{u=0}\Big]\\ &= \mathrm{tr}\Big[\big(\hat{\rho}_B^{\pi'_{m+1}}(x)-\rho_\theta\big)\frac{\mathrm{d}}{\mathrm{d}u}f'(\hat{\rho}_B^{\pi}(x))\Big|_{u=0}\Big].\end{aligned}$$

So, plugging this in the second term of (3.11), we have

$$\begin{aligned}&\int_\Theta \mathrm{d}\pi'_{m+1}(\theta)\int_{\mathcal{X}}\mathrm{d}p(x|\theta)\,\mathrm{tr}\left[\big(\hat{\rho}_B^{\pi'_{m+1}}(x)-\rho_\theta\big)\frac{\mathrm{d}}{\mathrm{d}u}f'(\hat{\rho}_B^{\pi}(x))\Big|_{u=0}\right]\\ &=\mathrm{tr}\left[\int_{\mathcal{X}}\int_\Theta \mathrm{d}\pi'_{m+1}(\theta)\mathrm{d}p(x|\theta)\big(\hat{\rho}_B^{\pi'_{m+1}}(x)-\rho_\theta\big)\frac{\mathrm{d}}{\mathrm{d}u}f'(\hat{\rho}_B^{\pi}(x))\Big|_{u=0}\right]\\ &=\mathrm{tr}\left[\int_{\mathcal{X}}\left(\mathrm{d}p_{\pi'_{m+1}}(x)\hat{\rho}_B^{\pi'_{m+1}}(x)-\int_\Theta \mathrm{d}\pi'_{m+1}(\theta)\mathrm{d}p(x|\theta)\rho_\theta\right)\frac{\mathrm{d}}{\mathrm{d}u}f'(\hat{\rho}_B^{\pi}(x))\Big|_{u=0}\right]\\ &=0. \qquad (3.12)\end{aligned}$$

Thus, applying the limit $m\to\infty$ we arrive at the following inequality,

$$\begin{aligned}0 \;\geq\; &\lim_{m\to\infty}\int_{\mathcal{X}}\mathrm{d}p(x|\theta_0)D_f\big(\rho_{\theta_0},\hat{\rho}_B^{\pi'_{m+1}}(x)\big)-\\ &\int_\Theta \mathrm{d}\pi'_{m+1}(\theta)\int_{\mathcal{X}}\mathrm{d}p(x|\theta)D_f\big(\rho_\theta,\hat{\rho}_B^{\pi'_{m+1}}(x)\big), \qquad (3.13)\end{aligned}$$

which implies that

$$\begin{aligned}&\lim_{m\to\infty}\int_{\mathcal{X}}\mathrm{d}p(x|\theta_0)D_f\big(\rho_{\theta_0},\hat{\rho}_B^{\pi'_{m+1}}(x)\big)\leq\\ &\lim_{m\to\infty}\int_\Theta \mathrm{d}\pi'_{m+1}(\theta)\int_{\mathcal{X}}\mathrm{d}p(x|\theta)D_f\big(\rho_\theta,\hat{\rho}_B^{\pi'_{m+1}}(x)\big). \qquad (3.14)\end{aligned}$$

So, we have

$$\lim_{m\to\infty}R(\rho_{\theta_0},\hat{\rho}_B^{\pi'_{m+1}}) \;\leq\; \lim_{m\to\infty}\int_\Theta \mathrm{d}\pi'_{m+1}(\theta)R(\rho_\theta,\hat{\rho}_B^{\pi'_{m+1}}),\quad \forall\theta_0\in\Theta.$$

The lower semi-continuity of Bregman divergence implies that

$$R(\rho_{\theta_0}, \lim_{m\to\infty} \hat{\rho}_B^{\pi'_{m+1}}) \leq \lim_{m\to\infty} \int_\Theta \mathrm{d}\pi'_{m+1}(\theta) R(\rho_\theta, \hat{\rho}_B^{\pi'_{m+1}}).$$

Thus, we have

$$\sup_{\theta_0} R(\rho_{\theta_0}, \lim_{m\to\infty} \hat{\rho}_B^{\pi'_{m+1}}) \leq \lim_{m\to\infty} \int_\Theta \mathrm{d}\pi'_{m+1}(\theta) R(\rho_\theta, \hat{\rho}_B^{\pi'_{m+1}}).$$

But, the other direction of the inequality above is true trivially i.e.

$$\sup_{\theta_0} R(\rho_{\theta_0}, \lim_{m\to\infty} \hat{\rho}_B^{\pi'_{m+1}}) \geq \lim_{m\to\infty} \int_\Theta \mathrm{d}\pi'_{m+1}(\theta) R(\rho_\theta, \hat{\rho}_B^{\pi'_{m+1}}).$$

Therefore, we obtain

$$\sup_{\theta_0} R(\rho_{\theta_0}, \lim_{m\to\infty} \hat{\rho}_B^{\pi'_{m+1}}) = \lim_{m\to\infty} \int_\Theta \mathrm{d}\pi'_{m+1}(\theta) R(\rho_\theta, \hat{\rho}_B^{\pi'_{m+1}}). \tag{3.15}$$

But,

$$\lim_{m\to\infty} \int_\Theta \mathrm{d}\pi'_{m+1}(\theta) R(\rho_\theta, \hat{\rho}_B^{\pi'_{m+1}}) = \lim_{m\to\infty} \sup_{\pi\in\mathcal{P}_{\mu/n_{m+1}}} \int_\Theta \mathrm{d}\pi(\theta) R(\rho_\theta, \hat{\rho}_B^{\pi}).$$

By Lemma 17, the limit of the suprema over subsets $\mathcal{P}_{\mu/n_{m+1}}$ can be replaced by a supremum over the set $\mathcal{P}(\Theta)$ since the sequence of subsets $\mathcal{P}_{\mu/n_{m+1}}$ is dense in $\mathcal{P}(\Theta)$. Thus, we have

$$\begin{aligned}\lim_{m\to\infty} \int_\Theta \mathrm{d}\pi'_{m+1}(\theta) R(\rho_\theta, \hat{\rho}_B^{\pi'_{m+1}}) &= \sup_{\pi\in\mathcal{P}(\Theta)} \int_\Theta \mathrm{d}\pi(\theta) R(\rho_\theta, \hat{\rho}_B^{\pi}) \\ &= \sup_{\pi\in\mathcal{P}(\Theta)} \inf_{\hat{\rho}} \int_\Theta \mathrm{d}\pi(\theta) R(\rho_\theta, \hat{\rho}). \end{aligned} \tag{3.16}$$

Using the minimax theorem for lower semi-continuous and quasi-convex functions [(Sion, 1958, Theorem 3.4)], we can exchange the infimum and the supremum to obtain

$$\sup_{\pi\in\mathcal{P}(\Theta)} \inf_{\hat{\rho}} \int_\Theta \mathrm{d}\pi(\theta) R(\rho_\theta, \hat{\rho}) = \inf_{\hat{\rho}} \sup_{\pi\in\mathcal{P}(\Theta)} \int_\Theta \mathrm{d}\pi(\theta) R(\rho_\theta, \hat{\rho}) = \inf_{\hat{\rho}} \sup_{\Theta} R(\rho_\theta, \hat{\rho}).$$

Thus, by (3.15) and (3.16) we have the result

$$\inf_{\hat{\rho}} \sup_{\theta} R(\rho_\theta, \hat{\rho}) = \sup_{\theta} R(\rho_\theta, \lim_{m\to\infty} \hat{\rho}_B^{\pi'_{m+1}}).$$

□

Theorem 1 and Theorem 2 are based on the assumption that the underlying POVM is fixed. However, in general, the risk depends on the POVM P, i.e. $R(\rho_\theta, \hat{\rho}) \equiv R_P(\rho_\theta, \hat{\rho})$. One way of defining an optimal POVM could be to minimize the worst-case risk over $\mathcal{P}$, the convex set of all POVMs. The POVM that minimizes the worst-case risk is called a *minimax* POVM.

Definition 4 (Minimax POVM)**.** *A POVM P^* is minimax if:*

$$\inf_{P\in\mathcal{P}} \inf_{\hat{\rho}} \sup_{\theta} R_P(\rho_\theta, \hat{\rho}) = \inf_{\hat{\rho}} \sup_{\theta} R_{P^*}(\rho_\theta, \hat{\rho}) \tag{3.17}$$

where ρ_θ is the estimand, $\hat{\rho} : \mathcal{X} \mapsto \mathcal{S}(\mathcal{H})$ is an estimator with risk $R_P(\rho_\theta, \hat{\rho})$ which is a function of the POVM P, and $\mathcal{P}$ is the convex set of all POVMs on the measurement outcome space $\mathcal{X}$.

We will obtain a minimax POVM for a restricted problem in the next chapter.

4

Covariant state estimation

While it remains unclear as to how one could obtain a minimax POVM for general state estimation, if we restrict ourselves to the case of *covariant state estimation* the situation simplifies.

In the covariant state estimation problem, as discussed in Ref. [Holevo (1982)], one is given a fixed state ρ_{θ_0} and is interested in estimating all the states ρ_θ that lie in the orbit $\{V_g \rho_{\theta_0} V_g^\dagger\}$, where $g \in G$ is a parametric group of transformations of the parameter space Θ and $g \mapsto V_g$ is a (continuous) projective unitary representation of G. One can think of this as representing the following physical scenario. Given that the parameter θ labels the quantum states of the Hilbert space $\mathcal{H}$, θ can be assumed to be describing some aspects of the preparation procedure for the state ρ_θ—a transformation g of the parameter θ_0 results in the preparation of the state $\rho_\theta = V_g \rho_{\theta_0} V_g^\dagger$ where $\theta = g\theta_0$. Covariant state estimation thus corresponds to the estimation of the state ρ_θ with the measurement outcome space $\mathcal{X}$ being identical to the parameter space Θ. Let us first define a *covariant* measurement.

Definition 5 (Covariant measurement)**.** *Let G be a parametric group of trans-*

formations of a set Θ and $g \mapsto V_g$ be a (continuous) projective unitary representation of G in a Hilbert space $\mathcal{H}$. Let $M(d\hat{\theta})$ be a positive operator-valued measure defined on the σ-algebra $\mathcal{A}(\Theta)$ of Borel subsets of Θ. Then $M(d\hat{\theta})$ is covariant with respect to the representation $g \mapsto V_g$ if

$$V_g^\dagger M(B) V_g = M(B_{g^{-1}}), \quad g \in G, \tag{4.1}$$

for any $B \in \mathcal{A}(\Theta)$, where $B_g = \{\theta' : \theta' = g\theta, \ \theta \in B\}$.

If $M(d\hat{\theta})$ is covariant, then

$$\operatorname{tr} M(B)\rho_\theta = \operatorname{tr} \rho_0 V_g^\dagger M(B) V_g = \operatorname{tr} \rho_0 M(B_{g^{-1}}).$$

Thus,

$$\Pr[\hat{\theta} \in B |\ g\theta_0] = \Pr[\hat{\theta} \in B_{g^{-1}} |\ \theta_0],$$

i.e. a covariant measurement preserves the probability distribution under the transformation of the state. We refer the reader to Ref. [Holevo (1982)] for a more detailed discussion on covariant measurements.

Before we start building towards the proof of Theorem 3, let us look at some of the properties of the parametric group G to understand the situation better. First, the group G is chosen to act transitively on Θ. This ensures that the map $g \mapsto g\theta_0$ maps G onto the whole Θ. Second, G is assumed to be unimodular which implies that there exists an invariant measure μ on G. Third, G is assumed to be compact which ensures that the measure $\mu < \infty$. The measure μ is normalized as $\mu(G) = 1$. Now, we are interested in an invariant measure ν on the Σ-algebra $\mathcal{A}(\Theta)$ on Θ such that

$$\nu(B) = \nu(B_g), \quad B \in \mathcal{A}(\Theta),$$

where $B_g = \{\theta' : \theta' = g\theta, \ \theta \in B\}$. If G_0, the stationary subgroup of G, is unimodular then such a measure ν exists and if G_0 is compact then ν

is finite and can be constructed from μ by demanding that the following relation holds for all integrable functions f on Θ:

$$\int_G f(g\theta_0)\mathrm{d}\mu(g) = \int_\Theta f(\theta)\mathrm{d}\nu(\theta). \tag{4.2}$$

We now state Proposition 2.1 from Ref. [Holevo (1982)] as the following lemma that gives a relation between the two measures.

Lemma 2. *Let $M(d\theta)$ be a measurement covariant with respect to a projective unitary representation $g \mapsto V_g$ of the parametric group G acting on Θ. For any density operator $\rho \in \mathcal{H}$, and for any Borel set $B \in \mathcal{A}(\Theta)$*

$$\int_G \mathrm{tr}[V_g \rho V_g^\dagger M(B)] d\mu(g) = \nu(B) \tag{4.3}$$

Let us pause here to look at an example.

Example 3. *Let us assume that we are interested in estimating all those states in $\mathbb{C}^2$ that lie on the Bloch sphere. Thus, the parameter space Θ is $\mathbb{S}^2$. This is a covariant estimation problem with the parametric group of transformations on $\mathbb{S}^2$ being SO(3). Its projective unitary representation is the quotient subgroup SU(2)/U(1). Let us assume that the initial state ρ_{θ_0} is $|0\rangle\langle 0|$. Then, the elements of SU(2)/U(1) generate all the states on the Bloch sphere that are parametrized by a set of two parameters: the latitude θ[1] and azimuth ϕ, with the states being identified as $|\theta, \phi\rangle$. Note that an element of SU(2)/U(1) can be written in terms of these as*

$$U_{\theta,\phi} = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2}e^{-i\phi} \\ \sin\frac{\theta}{2}e^{i\phi} & \cos\frac{\theta}{2} \end{bmatrix}.$$

It can be shown [(Holevo, 1982, Theorem 2.1)] (stated as Lemma 18 for Ref.) that starting from a positive operator P_0 that commutes with all the elements of the stationary subgroup of SU(2)/U(1) such that it satisfies Equation (A.4)*, setting*

[1] We apologize for the redundancy, but it is best to stick to conventional symbols.

$M(\theta,\phi) = U_{\theta,\phi} P_0 U^{\dagger}_{\theta,\phi}$ implies that the measurement defined with $M(\theta,\phi)$ as the operator-valued density with respect to the uniform measure on Θ is covariant. In this case, $P_0 = 2|0\rangle\langle 0|$ and the operator-valued density is

$$M(\theta,\phi) = 2\begin{bmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{bmatrix} \cdot \begin{bmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2}e^{-i\phi} \end{bmatrix} = 2\begin{bmatrix} \cos^2\frac{\theta}{2} & \cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{-i\phi} \\ \cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{i\phi} & \sin^2\frac{\theta}{2} \end{bmatrix}.$$

It is straightforward to verify that $\frac{1}{4\pi}\int_{S^2} M(\theta,\phi)\sin\theta d\theta d\phi = \mathbb{I}$.

Having defined and illustrated the problem of covariant state estimation, we now recall Holevo's theorem [(Holevo, 1982, Theorem 3.1)], which states that for every loss function that is invariant under the group transformation g, the minimax risk as well as the average risk attain their minima at a covariant measurement. But, the analysis in Ref. [Holevo (1982)] is done for loss functions expressed as functions of the true parameter and the estimator of the parameter. It can be recast in terms of the general framework involving estimators that are functions of the parameter, $\hat{\rho} : \Theta \mapsto \mathcal{D}(\mathcal{H})$ by simply choosing the domain of the loss function to be the set of density matrices $\mathcal{S}(\mathcal{H})$ as opposed to the parameter space Θ. We thus state it as the following lemma which is the main ingredient of the proof of Theorem 3.

Lemma 3 (Theorem 3.1, [Holevo (1982)]). *] In the quantum covariant statistical estimation problem, given an estimator $\hat{\rho}$ of the state, the minima of the average risk $r_P(\nu,\hat{\rho})$ with respect to the uniform Haar measure ν on Θ and the worst case risk $\sup_\theta R_P(\rho_\theta,\hat{\rho})$ for all $\Theta-$measurements are achieved on a covariant measurement. Moreover, for any covariant measurement P_c, we have*

$$r_{P_c}(\nu,\hat{\rho}) = \sup_\theta R_{P_c}(\rho_\theta,\hat{\rho}) = R_{P_c}(\rho_\theta,\hat{\rho}), \quad \theta \in \Theta \tag{4.4}$$

Note: A covariant measurement is *not* a unique minimum for either the average or the worst-case risk.

The above theorem implies that for any measurement P, there exists a covariant measurement that minimizes the average risk as well as the worst case risk for a fixed estimator $\hat{\rho}$. But, we know that for a fixed measurement the average risk is minimized by the Bayes estimator $\hat{\rho}_B$. Thus, the Bayes estimator minimizes the average risk for a covariant measurement. However, the invariance of the loss function implies that the Bayes estimator must be covariant under the group transformations as shown below.

Lemma 4. *The Bayes estimator is covariant under the group transformations V_g, i.e.*

$$\hat{\rho}_B(B_g) = V_g \hat{\rho}_B(B) V_g^\dagger, \quad B \in \mathcal{A}(\Theta).$$

Proof. Recalling the invariance property of the loss function: $L(\rho_\theta, \hat{\rho}(x)) = L(\rho_{g\theta}, \hat{\rho}(gx)) = L(V_g \rho_\theta V_g^\dagger, V_g \hat{\rho}(x) V_g^\dagger)$, let us verify for the case of Bayes estimator. Recalling Equation (2.13), we have

$$\hat{\rho}_B(B_g) \;=\; \frac{\int_\Theta \mathrm{d}\nu(\theta)\, \mathrm{tr}\, \rho_\theta P(B_g) \rho_\theta}{\int_\Theta \mathrm{d}\nu(\theta)\, \mathrm{tr}\, \rho_\theta P(B_g)}.$$

As we are interested in a covariant measurement $P(B_g) = V_g P(B) V_g^\dagger$, therefore

$$\begin{aligned}
\hat{\rho}_B(B_g) &= \frac{\int_\Theta \mathrm{d}\nu(\theta) \rho_\theta\, \mathrm{tr}\, \rho_\theta V_g P(B) V_g^\dagger}{\int_\Theta \mathrm{d}\nu(\theta)\, \mathrm{tr}\, \rho_\theta V_g P(B) V_g^\dagger} \\
&= \frac{\int_\Theta \mathrm{d}\nu(\theta) \rho_\theta\, \mathrm{tr}\, V_g^\dagger \rho_\theta V_g P(B)}{\int_\Theta \mathrm{d}\nu(\theta)\, \mathrm{tr}\, V_g^\dagger \rho_\theta V_g P(B)} \\
&= \frac{\int_\Theta \mathrm{d}\nu(\theta) \rho_\theta\, \mathrm{tr}\, \rho_{g^{-1}\theta} P(B)}{\int_\Theta \mathrm{d}\nu(\theta)\, \mathrm{tr}\, \rho_{g^{-1}\theta} P(B)}.
\end{aligned}$$

By the invariance of ν and the fact that $\rho_\theta = V_g \rho_{g^{-1}\theta} V_g^\dagger$, we finally obtain

$$\begin{aligned}\hat{\rho}_B(B_g) &= \frac{\int_\Theta \mathrm{d}\nu(g^{-1}\theta) V_g \rho_{g^{-1}\theta} V_g^\dagger \operatorname{tr} \rho_{g^{-1}\theta} P(B)}{\int_\Theta \mathrm{d}\nu(g^{-1}\theta) \operatorname{tr} \rho_{g^{-1}\theta} P(B)} \\ &= V_g \left\{ \frac{\int_\Theta \mathrm{d}\nu(g^{-1}\theta) \rho_{g^{-1}\theta} \operatorname{tr} \rho_{g^{-1}\theta} P(B)}{\int_\Theta \mathrm{d}\nu(g^{-1}\theta) \operatorname{tr} \rho_{g^{-1}\theta} P(B)} \right\} V_g^\dagger = V_g \hat{\rho}_B(B) V_g^\dagger.\end{aligned}$$

□

Thus, we have established two things about a covariant measurement. First, that the risk of a covariant measurement is independent of the state ρ_θ and second, that it minimizes the average as well as the worst-case risk among all measurements. But, the problem of finding a minimax POVM is closely tied to obtaining a least favourable prior which in turn is tied to the underlying measurement. The following lemma gives a least favourable prior and the corresponding measurement in the context of covariant state estimation.

Lemma 5. *The uniform measure on the parameter space Θ is a least favourable prior for covariant measurements.*

Proof. As the Bayes estimator $\hat{\rho}_B^\pi$ minimizes the average risk with respect to the prior π,

$$\sup_\theta R_{P_c}(\rho_\theta, \rho_B^\nu) = \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_{P_c}(\rho_\theta, \rho_B^\nu) \geq \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_{P_c}(\rho_\theta, \rho_B^\pi).$$

However, by Lemma 3, we know that for a covariant measurement the risk is independent of the state ρ_θ, i.e.

$$\sup_\theta R_{P_c}(\rho_\theta, \rho_B^\nu) = \int_\Theta \mathrm{d}\nu(\theta) R_{P_c}(\rho_\theta, \rho_B^\nu).$$

This implies that

$$\int_\Theta \mathrm{d}\nu(\theta) R_{P_c}(\rho_\theta, \rho_B^\nu) \geq \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_{P_c}(\rho_\theta, \rho_B^\pi).$$

The other direction of the above inequality holds trivially, i.e.

$$\int_\Theta \mathrm{d}\nu(\theta) R_{P_c}(\rho_\theta, \rho_B^\nu) \;\leq\; \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_{P_c}(\rho_\theta, \rho_B^\pi).$$

Therefore,

$$\int_\Theta \mathrm{d}\nu(\theta) R_{P_c}(\rho_\theta, \rho_B^\nu) = \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_{P_c}(\rho_\theta, \rho_B^\pi),$$

and so ν is a least favourable prior for a covariant measurement P_c. □

The only remaining ingredient needed to prove Theorem 3 is the following lemma.

Lemma 6. *The Bayes estimator for a covariant measurement P_c is*

$$\hat{\rho}_B(B) = \frac{1}{\nu(B)} \operatorname{tr}_{R'} \left[\mathbb{I}^R \otimes P_c^{R'}(B) \int_G d\mu(g) \left(V_g \rho_0 V_g^\dagger\right)^{\otimes 2} \right], \quad B \in \mathcal{A}(\Theta). \tag{4.5}$$

Proof. Recalling Equation (2.13), the Bayes estimator for a covariant measurement P_c is

$$\hat{\rho}_B(B) \;=\; \frac{\int_\Theta \mathrm{d}\nu(\theta) \operatorname{tr}[\rho_\theta P_c(B)] \rho_\theta}{\int_\Theta \mathrm{d}\nu(\theta) \operatorname{tr} \rho_\theta P_c(B)}, \quad B \in \mathcal{A}(\Theta).$$

Using Lemma 2, the denominator in the above expression is

$$\int_\Theta \mathrm{d}\nu(\theta) \operatorname{tr} \rho_\theta P_c(B) = \nu(B),$$

while the numerator is

$$\begin{aligned} \int_\Theta \mathrm{d}\nu(\theta) \operatorname{tr}[\rho_\theta P_c(B)] \rho_\theta \;&=\; \int_G \mathrm{d}\mu(g) \operatorname{tr}[\rho_{g\theta_0} P_c(B)] \rho_{g\theta_0} \\ &=\; \int_G \mathrm{d}\mu(g) \operatorname{tr}[V_g \rho_0 V_g^\dagger P_c(B)] V_g \rho_0 V_g^\dagger \\ &=\; \operatorname{tr}_{R'} \left[\mathbb{I}^R \otimes P_c^{R'}(B) \int_G \mathrm{d}\mu(g) \left(V_g \rho_0 V_g^\dagger\right)^R \otimes \left(V_g \rho_0 V_g^\dagger\right)^{R'} \right]. \end{aligned}$$

□

4.1 Minimax measurement for covariant estimation

Now that we have a class of measurements and the corresponding least favourable prior, in order to show that it is minimax, we have to show that this class of measurements also minimizes the average risk with respect to such a least favourable prior.

Theorem 3. *There exists a covariant measurement that is minimax for covariant state estimation.*

Proof. Recalling Definition 4 of a minimax POVM and the fact that the Bayes estimator minimizes the average risk, we have

$$\begin{aligned}\inf_P \inf_{\hat{\rho}} \sup_\theta R_P(\rho_\theta, \hat{\rho}) &= \inf_P \inf_{\hat{\rho}} \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_P(\rho_\theta, \hat{\rho}) \\ &\geq \inf_P \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_P(\rho_\theta, \rho_B^\pi).\end{aligned}$$

But, as

$$\sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_P(\rho_\theta, \rho_B^\pi) \geq \int_\Theta \mathrm{d}\mu(\theta) R_P(\rho_\theta, \rho_B^\mu), \quad \forall \mu \in \mathcal{P}(\Theta),$$

it implies that the same holds for the uniform Haar measure ν as well. Thus,

$$\inf_P \inf_{\hat{\rho}} \sup_\theta R_P(\rho_\theta, \hat{\rho}) \geq \inf_P \int_\Theta \mathrm{d}\nu(\theta) R_P(\rho_\theta, \rho_B^\nu).$$

Now, we know from Lemma 3 that

$$\inf_P \int_\Theta \mathrm{d}\nu(\theta) R_P(\rho_\theta, \rho_B^\nu) = \int_\Theta \mathrm{d}\nu(\theta) R_{P_c}(\rho_\theta, \rho_B^\nu),$$

where P_c is a covariant measurement that minimizes the average risk. Also, by Lemma 5, ν is a least favourable prior which means that $\hat{\rho}_B^\nu$ is a minimax estimator. Therefore, we have

$$\int_\Theta \mathrm{d}\nu(\theta) R_{P_c}(\rho_\theta, \rho_B^\nu) = \sup_\theta R_c(\rho_\theta, \rho_B^\nu) = \inf_{\hat{\rho}} \sup_\theta R_{P_c}(\rho_\theta, \hat{\rho}).$$

Thus, we obtain

$$\inf_P \inf_{\hat{\rho}} \sup_\theta R_P(\rho_\theta, \hat{\rho}) \geq \inf_{\hat{\rho}} \sup_\theta R_{P_c}(\rho_\theta, \hat{\rho}).$$

The other direction of the inequality above holds trivially, i.e.

$$\inf_P \inf_{\hat{\rho}} \sup_\theta R_P(\rho_\theta, \hat{\rho}) \leq \inf_{\hat{\rho}} \sup_\theta R_{P_c}(\rho_\theta, \hat{\rho})$$

Hence, we have proved that P_c is a minimax POVM, i.e.

$$\inf_P \inf_{\hat{\rho}} \sup_\theta R_P(\rho_\theta, \hat{\rho}) = \inf_{\hat{\rho}} \sup_\theta R_{P_c}(\rho_\theta, \hat{\rho}).$$

□

As the risk for a covariant measurement is independent of the state ρ_θ (by Lemma 3) and depends only on the estimator (the Bayes estimator in this case, which is a function of $\int_G \mathrm{d}\mu(g)\left(V_g \rho_0 V_g^\dagger\right)^{\otimes 2}$), we have the following corollary.

Corollary 1. *Given a minimax covariant measurement $\mathcal{P}_c$, if there exists a measurement $\mathcal{P}'_c$ which is covariant under a subgroup H of G such that $\{V_h |\ h \in H\}$, where V_h is the projective unitary representation of the subgroup H, forms a unitary 2-design, i.e.*

$$\mathcal{P}_c(B) = V_h^\dagger \mathcal{P}_c(B_{g^{-1}}) V_h, \quad B \in \mathcal{A}(\Theta);\ h \in H,$$

where $B_{g^{-1}} = \{g^{-1}\theta |\ \theta \in B\}$, and $\mathcal{P}_c$ and $\mathcal{P}'_c$ have the same seed, then $\mathcal{P}'_c$ is also minimax.

In order to understand the above corollary better let us look at what it means for Example 3.

Example 3 (continued). *Now, since any state $|\theta, \phi\rangle$ in $\mathbb{S}^2$ can be generated by elements of SU(2)/U(1), the following equivalence holds:*

$$\frac{1}{4\pi} \int_{\mathbb{S}^2} |\theta, \phi\rangle\langle\theta, \phi| \sin\theta d\theta d\phi = \int_{SU(2)/U(1)} U_{\theta,\phi} |0\rangle\langle 0| U_{\theta,\phi}^\dagger dU_{\theta,\phi},$$

where $dU_{\theta,\phi}$ is the Haar measure on SU(2)/U(1). Infact, the above implies that

$$\frac{1}{4\pi}\int_{S^2}\left(|\theta,\phi\rangle\langle\theta,\phi|\right)^{\otimes 2}\sin\theta d\theta d\phi = \int_{SU(2)/U(1)}\left(U_{\theta,\phi}|0\rangle\langle 0|U_{\theta,\phi}^{\dagger}\right)^{\otimes 2}dU_{\theta,\phi}.$$

Now, the above equivalence along with [(Derakhshani, 2008, Theorem 3.3.1)] implies that one can construct a unitary 2-design from a quantum 2-design. Thus, the set of unitary matrices that generate the set of eigenstates of the Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ is a unitary 2-design given as below.

$$\begin{aligned}
U_{0,0} &= \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}, U_{\pi,0} = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},\\
U_{\pi/2,0} &= \frac{1}{\sqrt{2}}\begin{bmatrix}1 & -1\\ 1 & 1\end{bmatrix}, U_{\pi/2,\pi} = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ & \end{bmatrix},\\
U_{\pi/2,\pi/2} &= \frac{1}{\sqrt{2}}\begin{bmatrix}1 & i\\ i & 1\end{bmatrix}, U_{\pi/2,3\pi/2} = \frac{1}{\sqrt{2}}\begin{matrix}1 & -i\\ -i & 1\end{matrix}\Bigg].
\end{aligned}$$

The corresponding measurement that is covariant under the above unitary 2-design is then obtained via $M_{\theta,\phi} = U_{\theta,\phi}P_0U_{\theta,\phi}^{\dagger}$. It is straightforward to see that the corresponding $M_{\theta,\phi}$ are the same as the Pauli measurements apart from a normalization constant. This measurement is thus minimax.

Note: In the above example we obtained a minimax POVM—a covariant measurement for the parameter space $\mathbb{S}^2$ which describes only pure qubit states. There is no a-priori reason to believe that the same measurement would also be minimax for estimating an arbitrary state of a qubit. However, curiously, it happens to be true for a qubit as we will see in the next chapter.

5

Optimal state estimation for qubits

We look at the single qubit case as studied in Ref. [Koyama *et al.* (2017)] wherein the authors obtain such a minimax POVM with relative entropy as the distance-measure. We generalize their results to squared-distance $\|\rho - \sigma\|^2 = \mathrm{tr}(\rho - \sigma)^2$. However, the proof does not follow the generalized treatment in terms of Bregman divergence as done in the previous sections.

To begin with, let us write the most general expression for a POVM on $\mathbb{C}^2$. Recalling Lemma 1, we can write any POVM, see Definition 1, as an operator-valued density, i.e.

$$P(B) = \int_B \mu(dx) M(x),$$

where $B \in \sigma(\mathcal{X})$, $M(x) \geq 0$, $\mathrm{Tr}[M(x)] = 2$ and $\mu(\mathcal{X}) = 1$. Since positive operators can be expanded in the Pauli basis $\{\mathbb{I}, \sigma_x, \sigma_y, \sigma_z\}$ with real coefficients, $M(\vec{x}) = \alpha_0 \mathbb{I} + \vec{x} \cdot \vec{\sigma}$, but the trace 1 condition on $M(\vec{x})$ implies

$\alpha_0 = 1/2$. Without loss of generality,

$$M(\vec{x}) = (\mathbb{I} + \vec{x} \cdot \vec{\sigma}).$$

Thus, the most general form of a POVM element on $\mathbb{C}^2$ is

$$P(B) \quad = \quad \int_B (\mathbb{I} + \vec{x} \cdot \vec{\sigma}) \mathrm{d}\mu(\vec{x}). \tag{5.1}$$

Now that we have obtained the general expression for a POVM on $\mathbb{C}^2$, we next evaluate the Bayes estimator which in turn is needed to evaluate the risk $R_P(\rho_\theta, \rho_B^\pi)$. Recalling that the Bayes estimator is given as

$$\rho_B^\pi(x) \quad = \quad \int_\Theta \frac{\mathrm{d}p(x|\theta)}{\mathrm{d}p_\pi(x)} \rho_\theta \mathrm{d}\pi(\theta).$$

Recalling the differential form of Born's rule (2.7), and using the Bloch sphere notation of ρ_θ, $\rho_\theta = \frac{1}{2}(\mathbb{I} + \vec{\theta} \cdot \vec{\sigma})$, it is a straightforward calculation to obtain

$$\mathrm{tr}\, M(\vec{x}) \rho_\theta = \mathrm{d}\mu(\vec{x})(1 + \vec{x} \cdot \vec{\theta}). \tag{5.2}$$

However, to be able to further simplify the Bayes estimator, we need to impose some restrictions on the prior π defined on the parameter space Θ (which in this case is $\mathbb{R}^3$). In particular, we choose a uniform prior π^* supported only on pure states, i.e. $\pi(\theta)$ is zero for all vectors $\vec{\theta}$ with $\|\theta\| < 1$ but is uniformly distributed on the set of unit vectors with $\|\theta\| = 1$. It can be verified that such a prior has the following two properties :

1. $\mathbb{E}_{\pi^*}[\theta_i] = 0, \quad \forall i \in \{x, y, z\}$.
2. $\mathbb{E}_{\pi^*}[\theta_i \theta_j] = \frac{1}{3}\delta_{ij} \quad \forall i, j \in \{x, y, z\}$.

By property (1) of the prior π^*, we have

$$p_\pi(B) = \int_\Theta \int_B \mathrm{d}\mu(\vec{x})(1 + \vec{x} \cdot \vec{\theta}) \pi^*(\theta) \mathrm{d}\theta = \mu(B). \tag{5.3}$$

Thus, the Bayes estimator reduces to

$$\begin{aligned}
\rho_B^{\pi^*}(\vec{x}) &= \int_\Theta \frac{1}{\frac{\mathrm{d}p_{\pi^*}(x)}{\mathrm{d}p(x|\theta)}} \rho_\theta \mathrm{d}\pi^*(\theta) \\
&= \int_\Theta \frac{1}{\frac{\mathrm{d}\mu(x)}{\mathrm{d}p(x|\theta)}} \rho_\theta \mathrm{d}\pi^*(\theta) \\
&= \int_\Theta \frac{\mathrm{d}p(x|\theta)}{\mathrm{d}\mu(x)} \rho_\theta \mathrm{d}\pi^*(\theta) \\
&= \int_\Theta \rho_\theta \mathrm{d}\pi^*(\theta) \,\mathrm{tr}\, M(x)\rho_\theta \\
&= \frac{1}{2}\int_\Theta \mathrm{d}\pi^*(\theta)(1+\vec{x}\cdot\vec{\theta})(\mathbb{I}+\vec{\theta}\cdot\vec{\sigma}) \\
&= \frac{1}{2}\Big(\mathbb{I} + \int_\Theta \mathrm{d}\pi^*(\theta)(\vec{x}\cdot\vec{\theta})(\vec{\theta}\cdot\vec{\sigma})\Big) \\
&= \frac{1}{2}\Big(\mathbb{I} + \frac{1}{3}\vec{x}\cdot\vec{\sigma}\Big).
\end{aligned}$$

Now, recalling that the risk is a function of the POVM P, i.e.

$$R_P(\rho_\theta, \rho_B^{\pi^*}) = \int_{\mathcal{X}} \mathrm{d}\mu(\vec{x}) \,\mathrm{tr}\, M(\vec{x})\rho_\theta \; D_f(\rho_\theta, \rho_B^{\pi^*}(\vec{x})), \tag{5.4}$$

we evaluate the risk for both relative entropy and Hilbert-Schmidt distance below.

Lemma 7. *The risk for relative entropy and Hilbert-Schmidt distance are given as*

$$R_P^{rel}(\rho_\theta, \rho_B^{\pi^*}) = -h\left(\frac{1+\|\theta\|}{2}\right) + \frac{1}{2}\log\frac{9}{2} - \frac{\log 2}{2}\int_{\mathcal{X}} d\mu(\vec{x}) \sum_{j,k} \theta_j\theta_k x_j x_k, \quad \textit{and}$$

$$\begin{aligned}
R_P^{sq}(\rho_\theta, \rho_B^{\pi^*}) = \frac{1}{2}\Big\{ \|\vec{\theta}\|^2 + \frac{1}{9}\int_{\mathcal{X}} d\mu(\vec{x})\|\vec{x}\|^2 + \frac{1}{9}\int_{\mathcal{X}} d\mu(\vec{x})\|\vec{x}\|^2\vec{x}\cdot\vec{\theta} - \\
\frac{2}{3}\int_{\mathcal{X}} d\mu(\vec{x}) \sum_{j,k} \theta_j\theta_k x_j x_k\Big\},
\end{aligned}$$

respectively.

Proof. (a) For *relative entropy*, see (Koyama *et al.*, 2017, pg. 11).
(b) For *Hilbert-Schmidt distance*, substituting $f = \|A\|_1^2$ in (5.4), we get

$$D_{sq}(\rho_\theta, \rho_B^{\pi^*}(x)) \;=\; \mathrm{tr}\left(\rho_\theta - \rho_B^{\pi^*}(x)\right)^2.$$

Thus,

$$\begin{aligned} D_{sq}(\rho_\theta, \rho_B^{\pi^*}(B)) &= \frac{1}{2}\,\mathrm{tr}\left[\begin{bmatrix} 1+\theta_z & \theta_x - i\theta_y \\ \theta_x + i\theta_y & 1-\theta_z \end{bmatrix} - \begin{bmatrix} 1+z/3 & (x-iy)/3 \\ (x+iy)/3 & 1-z/3 \end{bmatrix}\right]^2 \\ &= \frac{1}{2}\,\mathrm{tr}\left[(\theta_z - z/3)\sigma_z + (\theta_x - x/3)\sigma_x + (\theta_y - y/3)\sigma_y\right]^2 \\ &= \frac{1}{2}\Big((\theta_z - z/3)^2 + (\theta_x - x/3)^2 + (\theta_y - y/3)^2\Big) \\ &= \frac{1}{2}\Big(\|\vec{\theta}\|^2 + \frac{1}{9}\|\vec{x}\|^2 - \frac{2}{3}\vec{x}\cdot\vec{\theta}\Big). \end{aligned}$$

This implies that the risk is

$$R_P^{sq}(\rho_\theta, \rho_B^{\pi^*}) = \frac{1}{2}\int_{\mathcal{X}} \mathrm{d}\mu(\vec{x})(1 + \vec{x}\cdot\vec{\theta})\Big(\|\vec{\theta}\|^2 + \frac{1}{9}\|\vec{x}\|^2 - \frac{2}{3}\vec{x}\cdot\vec{\theta}\Big).$$

We can write the above using the property of a general POVM on $\mathbb{C}^2$, i.e. $\int_{\mathcal{X}} \mathrm{d}\mu(\vec{x})\vec{x} = 0$ as

$$\begin{aligned} R_P^{sq}(\rho_\theta, \rho_B^{\pi^*}) &= \frac{1}{2}\Big\{\|\vec{\theta}\|^2 + \frac{1}{9}\int_{\mathcal{X}} \mathrm{d}\mu(\vec{x})\|\vec{x}\|^2 + \frac{1}{9}\int_{\mathcal{X}} \mathrm{d}\mu(\vec{x})\|\vec{x}\|^2\vec{x}\cdot\vec{\theta} - \\ &\qquad \frac{2}{3}\int_{\mathcal{X}} \mathrm{d}\mu(\vec{x})\sum_{j,k}\theta_j\theta_k x_j x_k\Big\}. \end{aligned}$$

Note: Although in Ref. [Koyama et al. *(2017)] it is assumed that the POVM P is rank-1, the above expressions hold in general for any POVM P, i.e. the vector* $\vec{x}$ *in* (5.1) *need not be a unit vector.* □

Lemma 8. *For any POVM P, the average risk of the Bayes estimator with respect to the prior* π^* *satisfies the inequalities:*

$$\begin{aligned} \int_\Theta d\pi^*(\theta) R_P^{rel}(\rho_\theta, \rho_B^{\pi^*}) &\geq \frac{1}{2}\log\frac{9}{2} - \frac{1}{6}\log 2, \\ \int_\Theta d\pi^*(\theta) R_P^{sq}(\rho_\theta, \rho_B^{\pi^*}) &\geq \frac{2}{9}, \end{aligned}$$

for relative entropy and Hilbert-Schmidt distance respectively.

Proof. (a) For *relative entropy* :
From Lemma 7 and the properties of the prior π^* we get

$$\begin{aligned}\int_\Theta \mathrm{d}\pi^*(\theta) R_P^{rel}(\rho_\theta, \rho_B^{\pi^*}) &= \int_\Theta \mathrm{d}\pi^*(\theta)\Big\{ -h\left(\frac{1+\|\theta\|}{2}\right) + \frac{1}{2}\log\frac{9}{2} - \\ &\qquad \frac{\log 2}{2}\int_{\mathcal{X}} \mathrm{d}\mu(\vec{x}) \sum_{j,k} \theta_j\theta_k x_j x_k \Big\} \\ &= \frac{1}{2}\log\frac{9}{2} - \frac{\log 2}{2}\int_{\mathcal{X}} \mathrm{d}\mu(\vec{x}) \sum_{j,k} \frac{\delta_{jk}}{3} x_j x_k \\ &= \frac{1}{2}\log\frac{9}{2} - \frac{1}{6}\log 2 \sum_j \mathbb{E}_\mu[r_j^2].\end{aligned}$$

However, since $\sum_j r_j^2 \leq 1$, it implies $\sum_j \mathbb{E}_\mu[r_j^2] \leq 1$, and we obtain the required inequality :

$$\int_\Theta \mathrm{d}\pi^*(\theta) R_P^{rel}(\rho_\theta, \rho_B^{\pi^*}) \geq \frac{1}{2}\log\frac{9}{2} - \frac{1}{6}\log 2.$$

(b) For *Hilbert-Schmidt distance* :
From Lemma 7 and the properties of the prior π^* we get

$$\begin{aligned}\int_\Theta \mathrm{d}\pi^*(\theta) R_P^{f_2}(\rho_\theta, \rho_B^{\pi^*}) &= \int_\Theta \mathrm{d}\pi^*(\theta)\frac{1}{2}\Big\{ \|\vec{\theta}\|^2 + \frac{1}{9}\int_{\mathcal{X}} \mathrm{d}\mu(\vec{x})\|\vec{x}\|^2 + \frac{1}{9}\int_{\mathcal{X}} \mathrm{d}\mu(\vec{x})\|\vec{x}\|^2 \vec{x}\cdot\vec{\theta} - \\ &\qquad \frac{2}{3}\int_{\mathcal{X}} \mathrm{d}\mu(\vec{x}) \sum_{j,k} \theta_j\theta_k x_j x_k \Big\} \\ &= \frac{1}{2}\Big\{ 1 + \frac{1}{9}\sum_j \mathbb{E}_\mu[r_j^2] - \frac{2}{9}\sum_j \mathbb{E}_\mu[r_j^2] \Big\} \\ &= \frac{1}{2}\Big\{ 1 - \frac{1}{9}\sum_j \mathbb{E}_\mu[r_j^2] \Big\}.\end{aligned}$$

Again, as $\sum_j r_j^2 \leq 1$, it implies $\sum_j \mathbb{E}_\mu[r_j^2] \leq 1$, and we obtain the required inequality :

$$\int_\Theta \mathrm{d}\pi^*(\theta) R_P^{f_2}(\rho_\theta, \rho_B^{\pi^*}) \geq \frac{1}{2}\big(1 - \frac{1}{9}\big) = \frac{4}{9}.$$

□

Lemma 9. *For any POVM P^* that satisfies $\mathbb{E}_\mu[r_i r_j] = \frac{1}{3}\delta_{ij}$, the average risk of the Bayes estimator coincides with the worst-case risk:*

$$\int_\Theta d\pi^*(\theta) R_{P^*}(\rho_\theta, \rho_B^{\pi^*}) = \sup_\theta R_{P^*}(\rho_\theta, \rho_B^{\pi^*}).$$

Proof. (i) (a) For *relative entropy* : (a) See [(Koyama *et al.*, 2017, pg. 11)].

(b) For *Hilbert-Schmidt* distance:

As $\mathbb{E}_\mu[r_i r_j] = \frac{1}{3}\delta_{ij}$, it implies $\sum_j \mathbb{E}_\mu[r_j^2] = 1$, and thus by Lemma 8,

$$\int_\Theta \mathrm{d}\pi^*(\theta) R^{f_2}_{P^*}(\rho_\theta, \rho_B^{\pi^*}) = \frac{4}{9}.$$

Now, for such a POVM P^*, $\|\vec{x}\|^2 = 1$, and the risk, see Lemma 7, becomes

$$R^{sq}_{P^*}(\rho_\theta, \rho_B^{\pi^*}) \;=\; \frac{1}{2}\Big(\|\vec{\theta}\|^2 + \frac{1}{9} - \frac{2}{9}\|\vec{\theta}\|^2\Big).$$

Clearly,

$$\max_{\|\theta\|} R^{sq}_{P^*}(\rho_\theta, \rho_B^{\pi^*}) = \frac{4}{9}, \text{at } \|\vec{\theta}\| = 1.$$

This implies that

$$\int_\Theta \mathrm{d}\pi^*(\theta) R_{P^*}(\rho_\theta, \rho_B^{\pi^*}) = \sup_\theta R_{P^*}(\rho_\theta, \rho_B^{\pi^*}),$$

for both relative entropy and squared-distance. □

Lemma 10. *The uniform Haar measure on $\mathbb{S}^2$ is a least favourable prior for spherical 2-designs in $\mathbb{C}^2$.*

Proof. Firstly, note that a POVM P^* with $\mathbb{E}_\mu[r_i r_j] = \frac{1}{3}\delta_{ij}$ is a spherical 2-design. (See Definition 8 of spherical t-designs. Examples of spherical 2-designs include the SIC-POVM [Renes *et al.* (2004)] on $\mathbb{C}^2$ as well as the POVM defined through the Pauli measurements.) It can be seen from Lemma 7 that the risk is a polynomial function of degree 2 in the variables x, y, z. It is straightforward to see that the average of the typical term $x_i x_j$ with respect to the Haar measure on $\mathbb{S}^2$ is $\frac{\delta_{ij}}{3}$. Thus, any POVM with $\mathbb{E}_\mu[x_i x_j] = \frac{1}{3}\delta_{ij}$ is a spherical 2-design. Let us now proceed with the proof of the lemma. As the Bayes estimator $\hat{\rho}_B^\pi$ minimizes the average risk with respect to the prior π,

$$\sup_\theta R_{P^*}(\rho_\theta, \rho_B^{\pi^*}) = \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_{P^*}(\rho_\theta, \rho_B^{\pi^*}) \geq \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_{P^*}(\rho_\theta, \rho_B^{\pi}).$$

However, we just proved in Lemma 9 that

$$\begin{aligned} \sup_\theta R_{P^*}(\rho_\theta, \rho_B^{\pi^*}) &= \int_\Theta \mathrm{d}\pi^*(\theta) R_{P^*}(\rho_\theta, \rho_B^{\pi^*}), \\ \implies \int_\Theta \mathrm{d}\pi^*(\theta) R_{P^*}(\rho_\theta, \rho_B^{\pi^*}) &\geq \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_{P^*}(\rho_\theta, \rho_B^{\pi}). \end{aligned}$$

The other direction of the above inequality holds trivially, i.e.

$$\begin{aligned} \int_\Theta \mathrm{d}\pi^*(\theta) R_{P^*}(\rho_\theta, \rho_B^{\pi^*}) &\leq \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_{P^*}(\rho_\theta, \rho_B^{\pi}), \\ \implies \int_\Theta \mathrm{d}\pi^*(\theta) R_{P^*}(\rho_\theta, \rho_B^{\pi^*}) &= \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_{P^*}(\rho_\theta, \rho_B^{\pi}). \end{aligned}$$

Thus, π^* is a least favourable prior for a spherical 2-design in $\mathbb{C}^2$. □

Theorem 4. *Any spherical 2-design for $\mathbb{C}^2$ is a minimax POVM.*

Proof. Recalling Definition 8 of a minimax POVM and the fact that the

Bayes estimator minimizes the average risk, we have:

$$\begin{aligned}\inf_P \inf_{\hat{\rho}} \sup_\theta R_P(\rho_\theta, \hat{\rho}) &= \inf_P \inf_{\hat{\rho}} \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_P(\rho_\theta, \hat{\rho}) \\ &\geq \inf_P \sup_\pi \int_\Theta \mathrm{d}\pi(\theta) R_P(\rho_\theta, \rho_B^\pi) \\ &\geq \inf_P \int_\Theta \mathrm{d}\pi^*(\theta) R_P(\rho_\theta, \rho_B^{\pi^*}).\end{aligned}$$

Now, Lemma 8 and Lemma 9 together imply that the average risk with respect to π^* is minimized by the POVM P^*, i.e.

$$\inf_P \int_\Theta \mathrm{d}\pi^*(\theta) R_P(\rho_\theta, \rho_B^{\pi^*}) = \int_\Theta \mathrm{d}\pi^*(\theta) R_{P^*}(\rho_\theta, \rho_B^{\pi^*}).$$

Also, by Lemma 10, π^* is a least favourable prior which means that $\rho_B^{\pi^*}$ is a minimax estimator. Therefore, we have

$$\int_\Theta \mathrm{d}\pi^*(\theta) R_{P^*}(\rho_\theta, \rho_B^{\pi^*}) = \sup_\theta R_{P^*}(\rho_\theta, \rho_B^{\pi^*}) = \inf_{\hat{\rho}} \sup_\theta R_{P^*}(\rho_\theta, \hat{\rho}).$$

Thus, we obtain

$$\inf_P \inf_{\hat{\rho}} \sup_\theta R_P(\rho_\theta, \hat{\rho}) \geq \inf_{\hat{\rho}} \sup_\theta R_{P^*}(\rho_\theta, \hat{\rho}).$$

The other direction of the inequality above holds trivially, i.e.

$$\inf_P \inf_{\hat{\rho}} \sup_\theta R_P(\rho_\theta, \hat{\rho}) \leq \inf_{\hat{\rho}} \sup_\theta R_{P^*}(\rho_\theta, \hat{\rho})$$

Hence, we have proved that P^*, a spherical 2-design is a minimax POVM, i.e.

$$\inf_P \inf_{\hat{\rho}} \sup_\theta R_P(\rho_\theta, \hat{\rho}) = \inf_{\hat{\rho}} \sup_\theta R_{P^*}(\rho_\theta, \hat{\rho}).$$

□

Part II

Work in quasi-thermal processes for two-level systems

6

Overview & model

6.1 Background

A standard thermodynamic setting comprises of large systems with relatively short relaxation times wherein fluctuations in values of extensive quantities such as *work*, that follow the law of large numbers, are negligible and one only cares about averages [Callen (2006); Jarzynski (2011)]. Work is essentially a deterministic quantity in such scenarios. Non-equilibrium thermodynamics, on the other hand, is the study of *fluctuations* in work as one departs from the standard thermodynamic setting. Small systems with long relaxation times make the study of fluctuations inevitable since these are no longer just statistical noise. Within the framework of non-equilibrium statistical mechanics, fluctuations have been characterised using *fluctuation theorems* [Jarzynski (1997); Crooks (1999)] that play a key role in the control and study of biomolecular processes such as the folding of proteins [Dobson (2003)]. In fact, single molecule experiments involving stretching of biomolecules under external forces are a ripe avenue for the study of non-equilibrium phenomena [Alemany

and Ritort (2010); Bustamante *et al.* (2005); Kolomeisky and Fisher (2007); Liphardt *et al.* (2002)].

A complementary approach to non-equilibrium thermodynamics is the incipient field of one-shot statistical mechanics [Garner (2018); Åberg (2013); Dahlsten *et al.* (2011); Del Rio *et al.* (2011); Faist *et al.* (2015)] which draws techniques from one-shot information theory [Tomamichel (2015); Rényi (1961); Renner and Wolf (2004); Renner (2005)] to characterize processes that are far from equilibrium. And, within this non-equilibrium framework, work is analysed as a random variable. In the one-shot regime one considers single instances of the task at hand instead of looking at ensemble averages. Fluctuations in work have been studied in this regime in Ref. [Åberg (2013)] for a discrete classical model. The main question in consideration was what constituted truly work-like work extraction. The basic idea was that in order to define work for small systems in contrast to *heat*, one should be able to extract a fixed amount of work from a fixed system configuration. The author showed that for a system that is initially not in equilibrium with the ambient bath even the optimal process (that achieves maximum average work output) results in fluctuations as large as the average work itself. Such an optimal process is comprised of a) energy level transformations (quenches) rendering the system effectively thermal, and b) *reversible isothermal* processes [Åberg (2013)]. The latter is manifestly fluctuation-free because the system equilibrates at each infinitesimal step of a reversible process and equilibration washes away the fluctuations. Of course this is only possible since the time scale over which one performs the energy level transformations (during the isothermal process) is much larger than the relaxation time of the system. The question is what happens to these fluctuations when the system only *partially* thermalizes, i.e. when the system is driven externally over shorter time periods in comparison to its relaxation time scale.

The relaxation towards equilibrium can be studied within the framework of *collision models* which have been used to study open quantum system dynamics [Ziman *et al.* (2005); Scarani *et al.* (2002); Ciccarello (2017)]. Within these models the bath is treated as a composition of smaller non-interacting particles that are copies of the system in the thermal Gibbs state. Such a process of thermalization has been studied in Ref. [Scarani *et al.* (2002)] for a qubit in contact with a bath composed of non-interacting qubits. For a qubit in a general quantum state interacting with an ambient bath, thermalization was shown to be a two-component process comprising of decoherence and dissipation. And, a functional dependence on time was obtained for both of these processes. In the present work, we are interested in fluctuations in processes involving partial thermalizations for classical two-level systems and will limit ourselves to states diagonal in the energy eigenbasis. With this we come to the question we posed earlier regarding fluctuations in work for processes involving partial thermalizations.

While work along these lines has been done in Ref. [Ma *et al.* (2018a)] in the low-dissipation regime (where the system is driven for large but finite time), a more closely related numerical study on this question was undertaken in Ref. [Marathe and Dhar (2005)] where the authors studied a single Ising spin driven by an external magnetic field. They obtained work distributions using Monte Carlo simulations of the processes for different driving rates. The authors found that such processes have broad work distributions with significant probability for processes with negative dissipated work in general. They also verified work fluctuation theorems [Jarzynski (1997); Crooks (1999)] and derived analytic expressions for the distribution of work when the spin's energy gap was driven by the external field in the slow and fast limits. Another recent work [Bäumer *et al.* (2019)] looked into the same problem but again in the low-dissipation regime. We will discuss this further in Section 6.2.

Here, we investigate similar work extraction processes involving partial thermalizations for a single classical two-level system driven by an external magnetic field changing linearly in time. We derive an analytic expression for the average work yield of such a process as a function of the total time, τ. This expression reduces to the average work outputs of the corresponding adiabatic and isothermal processes in the $\tau \to 0$ and $\tau \to \infty$ limits, respectively. Next, in an attempt to characterize fluctuations in the average work yield, we provide a lower bound for the variance of work as a function of the total time duration of the process. This lower bound is saturated in the adiabatic and the isothermal limits thereby reproducing the result that isothermal processes are deterministic as was shown in Ref. [Åberg (2013)]. Even though an analytical expression for the variance of work seems intractable, we employ Jarzynski's fluctuation-dissipation relation [Jarzynski (1997)] to compare the dissipation in work ($\tau < \infty$) with our estimate of variance obtained by performing Monte Carlo simulations. We find that for a two-level system initially in equilibrium with the bath, the fluctuation-dissipation relation provides a good approximation which becomes exact as τ becomes large as was also noted in Ref. [Marathe and Dhar (2005)]. Finally, we investigate finite-time work extraction cycles inspired by the Carnot cycle, replacing the ideal isothermal reversible processes with the realistic ones involving partial thermalizations. We then numerically optimize the power output of such finite-time work extraction cycles over different sets of constraints and parameters keeping the time period of the cycles fixed and provide comparisons between those scenarios.

6.2 Model

Given an ambient bath at temperature T_h and a two-level system such that its energy gap δ can only be driven within a fixed range between

δ_{min} and δ_{max} (for example by an external magnetic field), let us assume that the time period of the external driving is much shorter compared to the relaxation time of the system interacting with the bath, and that the spectral density of the bath is constant over the given range of values for δ. Without loss of generality, let us further assume that the ground state energy is zero. For a two-level system with an energy gap δ one can always define a temperature such that the occupation probability of the excited state is given by the corresponding Gibbs distribution at that temperature. We choose time as the independent quantity under these settings and denote it by the continuous variable t. This brings to the question of how one could extract work under these settings. To this end, we study finite-time work extraction processes involving *partial thermalizations*. Partial thermalization encapsulates a finite time restriction for the system's equilibration with the bath and can be studied by considering a randomized model of interaction between the two—a collision model [Ziman *et al.* (2005); Scarani *et al.* (2002); Ciccarello (2017)]. Such models are based on the assumption that the bath is composed of smaller non-interacting particles that are copies of the system in the thermal Gibbs state. The system-bath interaction is then modelled as a sequence of collisions between the system and bath particles where each collision itself is considered to be a joint unitary on the system and the bath particle in question. The additional assumptions of the bath being initially uncorrelated and the system colliding with exactly one bath particle at a time result in a Markovian dynamics for the system which in turn can be translated to a Lindblad master equation in the continuous time limit [Ziman *et al.* (2005); Brun (2002)]. The process of partial thermalization was studied in Ref. [Scarani *et al.* (2002)] within the framework of a collision model and was shown to be composed of dissipation and decoherence for a general quantum state. For states that are diagonal in the energy eigenbasis thermalization simply amounts to dissipation and the state of

a two-level system can be described by the occupation probabilities $p(t)$ for the excited state and $1 - p(t)$ for the ground state. Denoting the thermal Gibbs occupation probability for the excited state by $\gamma(t)$, the thermalization process is given by the following equation as per Ref.[Scarani *et al.* (2002)]:

$$p(t) = e^{-\kappa t} p(0) + \left(1 - e^{-\kappa t}\right)\gamma(t), \tag{6.1}$$

where κ is the thermalization rate (dissipation), the inverse of the relaxation time T_1 [Scarani *et al.* (2002)]. One can interpret $1 - e^{-\kappa t}$ as the probability of collision between the qubit and a bath particle, denoting it by λ. The case $\lambda = 1$ corresponds to exact thermalization and $\lambda = 0$ corresponds to no thermalization. Thus, for sufficiently short interaction times Δt, the probability λ with which the system interacts with the bath particles (and thermalizes) is linear in Δt, i.e. $\lambda = \kappa \Delta t$. Microscopically, partial thermalization is a time-dependent Markov process on a finite state space—the ground and excited states of our two-level system. The system with energy gap $\delta(t)$ at time t interacts with the bath for a time Δt and with probability $\kappa \Delta t$ it collides with a bath particle. If the system thermalizes then it can change its state such that the occupation probability for the excited state is $\gamma_h\big(\delta(t + \Delta t)\big)$, the thermal Gibbs weight associated with the excited state $\delta(t + \Delta t)$ for the bath temperature T_h. Work is done when the system is in the excited state and its energy gap is changed from $\delta(t)$ to $\delta(t + \Delta t)$.

We can thus build a finite-time work extraction process that involves a series of infinitesimal level transformations and partial thermalizations, along the lines of Ref.[Åberg (2013)]. A discrete version of such a process at a given time t is, therefore, composed of a series of two steps:

1. Level transformation: changing the energy gap $\delta(t)$ by an infinitesimal amount to $\delta(t + \Delta t)$ keeping the occupation probabilities fixed.

2. Partial thermalization: changing the state of the system such that with probability $1-\kappa\Delta t$ it stays in the same state, while with probability $\kappa\Delta t$ it thermalises with respect to the bath.

The above defines a time-dependent Markov process and corresponds to the Markov diagram in Fig. 6.1.

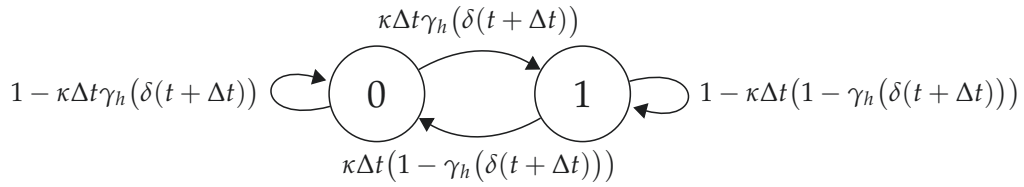


Figure 6.1: Markov chain representing partial thermalization during a finite-time work extraction process when the energy gap changes from $\delta(t)$ to $\delta(t+\Delta t)$. The states 0 and 1 denote the ground and excited states of the two level system, respectively. Each arrow is labelled by the corresponding transition probability.

A continuous version of Fig. 6.1 can then be simply obtained as per the following lemma.

Lemma 11. *Given a two-level system undergoing partial thermalization with a hot bath at temperature T_h (characterized by short system-bath interaction times), the occupation probability p for its excited state evolves according to the following equation:*

$$\frac{dp(t)}{dt} = \kappa\Big(\gamma_h\big(\delta(t)\big) - p(t)\Big), \tag{6.2}$$

where $\gamma_h\big(\delta(t)\big) = \frac{1}{1+e^{\delta(t)/T_h}}$, the Gibbs weight associated with the instantaneous excited state energy $\delta(t)$.

Proof. According to Fig. 6.1, the total probability of being in the excited state $p(t+\Delta t)$ at time step $t+\Delta t$ can be obtained using the law of total probability:

$$\begin{aligned} p(t+\Delta t) &= p_{01}(t+\Delta t)\big(1-p(t)\big) + \\ & \quad p_{11}(t+\Delta t)p(t), \end{aligned} \tag{6.3}$$

where $p_{01}(t+\Delta t)$ is the conditional probability for the system to be in the excited state at time $t+\Delta t$ when it was in the ground state at time t, and $p_{11}(t+\Delta t)$ is the conditional probability for the system to be in the excited state at time $t+\Delta t$ when it was in the excited state at time t. Plugging in the corresponding expressions using Fig. 6.1 we have

$$p(t+\Delta t) = (1-\kappa\Delta t)p(t) + \kappa\Delta t\gamma_h\big(\delta(t+\Delta t)\big). \tag{6.4}$$

Re-arranging the terms we obtain

$$p(t+\Delta t) - p(t) = \kappa\Delta t\Big(\gamma_h\big(\delta(t+\Delta t)\big) - p(t)\Big), \tag{6.5}$$

which after dividing by Δt reduces to (6.2) in the limit $\Delta t \to 0$. □

As an aside, we would like to make a comment on the model of partial thermalization as in Ref. [Bäumer *et al.* (2019)]. The authors consider a situation where the probability of interaction between the system and the bath is fixed. If we were to do the same then we would have to replace $\kappa\Delta t$ by a constant, let us say λ. Then (6.5) would yield

$$p(t+\Delta t) - p(t) = \lambda\Big(\gamma_h\big(\delta(t+\Delta t)\big) - p(t)\Big), \tag{6.6}$$

which in the limit $\Delta t \to 0$ would simply give

$$p(t) = \gamma_h\big(\delta(t+\Delta t)\big). \tag{6.7}$$

This implies that the system would be in the thermal Gibbs state at each infinitesimal step of the process. Naturally, one would obtain an isothermal reversible process with no fluctuations.

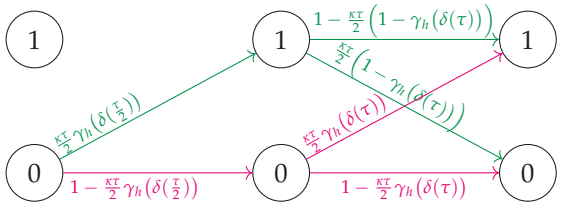
So, given that we have a general work extraction process involving partial thermalizations, let us make the following assumption in order to completely specify the model.

Assumption 1. *The energy gap $\delta(t)$ is driven at a constant rate.*

We are now ready to derive the results. But, before we move on, let us first look at an example of a discrete version of this problem for an intuitive understanding of the underlying Markov process which would also inform our derivations in Section 7.1.2.

Example 4. *Let $\epsilon = \delta_{max} - \delta_{min}$ be the range over which we can vary δ as a function of time t and let us choose $\delta(0) = \delta_{max}$. Let $p(0)$ to be a constant p_0 and let the total time of the process be τ. Then, $\delta(\tau) = \delta_{min}$ and $p(\tau)$ would be determined by Lemma 11. Now, a work extraction process involving partial thermalization corresponds to a curve on the $\delta - p$ plane. The discretization of this process is a discretization of that curve. So, let us divide the range ϵ for δ into $L = 2$ equal steps. Then, the change in δ at each step would be $\Delta\delta = -\epsilon/2$ and the extracted work during each step would be $w_{ex} = \epsilon/2$. Moreover, Assumption 1 under the above boundary conditions gives $d\delta/dt = -\epsilon/\tau$ which implies that $\Delta t = \tau/2$ for each step. Each of these discrete steps itself is composed of two steps: a level transformation and then a partial thermalization. Let us say that the system is in the ground state at time $t = 0$, see the Markov chain in Fig. 6.2. Clearly, since the system starts in the ground state, the work done in the first step during the level transformation denoted by $w^{t=\tau/2}$ is zero, first row in the second column of the table. Next, the system thermalizes with respect to the hot bath with probability $\kappa\tau/2$. The work done during this partial thermalization is dissipated as heat and thus its contribution is zero. Upon partial thermalization we might transition to the excited state or remain in the ground state. The two possible paths are shown in the Markov chain in Fig. 6.2. If we transition to the excited state then the work done during the level transformation in the second step denoted by $w^{t=\tau}$ would be $\epsilon/2$, second row in the fourth column. In the*

end, partial thermalization in the second step would again lead to two different paths with zero work contributions. A complete distribution can be obtained by going through all such paths, enlisted in the table in Fig. 6.2.



state at $t=0$	$w^{t=\tau/2}$	state at $t=\tau/2$	$w^{t=\tau}$	w_{ex}	$\Pr[W_{ex}=w_{ex}]$
0	0	0	0	0	$(1-p_0)\left(1-\frac{\kappa\tau}{2}\gamma_h(\delta(\frac{\tau}{2}))\right)$
0	0	1	$\epsilon/2$	$\epsilon/2$	$(1-p_0)\frac{\kappa\tau}{2}\gamma_h(\delta(\frac{\tau}{2}))$
1	$\epsilon/2$	0	0	$\epsilon/2$	$p_0\frac{\kappa\tau}{2}\left(1-\gamma_h(\delta(\frac{\tau}{2}))\right)$
1	$\epsilon/2$	1	$\epsilon/2$	ϵ	$p_0\left(1-\frac{\kappa\tau}{2}(1-\gamma_h(\delta(\frac{\tau}{2})))\right)$

Figure 6.2: *The Markov chain above shows two specific paths corresponding to the work extraction process given in Example 4, where the ground and excited states of the two level system are denoted by 0 and 1, respectively. Each arrow is labelled by the corresponding transition probability. The table lists all possible paths for such a process with each row corresponding to a specific path. The first and third columns denote the state of the system at the beginning of each step which determines the work done during that step, namely $w^{t=\tau/2}$ and $w^{t=\tau}$ in the second and the fourth columns, respectively. W_{ex} is the random variable for extracted work and takes values w_{ex} which is the sum of work done at each step along a given path. $\Pr[W_{ex}=w_{ex}]$ is the probability that W_{ex} takes the value w_{ex} and can be obtained using the transition probabilities for each step as shown in Fig. 6.1.*

7

Average work and variance

7.1 Analytical results

In this section, we derive an expression for average work done during work extraction processes involving partial thermalizations (Section 7.1.1) and prove that they are *not* fluctuation-free in general (Section 7.1.2).

7.1.1 Average work

Let us denote the work done during a general thermodynamic process by the random variable W. Work is done when a two-level system is in the excited state during a level transformation. Depending upon whether this transformation decreases or increases the energy gap, one obtains negative or positive values of W corresponding to a net work gain or a net work cost. We shall denote a net work gain by the random variable W and refer to it as just work done unless stated otherwise. Thus, the average work done during a process where the energy gap of the system is driven from δ_{max} to δ_{min} as it partially thermalizes with an ambient bath

for a time τ is given by

$$\mu_W(\tau) = -\int_{\delta_{max}}^{\delta_{min}} p(\delta)\mathrm{d}\delta, \tag{7.1}$$

where $p(\delta)$ is the probability of the system to be in the excited state when the energy gap is δ. Let us first list a few ingredients that would come in handy in deriving the main result, i.e. an expression for average work, Theorem 5.

Definition 6. *Given the energy gap $\delta(t)$ of a two-level system at time $t \leq \tau$, we define the function*

$$\mathcal{G} : t \mapsto -\sum_{n=1}^{\infty} \frac{\left(-\frac{\delta(t)}{T_h}\right)^n}{\left(\frac{n\epsilon}{\kappa\tau T_h} + 1\right)}, \tag{7.2}$$

where $\epsilon = \delta_{\max} - \delta_{\min}$, κ is the thermalization rate, and T_h is the temperature of the ambient bath.

The function $\mathcal{G}$ is a monotone function in t. For δ monotonically decreasing in t, $\mathcal{G}$ monotonically increases. This follows by noting that $-e^{-\delta(t)}$ is also monotonically decreasing in t. We also make use of a few standard functions in the proofs that have been redefined in Section B.2 for completeness.

Lemma 12 (Time evolution of occupation probabilities under partial thermalization)**.** *Given a two-level system undergoing a work extraction process along with partial thermalizations with a bath at temperature T_h as per Assumption 1 such that its energy gap changes from δ_{max} to δ_{min} over a time τ, the occupation probability for the excited state at any time $0 < t < \tau$ is given by*

$$p(t) \;=\; p_0 e^{-\kappa t} + \mathcal{G}(t) - e^{-\kappa t}\mathcal{G}(0), \tag{7.3}$$

where $\epsilon = \delta_{max} - \delta_{min}$, $p_0 = p(0)$ and $\delta(t) = \delta_{max} - \epsilon t/\tau$.

Proof. Re-writing the differential equation for a general work extraction with partial thermalizations, (6.2), we have

$$\frac{\mathrm{d}p}{\mathrm{d}t} + \kappa p(t) = \kappa \gamma_h\big(\delta(t)\big), \tag{7.4}$$

which can be integrated along with the initial condition $p(0) = p_0$ to obtain

$$p(t) = p_0 e^{-\kappa t} + \kappa e^{-\kappa t} \int_0^t e^{\kappa t'} \gamma_h\big(\delta(t')\big)\, \mathrm{d}t'. \tag{7.5}$$

Given Assumption 1 and the boundary conditions $\delta(0) = \delta_{max}$ and $\delta(\tau) = \delta_{min}$, we have

$$\delta(t) = \delta_{max} - \frac{\epsilon}{\tau} t, \tag{7.6}$$

where $\epsilon = \delta_{max} - \delta_{min}$. Plugging $\gamma_h\big(\delta(t)\big) = \frac{1}{1+e^{\delta(t)/T_h}}$ and (7.6) in (7.5), we obtain

$$p(t) = p_0 e^{-\kappa t} + \kappa e^{-\kappa t} \int_0^t \frac{e^{\kappa t'}}{1 + e^{\frac{(\delta_{max} - \epsilon t'/\tau)}{T_h}}}\, \mathrm{d}t'. \tag{7.7}$$

The integral above is given in terms of the Hypergeometric function as in

(B.8). Thus,

$$\begin{aligned} p(t) &= p_0 e^{-\kappa t} + \kappa e^{-\kappa t} \left\{ \frac{e^{\left(\kappa + \frac{\epsilon}{\tau T_h}\right) t' - \frac{\delta_{max}}{T_h}}}{\kappa + \frac{\epsilon}{\tau T_h}} \times \right. \\ &\quad \left. {}_2F_1\left(1, \frac{\kappa\tau T_h}{\epsilon} + 1, \frac{\kappa\tau T_h}{\epsilon} + 2; -e^{-\frac{(\delta_{max} - \epsilon t'/\tau)}{T_h}}\right) \right|_0^t \Bigg\} \\ &= p_0 e^{-\kappa t} + \frac{\kappa\tau T_h}{\epsilon} \left\{ \frac{e^{-\frac{(\delta_{max} - \epsilon t/\tau)}{T_h}}}{\frac{\kappa\tau T_h}{\epsilon} + 1} \times \right. \\ &\quad {}_2F_1\left(1, \frac{\kappa\tau T_h}{\epsilon} + 1, \frac{\kappa\tau T_h}{\epsilon} + 2; -e^{-\frac{(\delta_{max} - \epsilon t/\tau)}{T_h}}\right) - \\ &\quad e^{-\kappa t} \frac{e^{-\frac{\delta_{max}}{T_h}}}{\frac{\kappa\tau T_h}{\epsilon} + 1} \times \\ &\quad \left. {}_2F_1\left(1, \frac{\kappa\tau T_h}{\epsilon} + 1, \frac{\kappa\tau T_h}{\epsilon} + 2; -e^{-\frac{\delta_{max}}{T_h}}\right) \right\}. \end{aligned} \tag{7.8}$$

Next, using (B.9) we can write

$$\begin{aligned} &\left(\frac{az}{a+1}\right) {}_2F_1(1, 1+a, 2+a; -z) \\ &= \left(\frac{az}{a+1}\right) \sum_{n=0}^{\infty} \frac{n!(1+a)_n}{(2+a)_n} \frac{(-z)^n}{n!} \\ &= -\sum_{n'=1}^{\infty} \frac{(-z)^{n'}}{\left(\frac{n'}{a} + 1\right)}. \end{aligned} \tag{7.9}$$

Using (7.9) we can write (7.8) in terms of the function $\mathcal{G}$, Definition 6, to obtain (7.3). □

We are now ready to derive the expression for average work.

Theorem 5 (Average work)**.** *The average work done by a two-level system during a work extraction process involving partial thermalizations with respect*

to a bath at temperature T_h, wherein its energy gap is driven from δ_{max} to δ_{min} as per Assumption 1 over a time τ, is given by

$$\begin{aligned}\mu_W(\tau) &= W_{iso}^{T_h} + \frac{W_{ad}}{\kappa\tau}\big(1 - e^{-\kappa\tau}\big) \\ &\quad - \frac{\epsilon}{\kappa\tau}\Big\{\mathcal{G}(\tau) - e^{-\kappa\tau}\mathcal{G}(0)\Big\},\end{aligned} \tag{7.10}$$

where $W_{iso}^{T_h}$ is the work done during the corresponding isothermal process, i.e. $W_{iso}^{T_h} = T_h \log\big(Z(\delta_{min})/Z(\delta_{max})\big)$, with Z being the partition function $Z : \delta \mapsto 1 + e^{-\delta/T_h}$, W_{ad} is the work done during the corresponding adiabatic process, i.e. $W_{ad} = \epsilon p_0$, where $p_0 = p(0)$ and $\epsilon = \delta_{max} - \delta_{min}$.

Proof. We start by noting that

$$\frac{\mathrm{d}p}{\mathrm{d}\delta} = \frac{\mathrm{d}p}{\mathrm{d}t}.\frac{\mathrm{d}t}{\mathrm{d}\delta} = -\frac{\kappa\tau}{\epsilon}\Big(\gamma_h(\delta) - p\Big), \tag{7.11}$$

where the last line follows from (6.2) & (7.6) and supressing the dependence on t. Integrating (7.11) with respect to δ from δ_{max} to δ_{min}, we have

$$\int_{\delta_{max}}^{\delta_{min}} p \; \mathrm{d}\delta = \int_{\delta_{max}}^{\delta_{min}} \gamma_h\big(\delta\big)\mathrm{d}\delta + \frac{\epsilon}{\kappa\tau}\int_{\delta_{max}}^{\delta_{min}} \frac{\mathrm{d}p}{\mathrm{d}\delta}\mathrm{d}\delta. \tag{7.12}$$

Then, plugging (7.12) in (7.1) implies

$$\mu_W(\tau) = -\int_{\delta_{max}}^{\delta_{min}} \gamma_h\big(\delta\big)\mathrm{d}\delta - \frac{\epsilon}{\kappa\tau}\int_{\delta_{max}}^{\delta_{min}} \frac{\mathrm{d}p}{\mathrm{d}\delta}\mathrm{d}\delta. \tag{7.13}$$

Substituting the expression for $\gamma_h(\delta)$ and evaluating the integral gives us the first term of (7.13) as

$$\int_{\delta_{max}}^{\delta_{min}} \gamma_h\big(\delta\big)\mathrm{d}\delta = -T_h \ln\frac{Z(\delta_{min})}{Z(\delta_{max})}, \tag{7.14}$$

where Z is the partition function. The expression above is simply the negative of the work done during the corresponding isothermal reversible process,

$$W_{iso}^{T_h} = T_h \ln \frac{Z(\delta_{min})}{Z(\delta_{max})}. \tag{7.15}$$

Next, we evaluate the integral in the second term in (7.13) using Lemma 12 together with the boundary conditions $p(\delta_{max}) = p_0$ and $p(\delta_{min}) = p(\tau)$. Thus, we have

$$\begin{aligned} \int_{\delta_{max}}^{\delta_{min}} \frac{\mathrm{d}p}{\mathrm{d}\delta}\, \mathrm{d}\delta &= p(\delta_{min}) - p(\delta_{max}) \\ = \quad & p_0\big(e^{-\kappa\tau} - 1\big) + \mathcal{G}(\tau) - e^{-\kappa t}\mathcal{G}(0). \end{aligned} \tag{7.16}$$

Now, if one changes the energy gap from δ_{max} to δ_{min} adiabatically the distribution of work is simply a two-point distribution, where $W = 0$ occurs with probability $1 - p_0$ and $W = \epsilon$ occurs with probability p_0. Thus, the average work done would be

$$W_{ad} = \epsilon p_0. \tag{7.17}$$

Plugging (7.14) and (7.16) in (7.13) together with (7.15) and (7.17) gives us the result. □

Corollary 2. *The expression for average work in Theorem 5 reduces to the adiabatic case in the limit $\tau \to 0$, i.e.*

$$\lim_{\tau\to 0} \mu_W(\tau) = W_{ad}, \tag{7.18}$$

and the isothermal case in the limit $\tau \to \infty$,

$$\lim_{\tau\to\infty} \mu_W(\tau) \quad = \quad W_{iso}^{T_h}. \tag{7.19}$$

Proof. Let us first derive the adiabatic limit, $\tau \to 0$:

$$\begin{aligned}\lim_{\tau\to 0}\mu_W(\tau) &= W_{iso}^{T_h} + \lim_{\tau\to 0}\Bigg\{\frac{W_{ad}}{\kappa\tau}\big(1-e^{-\kappa\tau}\big) + \\ &\qquad \frac{\epsilon}{\kappa\tau}\Big(\mathcal{G}(\tau) - e^{-\kappa\tau}\mathcal{G}(0)\Big)\Bigg\}. \end{aligned} \tag{7.20}$$

Let us first look at the second term in the limit

$$\begin{aligned}\lim_{\tau\to 0}\frac{1}{\tau}\big(1-e^{-\kappa\tau}\big) &= \lim_{\tau\to 0}\frac{1}{\tau}\left(1-\left(1-\kappa\tau+\frac{\kappa^2\tau^2}{2}-\cdots\right)\right) \\ &= \lim_{\tau\to 0}\left(\kappa-\frac{\kappa^2\tau}{2}+\cdots\right) = \kappa. \end{aligned} \tag{7.21}$$

So, we have

$$\begin{aligned}&\lim_{\tau\to 0}\mu_W(\tau) = W_{iso}^{T_h} + W_{ad} + \lim_{\tau\to 0}\ \frac{\epsilon}{\kappa\tau}\Bigg\{\mathcal{G}(\tau) - e^{-\kappa\tau}\mathcal{G}(0)\Bigg\} \\ = \ & W_{iso}^{T_h} + W_{ad} + T_h\Bigg\{-e^{-\frac{\delta_{min}}{T_h}}\ \Phi_L\Big(-e^{-\frac{\delta_{min}}{T_h}},1,1\Big) + \\ & e^{-\frac{\delta_{max}}{T_h}}\ \Phi_L\Big(-e^{-\frac{\delta_{max}}{T_h}},1,1\Big)\Bigg\}, \end{aligned} \tag{7.22}$$

where we have used Definition B.2.2 in the second step. Since, $z\,\Phi_L(z,1,1) = -\log(1-z)$, we have

$$\begin{aligned}&\lim_{\tau\to 0}\mu_W(\tau) = W_{iso}^{T_h} + W_{ad} + \\ &T_h\Bigg\{\log\big(1+e^{-\frac{\delta_{min}}{T_h}}\big) - \log\big(1+e^{-\frac{\delta_{max}}{T_h}}\big)\Bigg\}, \end{aligned} \tag{7.23}$$

where the first term cancels the third term due to (7.14), and thus we obtain (7.18). The isothermal limit, $\tau \to \infty$, can be similarly obtained

since

$$\lim_{\tau\to\infty}\mu_W(\tau) = W_{iso}^{T_h} - \lim_{\tau\to\infty}\Bigg\{ -\frac{W_{ad}}{\kappa\tau}\big(1-e^{-\kappa\tau}\big) + \frac{\epsilon}{\kappa\tau}\Big(\mathcal{G}(\tau) - e^{-\kappa\tau}\mathcal{G}(0)\Big)\Bigg\}, \tag{7.24}$$

and it is clear that the second term in the equation above would vanish in the limit $\tau \to \infty$. Furthermore, using Definition 6, we find that the third term would also vanish in the limit and so we recover (7.19). □

7.1.2 Lower bound on variance

We will now establish, by means of the following theorem, that fluctuations in work during processes involving partial thermalizations are non-zero, independent of Assumption 1.

Theorem 6 (Fluctuations in work)**.** *Consider a two-level system undergoing a work extraction process where the energy gap is driven from δ_{max} to δ_{min} in L discrete steps along with partial thermalizations over a finite time τ. Then, the following are true in general for the random variable W_L denoting the total work done during such a process:*

$$\lim_{L\to\infty}\Pr[W_L = 0] = \big(1-p_0\big)e^{-\kappa\int_0^\tau dt\gamma_h(\delta(t))}, \tag{7.25}$$

and

$$\lim_{L\to\infty}\Pr[W_L = \epsilon] = p_0 e^{-\kappa\int_0^\tau dt(1-\gamma_h(\delta(t))}, \tag{7.26}$$

where $\epsilon = \delta_{max} - \delta_{min}$, $L \to \infty$ is the continuous time limit, and p_0 is the initial excited state probability of the two-level system.

Proof. From Fig. 6.2, it is easy to see that the following expression holds for a discrete partial thermalization process composed of L steps such

that each step takes time Δt:

$$\Pr[W_L = 0] \;=\; (1-p_0)\prod_{l=1}^{L-1}\Big(1-\kappa\Delta t\gamma_h\big(\delta(l\Delta t)\big)\Big). \tag{7.27}$$

Taking log on both-sides of the above equation we have,

$$\begin{aligned}\log\Big(\Pr[W_L=0]\Big) \;&=\; \log(1-p_0) + \\ &\qquad \sum_{l=1}^{L-1}\log\Big(1-\kappa\Delta t\gamma_h\big(\delta(l\Delta t)\big)\Big) \\ &\overset{\Delta t\ll 1}{\simeq}\; \log(1-p_0) - \\ &\qquad \kappa\sum_{l=1}^{L-1}\Delta t\gamma_h\big(\delta(l\Delta t)\big).\end{aligned} \tag{7.28}$$

Taking the limit $\Delta t \to 0$ ($L \to \infty$) and observing that the second term above would thus be a Riemann sum, we obtain (7.25) by exponentiating the resulting expression (and noting that limit commutes with continuous functions). Similarily, the last row in Fig. 6.2 implies that

$$\Pr[W_L = \epsilon] = p_0\prod_{l=1}^{L-1}\Big(1-\kappa\Delta t\big(1-\gamma_h\big(\delta(l\Delta t)\big)\big)\Big). \tag{7.29}$$

Again, taking log on both-sides we have

$$\begin{aligned}&\log\Big(\Pr[W_L=\epsilon]\Big) \\ =\;& \log p_0 + \sum_{l=1}^{L-1}\log\Big(1-\kappa\Delta t\Big(1-\gamma_h\big(\delta(l\Delta t)\big)\Big)\Big) \\ \overset{\Delta t\ll 1}{\simeq}\;& \log p_0 - \kappa\sum_{l=1}^{L-1}\Delta t\Big(1-\gamma_h\big(\delta(l\Delta t)\big)\Big).\end{aligned} \tag{7.30}$$

Again, taking the limit $\Delta t \to 0$ ($L \to \infty$) results in an expression that gives (7.26) upon exponentiation. □

This result analytically establishes that the distribution of work is typically broad as was also found numerically in Ref. [Marathe and Dhar (2005)]. While the theorem above holds in general, a lower bound on the variance of work done by systems driven linearly in time (Assumption 1) can be obtained as a corollary to it.

Corollary 3 (Lower bound on variance of work)**.** *For a finite-time process as per Assumption 1 along with partial thermalizations, the variance of work is bounded from below as*

$$\sigma_W^2(\tau) \geq (1-p_0)\left(\frac{Z(\delta_{min})}{Z(\delta_{max})}\right)^{-\frac{\kappa\tau T_h}{\epsilon}} \mu_W^2(\tau) + p_0\, e^{-\kappa\tau}\left(\frac{Z(\delta_{min})}{Z(\delta_{max})}\right)^{\frac{\kappa\tau T_h}{\epsilon}} \Big(\epsilon + \mu_W(\tau)\Big)^2, \tag{7.31}$$

where Z is the partition function $Z : \delta \mapsto 1 + e^{-\delta/T_h}$ and $\mu_W(\tau)$ is the average work output of the process as given by Theorem 5. Moreover, the lower bound is saturated in the adiabatic limit,

$$\lim_{\tau\to 0} \sigma_W^2(\tau) = p_0(1-p_0)\epsilon^2, \tag{7.32}$$

as well as in the isothermal limit,

$$\lim_{\tau\to\infty} \sigma_W^2(\tau) = 0. \tag{7.33}$$

Proof. We will first derive expressions for the probabilities of work values $W = 0$ and $W = \epsilon$ when undergoing a finite-time process s per Assumption 1 along with partial thermalizations using Theorem 6. Using the expression for $\delta(t)$ as given by (7.6) we change the variable of integration to δ in (7.25) and obtain the following after taking log on both sides:

$$\begin{aligned} &\lim_{L\to\infty} \log\Big(\Pr[W_L = 0]\Big) \\ =\ &\log\Big(1-p_0\Big) + \frac{\kappa\tau}{\epsilon}\int_{\delta_{max}}^{\delta_{min}} \frac{\mathrm{d}\delta}{1+e^{\delta/T_h}}. \end{aligned} \tag{7.34}$$

Evaluating the integral and exponentiating the above we have

$$\lim_{L\to\infty} \Pr[W_L = 0] \;=\; (1-p_0)\left(\frac{Z(\delta_{min})}{Z(\delta_{max})}\right)^{-\frac{\kappa\tau T_h}{\epsilon}}, \tag{7.35}$$

where Z is the partition function. Similarly, (7.26) gives

$$\begin{aligned}&\lim_{L\to\infty} \log\Big(\Pr[W_L = \epsilon]\Big)\\ =\;& \log p_0 + \frac{\kappa\tau}{\epsilon}\int_{\delta_{max}}^{\delta_{min}} \frac{\mathrm{d}\delta}{1+e^{-\delta/T_h}}.\end{aligned} \tag{7.36}$$

Again, evaluating the integral and exponentiating the above we obtain

$$\lim_{L\to\infty} \Pr[W_L = \epsilon] \;=\; p_0\, e^{-\kappa\tau}\left(\frac{Z(\delta_{min})}{Z(\delta_{max})}\right)^{\frac{\kappa T T_h}{\epsilon}}. \tag{7.37}$$

Now that we have the expressions for $\Pr[W_L = 0]$ and $\Pr[W_L = \epsilon]$ it is straightforward to obtain a lower bound for the variance of work as the sum of these two contributions. Thus,

$$\begin{aligned}\sigma^2_{W_L}(\tau) \;\geq\; &\Pr[W_L = 0]\big(\mu_{W_L}(\tau)\big)^2 +\\ &\Pr[W_L = \epsilon]\big(\epsilon - \mu_{W_L}(\tau)\big)^2.\end{aligned} \tag{7.38}$$

Taking the limit $L \to \infty$ and assuming that W_L converges in probability to the random variable W for the continuous process, we have

$$\begin{aligned}\sigma^2_{W}(\tau) \;\geq\; \lim_{L\to\infty}\Bigg\{ &\Pr[W_L = 0]\big(\mu_{W}(\tau)\big)^2 +\\ &\Pr[W_L = \epsilon]\big(\epsilon - \mu_{W}(\tau)\big)^2\Bigg\}.\end{aligned} \tag{7.39}$$

Plugging (7.35) and (7.37) in the equation above gives (7.31). Let us now look at the lower bound in the following two limiting cases.

- Adiabatic limit, $\tau \to 0$:

$$\begin{aligned}
&\lim_{\tau\to 0}\Bigg\{(1-p_0)\left(\frac{Z(\delta_{min})}{Z(\delta_{max})}\right)^{-\frac{\kappa\tau T_h}{\epsilon}}\mu_W^2(\tau)+\\
&p_0\, e^{-\kappa\tau}\left(\frac{Z(\delta_{min})}{Z(\delta_{max})}\right)^{\frac{\kappa\tau T_h}{\epsilon}}\Big(\epsilon-\mu_W(\tau)\Big)^2\Bigg\}\\
=\;&\lim_{\tau\to 0}\Big\{(1-p_0)\mu_W^2(\tau)+p_0\Big(\epsilon-\mu_W(\tau)\Big)^2\Big\}\\
=\;&p_0(1-p_0)\epsilon^2, \qquad (7.40)
\end{aligned}$$

  where the last line follows from (7.18). Recall that the average work done when changing the energy gap from δ_{max} to δ_{min} adiabatically is given by (7.17). Moreover, the variance of work for an adiabatic process can be obtained by noting that the distribution of $W_{ad} \in \{0, \epsilon\}$ is simply $\{1-p_0, p_0\}$, i.e.

$$\begin{aligned}
\sigma_W^2(\tau=0) &= p_0(\epsilon-W_{ad})^2+(1-p_0)W_{ad}^2\\
&= p_0(1-p_0)\epsilon^2. \qquad (7.41)
\end{aligned}$$

  Therefore, (7.40) and (7.41) together imply that the lower bound is saturated in the said limit.

- Isothermal limit, $\tau \to \infty$:

$$\begin{aligned}
&\lim_{\tau\to\infty}\Bigg\{(1-p_0)\left(\frac{Z(\delta_{min})}{Z(\delta_{max})}\right)^{-\frac{\kappa\tau T_h}{\epsilon}}\mu_W^2(\tau)+\\
&p_0\, e^{-\kappa\tau}\left(\frac{Z(\delta_{min})}{Z(\delta_{max})}\right)^{\frac{\kappa\tau T_h}{\epsilon}}\Big(\epsilon-\mu_W(\tau)\Big)^2\Bigg\}. \qquad (7.42)
\end{aligned}$$

  Now, let us look at the relevant part in the first term of (7.42). Plug-

ging in the definition for the partition function Z, we have

$$\begin{aligned} &\lim_{\tau\to\infty}\left(\frac{Z(\delta_{min})}{Z(\delta_{max})}\right)^{-\frac{\kappa\tau T_h}{\epsilon}} \\ &= \lim_{\tau\to\infty}\left(\frac{1+e^{-\delta_{min}/T_h}}{1+e^{-\delta_{max}/T_h}}\right)^{-\frac{\kappa\tau T_h}{\epsilon}} \quad = \quad 0, \end{aligned} \tag{7.43}$$

as $1+e^{-\delta_{min}/T_h} > 1+e^{-\delta_{max}/T_h}$. Similarly, we look at the relevant part of the second term in (7.42) to obtain

$$\begin{aligned} &\lim_{\tau\to\infty} e^{-\kappa\tau}\left(\frac{Z(\delta_{min})}{Z(\delta_{max})}\right)^{\frac{\kappa\tau T_h}{\epsilon}} \\ &= \lim_{\tau\to\infty}\left(e^{-\epsilon/T_h}\left(\frac{1+e^{-\delta_{min}/T_h}}{1+e^{-\delta_{max}/T_h}}\right)\right)^{\frac{\kappa\tau T_h}{\epsilon}} \\ &= \lim_{\tau\to\infty}\left(\frac{1+e^{\delta_{min}/T_h}}{1+e^{\delta_{max}/T_h}}\right)^{\frac{\kappa\tau T_h}{\epsilon}} \\ &= 0, \end{aligned} \tag{7.44}$$

where we have used the fact that $\epsilon = \delta_{max} - \delta_{min}$ along with $1 + e^{\delta_{min}/T_h} < 1 + e^{\delta_{max}/T_h}$. Thus, we obtain

$$\lim_{\tau\to\infty}\sigma_W^2(\tau) \geq 0. \tag{7.45}$$

Moreover, from Ref. [Åberg (2013)], we know that isothermal work extraction is fluctuation-free, i.e.

$$\sigma_W^2(\tau=\infty) = 0. \tag{7.46}$$

Again, (7.45) and (7.46) together imply that the lower bound is saturated in this limit.

□

7.2 Numerical results

In this section we present the results of the Monte Carlo simulation for the Markov process, Fig. 6.1, to obtain estimates of the variance as a function of the time period of the process. Furthermore, for a two-level system that is initially in equilibrium with the bath, we find that the variance can be estimated using Jarzynski's fluctuation-dissipation relation.

7.2.1 Monte Carlo for variance of work

In order to compare the gap between the analytical lower bound obtained in Corollary 3 with the actual variance, we perform Monte Carlo simulations since an analytical derivation seems to be intractable owing to the time-dependent nature of the Markov process, Fig. 6.1. The Monte Carlo basically simulates a discrete version of the Markov process under Assumption 1, see Example 4. We plot the results of the same in Fig. 7.1. As a test of credibility, we find that the error-bars on our numerically obtained values of average work successfully envelop the analytical form as a function of τ (Theorem 5). The error bars were obtained using 10^4 independent runs. The independent runs were parallelized using GNU parallel [Tange (2018)].

7.2.2 Fluctuation-dissipation relation

A fluctuation-dissipation relation governing an irreversible thermodynamic process is a statement about the relation between the dissipated work (on average) when a system is driven away from equilibrium and the corresponding fluctuations of work during such a process. Jarzynski's

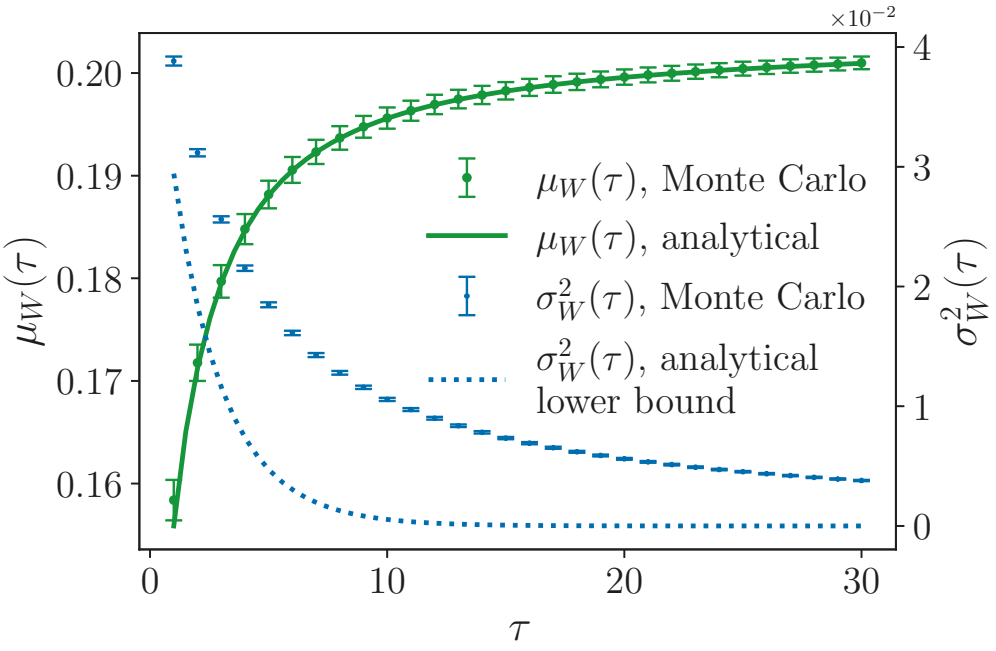


Figure 7.1: (Color online) On the x-axis we have total time of the work extraction process, τ. The solid green (gray) curve interpolates between the adiabatic $W_{ad} = 0.134$ and the isothermal $W_{iso}^{T_h} = 0.204$ limits. The dashed blue (black) curve also interpolates between the adiabatic $\sigma_W^2(\tau = 0) = 0.049$ and the isothermal $\sigma_W^2(\tau = \infty) = 0$ limits. The Monte Carlo simulations were done with $L = 1000$ steps, where L is the discretization (see Example 4) and for integer values of $\tau \in [1, 30]$. The parameter values used are $\delta_{max} = 1$, $\delta_{min} = 0.5$, $T_h = 2$, $p_0 = \frac{1}{1+e}$, and $\kappa = 1$.

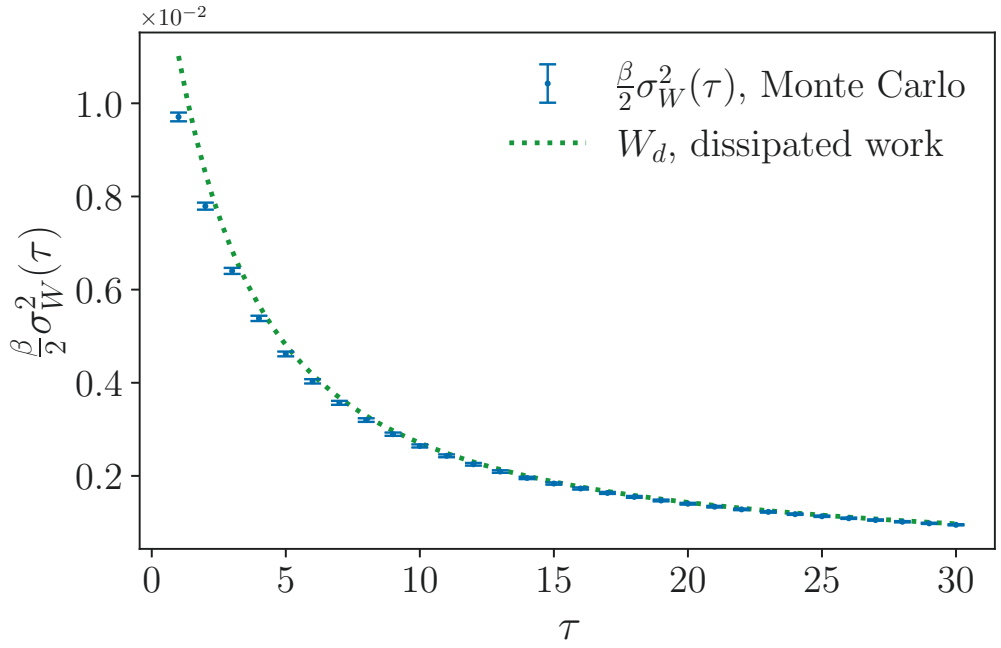


Figure 7.2: (Color online) Fluctuation-dissipation relation for finite-time processes. On the x-axis we have the total time of the work extraction process, τ. W_d is the dissipated work. The Monte Carlo simulations were done for $L = 1000$ steps, where L is the discretization (see Example 4) and for integer values of $\tau \in [1, 30]$. The parameter values used are $\delta_{max} = 1$, $\delta_{min} = 0.5$, $T_h = 2$, $p_0 = \frac{1}{1+e^{1/2}}$, and $\kappa = 1$.

[Jarzynski (1997)] much touted result gave such a relation in the weak system-bath interaction limit. Basically, once the system is in equilibrium with the ambient bath it is disconnected from the bath and then the work extraction process is performed which essentially amounts to changing the value of some relevant parameter (that governs the Hamiltonian) over a finite amount of time. When the time over which the process is carried out—the switching time—is large enough it renders the distribution of work Gaussian and the fluctuation-dissipation relation follows. Denoting the random variable for the work done during such an irreversible process by W and its mean and variance by μ_W and σ_W^2, respectively, the dissipated work is $W_{diss} = \mu_W - \Delta F$, the difference between the average work done during the process, μ_W, and the average work done during the corresponding reversible process i.e. the free-energy difference, ΔF. The fluctuation-dissipation relation can then be expressed as

$$W_{diss} = \frac{\beta}{2}\sigma_W^2, \tag{7.47}$$

where $\beta = 1/k_B T_h$ with T_h being the temperature of the ambient bath. This relation has been generalized [Miller *et al.* (2019); Scandi *et al.* (2020)] to the case where the system continues to be in contact with the bath during the work extraction process. Using Theorem 5 with $p_0 = 1/(1 + e^{\delta_{max}/T_h})$, we plot the dissipated work, $\mu_W(\tau) - \Delta F$, and the estimate of the variance from the Monte Carlo simulation as a function of the total time period of the process τ in Fig. 7.2. We observe that the dissipated work provides an upper bound for the variance of work in general. This bound is saturated in the limit of large τ in agreement with the aforementioned result of Refs. [Miller *et al.* (2019); Scandi *et al.* (2020)].

7.3 Distribution of work

This section is based on numerical analysis that was done using a different driving rate for the energy-gap $\delta(t)$; we assumed that the partial thermalization curve follows an isotherm at a lower temperature T_c, on an average[1]. However, the conclusions drawn for the distribution of work should hold in general (independent of the driving rate).

As the partial thermalization curve follows an isotherm on an average, $p(t) = \gamma_c(t)$, where $\gamma_c(t)$ is the corresponding Gibbs weight. Thus, the general expression for partial thermalization as given by (6.2) becomes

$$\frac{\mathrm{d}\gamma_c(t)}{\mathrm{d}t} = \kappa\big(\gamma_h(t) - \gamma_c(t)\big), \tag{7.48}$$

where $\gamma_c(t) = \frac{1}{1+e^{\delta(t)/T_c}}$. Taking the derivative in the above and rearranging the terms, we obtain

$$\delta'(t) = \kappa T_c \cdot \frac{\big(\gamma_c(t) - \gamma_h(t)\big)}{\gamma_c(t)\big(1-\gamma_c(t)\big)}. \tag{7.49}$$

For the numerical simulation, we want the system-bath interaction time, Δt, as the excited state's energy changes by an amount $\Delta\delta = \epsilon/L$ at each step. So, using (7.49), we have

$$\begin{aligned} \Delta t &= \Delta\delta \cdot \frac{\mathrm{d}t}{\mathrm{d}\delta} \\ &= \frac{\epsilon}{\kappa L T_c} \cdot \frac{\gamma_c(t)\big(1-\gamma_c(t)\big)}{\big(\gamma_c(t) - \gamma_h(t)\big)}. \end{aligned} \tag{7.50}$$

One can thus obtain the distribution for work using the probability with which the system thermalizes with the bath, $\lambda = \kappa\Delta t$, as shown in Fig. 7.3.

The numerically obtained distribution suggests that the asymptotic distribution ($L \to \infty$) might be uniform in the range $(0, \epsilon)$. If that were indeed

[1]For the sake of a neat visualization and in the hope of simplifications.

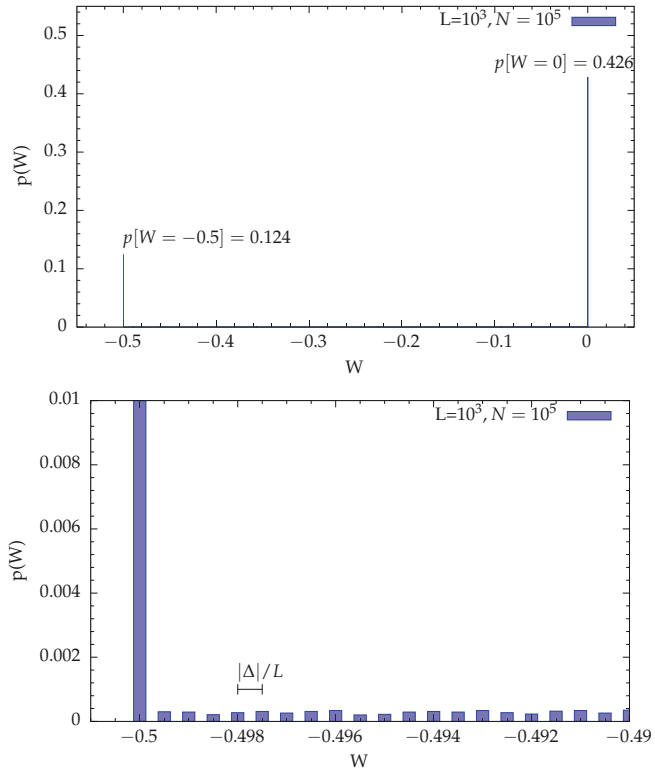


Figure 7.3: Distribution of work W along the isotherm T_c when partially thermalising with respect to the bath at T_h at different scales (negative signs indicate work gain). $p[W = 0]$ and $p[W = -0.5]$ are calculated analytically for $L = 10^3$ using the corresponding generalisation of expressions from Fig. 6.2 and are in agreement with the numerical values as seen in the plot with $\kappa = 1$.

the case then it would imply that $\Pr[W \in I]$ for any interval $I \subset (0, \epsilon)$ is proportional to $|I|$ and that the constant of proportionality is independent of I in the $L \to \infty$ limit. If for each possible value of $W \in (0, \epsilon)$, the probability was $\mathcal{O}(1/L)$ (for large but finite L), then

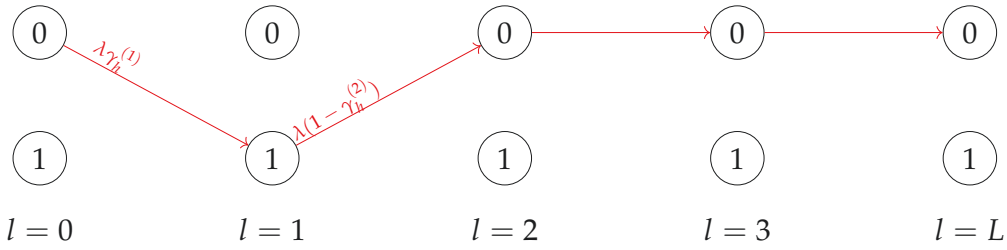
$$\Pr[W \in I] = \mathcal{O}\left(\frac{1}{L}\right) n_I, \quad \forall\ I \in (0, \epsilon), \tag{7.51}$$

where n_I is the number of work values in the interval I. Given that in our problem all possible work values are integer multiples of ϵ/L for finite L, we have $n_I = L \cdot |I|/\epsilon$ and

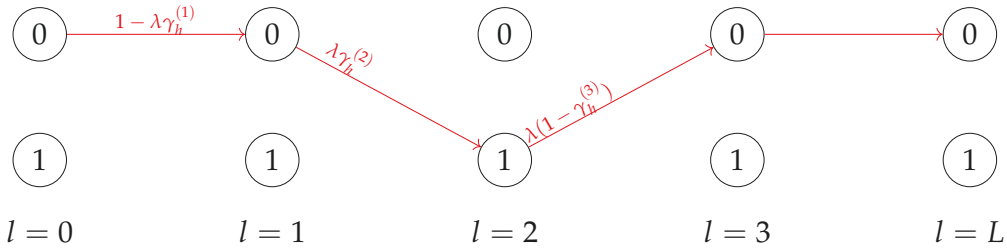
$$\Pr[W \in I] = \mathcal{O}(1). \tag{7.52}$$

So, if the constant of proportionality in the above was the same for all intervals $I \in (0, \epsilon)$ then one would be through. Hence, showing that the distribution is uniform in the range $(0, \epsilon)$ boils down to proving: a) that for each possible value of $W \in (0, \epsilon)$ the probability actually is $\mathcal{O}(1/L)$ and, b) that the constant that appears there is the same for all intervals I in the $L \to \infty$ limit.

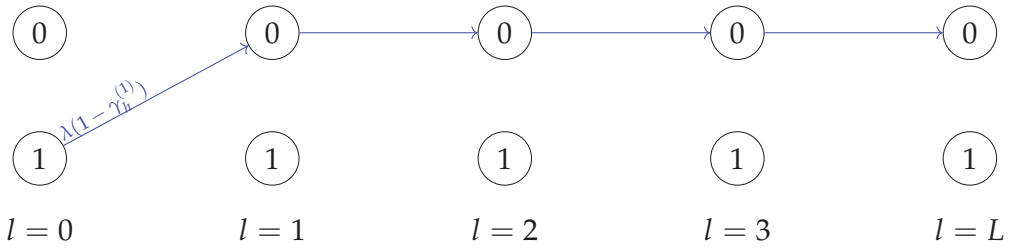
Let us begin by recalling Example 4 and looking at how the individual probabilities scale with L. For $W = \epsilon/L$, the following diagram represents a path in which the state starts at 0 and flips to 1 once and flips back to 0 in the next step.



The above corresponds to $W = \epsilon/L$. Obviously, the flips could happen after the first step, i.e.



Clearly, there are $L-1$ ways of flipping once starting at 0. But, there is exactly one path corresponding to $W = \epsilon/L$ starting at 1:



Therefore, as $\lambda \propto 1/L$, we have

$$\Pr\left[W = \epsilon/L \middle| \text{paths with two flips}\right] = \mathcal{O}\left(\frac{L-1}{L^2}\right),$$

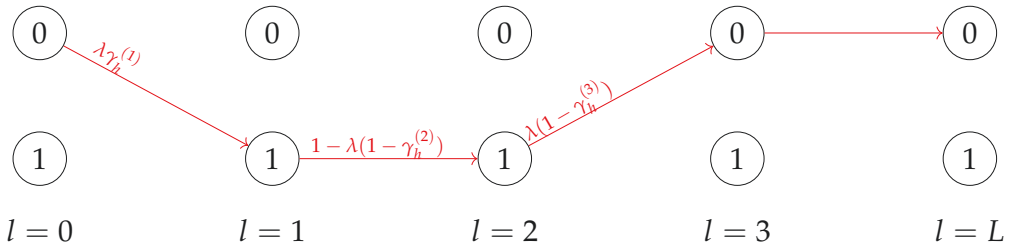
while

$$\Pr\left[W = \epsilon/L \middle| \text{paths with one flip}\right] = \mathcal{O}\left(\frac{1}{L}\right),$$

and so

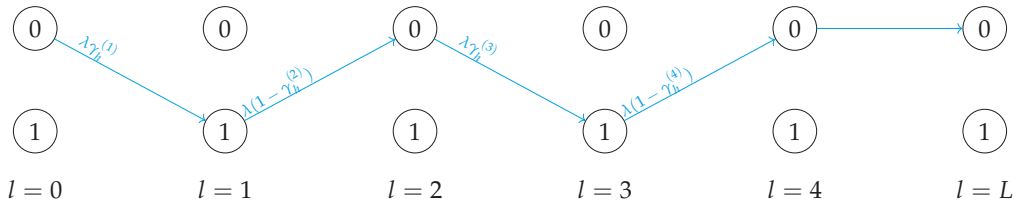
$$\Pr\left[W = \epsilon/L\right] = \mathcal{O}\left(\frac{1}{L}\right).$$

Next, for $W = 2\epsilon/L$, we could have the following diagrams corresponding to paths where the state starts at 0:



There are $\binom{L-2}{2}$ such paths as the first flip could happen at the second step, or the third, etc. and similarly for the second flip—really it is the

number of ways of choosing two points on the lower chain out of the available $L-2$ spots as such paths always start at 0. For example:



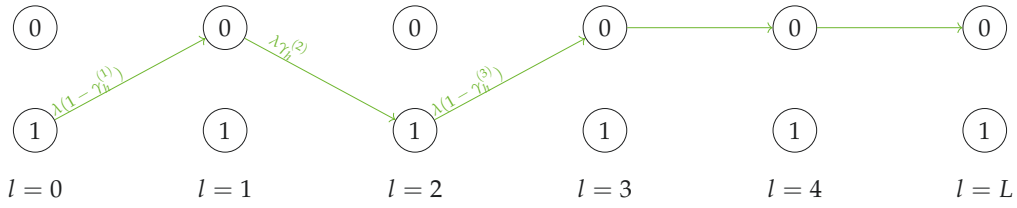
However, all paths that involve four flips can be neglected since

$$\Pr\left[W = 2\epsilon_L \middle| \text{paths with four flips}\right] = \mathcal{O}\left(\frac{L^2}{L^4}\right).$$

Thus,

$$\Pr\left[W = 2\epsilon_L \middle| \text{paths with two flips}\right] = \mathcal{O}\left(\frac{(L-1)/2}{L^2}\right),$$

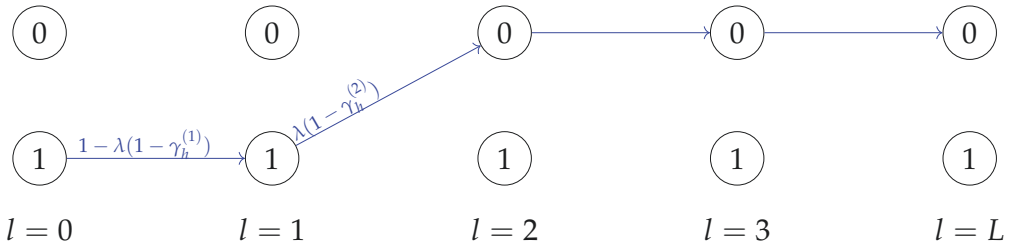
as there are $(L-2)/2$ paths that have exactly two flips i.e. the red ones. The third kind of paths are the ones for which the state starts in 1. The following is one such path:



As the second flip could happen at any of the next $L-3$ steps, there are $L-3$ such paths with exactly three flips starting at 1 and hence can be neglected as

$$\Pr\left[W = 2\epsilon_L \middle| \text{paths with three flips}\right] = \mathcal{O}\left(\frac{L-3}{L^3}\right).$$

The fourth kind of path is where the state starts at 1 and stays there and then flips and there is exactly one such path:



The above diagram implies that

$$\Pr\left[W = 2\epsilon_L \middle| \text{path with one flip}\right] = \mathcal{O}\Big(\frac{1}{L}\Big).$$

We could carry on like this but the counting process becomes intractable as we start looking at higher values of W. For example, for $W = \epsilon/2$, we find that the paths that were ignored in the above two cases (three flips and four flips) start contributing such that there seems to be no longer $\mathcal{O}(1)$ number of $\mathcal{O}(1/L)$ terms in $\Pr[W = \epsilon/2]$.

8

Optimal processes

We considered specific models for partial thermalization in Chapter 6 and Chapter 7. However, one might be interested in partial thermalization processes that are optimal in some sense—maximize average work for fixed time or minimize time given a fixed threshold for work output. We explore this question in this chapter, first by treating the probability of occupation for the excited state, p, as an independent variable in Section 8.1 and then, in terms of time t in Section 8.2.

8.1 p as independent variable

The average work done along a path $\delta(p)$ as in Fig. 8.1 with p as an independent variable is

$$W[\delta] = \int_{p_a}^{p_b} p\ \delta'(p)\mathrm{d}p, \tag{8.1}$$

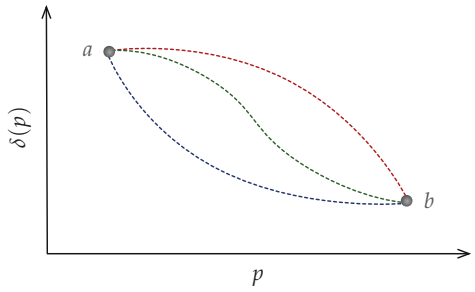


Figure 8.1: The dashed lines are various possible paths connecting the given initial and final points a and b each of which represents a partial thermalization model.

while the time taken along the same path can be obtained using (6.2) to obtain

$$T[\delta] = \int_{p_a}^{p_b} \frac{\mathrm{d}p}{\gamma_h(\delta) - p}\,, \tag{8.2}$$

where we have suppressed the dependence on time. First, let us minimize (8.2). The problem is that of variational calculus and the corresponding Euler-Lagrange equation is as below.

$$\frac{\partial}{\partial\delta}\left(\frac{1}{\gamma_h(\delta) - p}\right) - \frac{\mathrm{d}}{\mathrm{d}p}\frac{\partial}{\partial\delta'}\left(\frac{1}{\gamma_h(\delta) - p}\right) = 0. \tag{8.3}$$

Taking the derivative yields

$$\frac{1}{T_h}\frac{e^{\delta/T_h}}{\left(1 - p(1 + e^{\delta/T_h})\right)^2} = 0. \tag{8.4}$$

The solution to the above is $\delta(p) = -\infty$. As we know that isothermal processes at T_h for which $\delta(p) = T_h \ln\left(1/p - 1\right)$ take the maximum amount of time, i.e. infinitely long, the said solution must correspond to a minimum.

However, there are a few issues with the above problem: (a) The lagrangian in (8.2) is zeroeth order in δ' and is over-determined by the

boundary conditions $\delta(p_a) = \delta_a$, $\delta(p_b) = \delta_b$. (b) The zeroeth order solution is discontinuous and implies that the work done along the solution is infinite!

In order to deal with the discontinuity, instead of minimizing time, we could treat time as a constraint and maximize work. The problem is thus:

$$\begin{aligned} \text{Maximize: } W[\delta] &= \int_a^b p\ \delta'(p)\mathrm{d}p, \\ \text{under the constraint: } T[\delta] &= \int_a^b \frac{\mathrm{d}p}{\gamma_h(\delta) - p} = T, \\ \text{with boundary conditions: } \delta(p_a) &= \delta_a, \\ \delta(p_b) &= \delta_b. \end{aligned} \tag{8.5}$$

The Euler-Lagrange equation for the above problem is

$$\begin{aligned} \frac{\partial}{\partial\delta}\Big(p\ \delta'(p)\Big) - \frac{\mathrm{d}}{\mathrm{d}p}\frac{\partial}{\partial\delta'}\Big(p\ \delta'(p)\Big) = \lambda_1\Big\{ \frac{\partial}{\partial\delta}\left(\frac{1}{\gamma_h(\delta) - p}\right) - \\ \frac{\mathrm{d}}{\mathrm{d}p}\frac{\partial}{\partial\delta'}\left(\frac{1}{\gamma_h(\delta) - p}\right)\Big\}, \end{aligned} \tag{8.6}$$

where λ_1 is the lagrange multiplier for the constraint. The above gives

$$\begin{aligned} -1 &= \lambda_1\ \frac{\partial}{\partial\delta}\left(\frac{1}{\gamma_h(\delta) - p}\right) \\ &= -\lambda_1\ \frac{\frac{\partial}{\partial\delta}\Big(\gamma_h(\delta) - p\Big)}{\Big(\gamma_h(\delta) - p\Big)^2} \end{aligned} \tag{8.7}$$

Substituting for $\gamma_h(\delta)$, we have

$$\begin{aligned}\frac{\partial}{\partial\delta}\Big(\gamma_h(\delta)-p\Big) &= \frac{\partial}{\partial\delta}\left(\frac{1}{1+e^{\delta/T_h}}\right)\\ &= -\frac{\frac{\partial}{\partial\delta}\left(1+e^{\delta/T_h}\right)}{\left(1+e^{\delta/T_h}\right)^2}\\ &= -\frac{1}{T_h}\frac{e^{\delta/T_h}}{\left(1+e^{\delta/T_h}\right)^2}. \end{aligned} \tag{8.8}$$

Plugging (8.8) in (8.7) we get

$$-1 = \frac{\lambda_1}{T_h}\frac{e^{\delta/T_h}}{\left(1-p(1+e^{\delta/T_h})\right)^2}. \tag{8.9}$$

As is evident (8.9) is still ill-defined even though we have dealt with the discontinuity issue.[1] The boundary conditions can't be satisfied due to the fact as the problem is linear in $\delta'(p)$. We need a second-order differential equation in $\delta(p)$ to be able to satisfy our boundary conditions. One way to do so is to introduce a constraint that is non-linear in $\delta'(p)$. Thus, we have the following modified problem:

$$\begin{aligned}\text{Maximize: } W[\delta] &= \int_a^b p\ \delta'(p)\mathrm{d}p,\\ \text{under the constraints:}&\\ T[\delta] &= \int_a^b \frac{\mathrm{d}p}{\gamma_h(\delta)-p} = T,\\ \int_a^b \left(\delta'(p)\right)^2\mathrm{d}p &\leq C_2,\\ \text{with boundary conditions: } \delta(p_a) &= \delta_a,\\ \delta(p_b) &= \delta_b. \end{aligned} \tag{8.10}$$

[1]Swapping the objective and the constraint in (8.5) would still result in the same issue.

The above constrained optimization problem is defined only when the constraint is active i.e., when the strict equality holds as the solution for the inactive constraints is the same as that of the unconstrained problem which is ill-defined in this case. The Euler-Lagrange equation for the problem with equality constraint is

$$\begin{aligned}\frac{\partial}{\partial\delta}\Big(p\ \delta'(p)\Big) - \frac{\mathrm{d}}{\mathrm{d}p}\frac{\partial}{\partial\delta'}\Big(p\ \delta'(p)\Big) \;=\; & \lambda_1\Big\{\ \frac{\partial}{\partial\delta}\Big(\frac{1}{\gamma_h(\delta)-p}\Big) - \\ & \frac{\mathrm{d}}{\mathrm{d}p}\frac{\partial}{\partial\delta'}\Big(\frac{1}{\gamma_h(\delta)-p}\Big)\Big\} + \\ & \lambda_2\Big\{\ \frac{\partial}{\partial\delta}\Big(\big(\delta'(p)\big)^2\Big) - \\ & \frac{\mathrm{d}}{\mathrm{d}p}\frac{\partial}{\partial\delta'}\Big(\big(\delta'(p)\big)^2\Big)\Big\}. \qquad (8.11)\end{aligned}$$

The above equation simplifies to the following:

$$-1 = \frac{\lambda_1}{T_h}\frac{e^{\delta/T_h}}{\big(1-p(1+e^{\delta/T_h})\big)^2} - 2\lambda_2\delta''(p).$$

Redefining $\lambda_2 := -\lambda_2$ gives us

$$2\lambda_2\delta''(p) + \frac{\lambda_1}{T_h}\frac{e^{\delta/T_h}}{\big(1-p(1+e^{\delta/T_h})\big)^2} + 1 = 0. \qquad (8.12)$$

The constraint $\int_a^b \big(\delta'(p)\big)^2\mathrm{d}p = C_2$ can be interpreted as enforcing smoothness; recall that in the method of Lagrange multipliers, used to obtain the Euler-Lagrange equations, the constraints are introduced into the objective functional as an additive term. Thus, a large and positive value of the Lagrange multiplier λ_2 implies a large penalty in the form of positive work for a solution with a given amount of steepness.

Now, (8.12) can be solved numerically by treating λ_1 and λ_2 as parameters. But, there is no analytical way to prove that (8.12) has a solution

for any specific range of values of (λ_1, λ_2). To probe this numerically, we obtain[2] a landscape of possible solutions on a λ_1-λ_2 plot in Fig. 8.2.

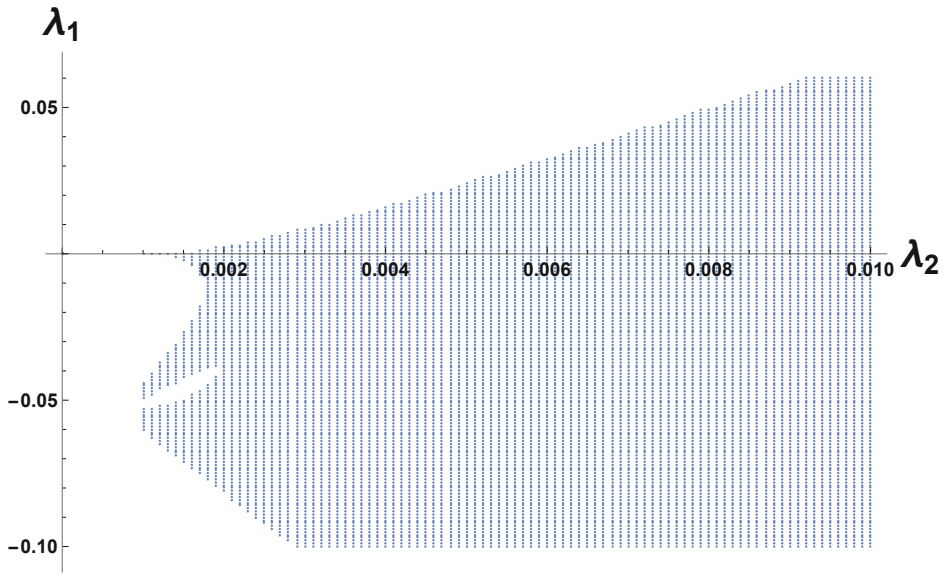


Figure 8.2: This is a plot of solutions for the variational calculus problem, see (8.12) for reference, where each solid dot represents existence of a solution while blank regions indicate no solutions.

While each pair of values of the parameters (λ_1, λ_2) (for which there exists a numerical solution) corresponds to a specific optimal path on the $\delta(p)$-p plot, Fig. 8.3, there is no continuity of solutions in (λ_1, λ_2) as is clear from Fig. 8.2. Even though we don't expect continuity of solutions for the whole (λ_1, λ_2) plane but only in some physically meaningful interval there is no clear way to establish it analytically.

[2]Using *Mathematica*.

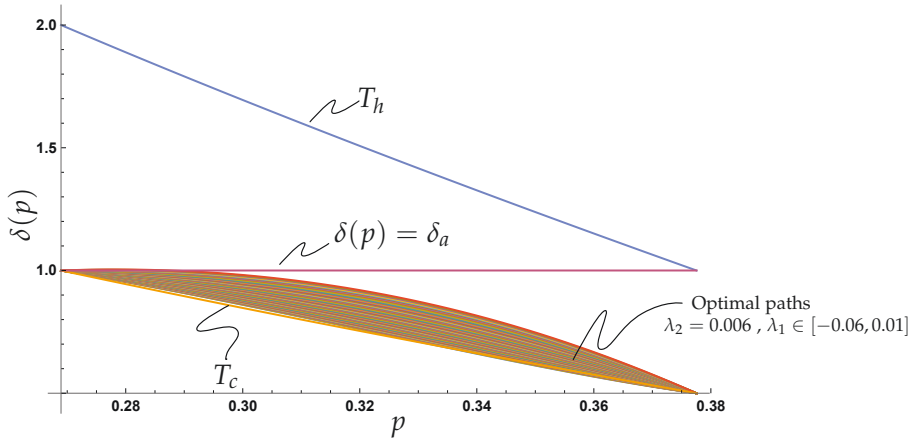


Figure 8.3: This is a p-δ plot with optimal partial thermalization processes for a range of values of (λ_1, λ_2). The isotherms at temperatures T_c and T_h are plotted for reference.

8.2 t as independent variable

In this section, we work with time t as the independent variable and rewrite the optimization problem in (8.10) to see if we can arrive any simplifications. As

$$\delta'(p) = \frac{\dot{\delta}(t)}{\dot{p}(t)},$$

we can write (8.1) using (6.2) in terms of t as

$$W[\delta] = \int_0^T \mathrm{d}t \; p(t)\dot{\delta}(t), \tag{8.13}$$

where T is the total duration. The time constraint becomes trivial and so we are left with the second constraint as in (8.10). The resulting Euler-

Langrange equation would thus be

$$\frac{\partial}{\partial\delta}\Big(p(t)\ \dot{\delta}(t)\Big) - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial\dot{\delta}}\Big(p(t)\ \dot{\delta}(t)\Big) = \lambda\Big\{\ \frac{\partial}{\partial\delta}\Big(\big(\dot{\delta}(t)\big)^2\Big) - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial\dot{\delta}}\Big(\big(\dot{\delta}(t)\big)^2\Big)\Big\}. \quad (8.14)$$

The above simplifies to the following equation:

$$\dot{p}(t) = -2\lambda\ddot{\delta}(t). \quad (8.15)$$

The boundary conditions are $\delta(0) = \delta_a$ and $\delta(T) = \delta_b$. Recalling (6.2) i.e.,

$$\dot{p}(t) = \gamma_h(t) - p(t), \quad (8.16)$$

a first-order ODE which can be solved along with the initial condition $p(0) = p_a$, we are still left with the condition $p(T) = p_b$ that needs to be enforced. Integrating (6.2) along with $p(0) = p_a$ gives us a solution that is a functional of $\delta(t)$:

$$p(t) = p_a + e^{-t}\int_0^t \mathrm{d}t'\ e^{t'}\gamma_h\big(\delta(t)\big). \quad (8.17)$$

So, the constraint $p(T) = p_b$ in turn results in a constraint on $\delta(t)$ i.e.

$$\int_0^T \mathrm{d}t'\ e^{t'}\gamma_h\big(\delta(t)\big) = (p_b - p_a)e^T, \quad (8.18)$$

under which we should optimize (8.13). Thus, we have the final problem as stated below.

$$\begin{aligned} \text{Maximize: } W[\delta] &= \int_0^T \mathrm{d}t\ p(t)\ \dot{\delta}(t), \\ \text{under the constraints:} & \\ \int_0^T \big(\dot{\delta}(t)\big)^2\mathrm{d}t &= C_2, \\ \int_0^T \mathrm{d}t\ e^t\gamma_h\big(\delta(t)\big) &= (p_b - p_a)e^T, \\ \text{with boundary conditions: } \delta(0) &= \delta_a, \\ \delta(T) &= \delta_b. \end{aligned} \quad (8.19)$$

The Euler-Lagrange equation for the above can be obtained as below.

$$\begin{aligned}\frac{\partial}{\partial\delta}\Big(p(t)\ \dot{\delta}(t)\Big) - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial\dot{\delta}}\Big(p(t)\ \dot{\delta}(t)\Big) \;&=\; \lambda_1\Big\{\ \frac{\partial}{\partial\delta}\Big(\big(\dot{\delta}(t)\big)^2\Big) - \\ &\quad \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial\dot{\delta}}\Big(\big(\dot{\delta}(t)\big)^2\Big)\Big\} + \\ &\quad \lambda_2\Big\{\ \frac{\partial}{\partial\delta}\Big(e^t\gamma_h\big(\delta(t)\big)\Big) - \\ &\quad \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial\dot{\delta}}\Big(e^t\gamma_h\big(\delta(t)\big)\Big)\Big\}. \qquad (8.20)\end{aligned}$$

Taking the derivatives above, we get

$$-\dot{p}(t) = 2\lambda_1\ddot{\delta}(t) - \frac{\lambda_2\ e^t}{T_h}\frac{e^{\delta/T_h}}{(1+e^{\delta/T_h})^2}. \qquad (8.21)$$

Plugging (6.2) on the left-hand-side, we obtain

$$-\gamma_h\big(\delta(t)\big) + p(t) = 2\lambda_1\ddot{\delta}(t) - \frac{\lambda_2\ e^t}{T_h}\frac{e^{\delta/T_h}}{(1+e^{\delta/T_h})^2}.$$

But since $p(t)$ is a functional in $\delta(t)$, (8.17), we get the following integro-differential equation:

$$\begin{aligned}p_a + e^{-t}\int_0^t \mathrm{d}t'\ e^{t'}\gamma_h\big(\delta(t)\big) \;&=\; 2\lambda_1\ddot{\delta}(t) - \frac{\lambda_2\ e^t}{T_h}\frac{e^{\delta/T_h}}{(1+e^{\delta/T_h})^2} + \\ &\quad \gamma_h\big(\delta(t)\big). \qquad (8.22)\end{aligned}$$

The above could be solved under the given boundary conditions however *Mathematica* is unable to do the integration directly. It needs to be brought into an ODE form which is also not going to work here as revealed by differentiating (8.22) once. In any case, there is still the problem of not being able to establish that the above would have solutions for any given pair of values of (λ_1, λ_2).

9

Application: finite-time heat engines

Finite-time heat engines are characterized by their non-zero power output in contrast to the ideal Carnot engine. In this section we discuss finite-time heat engines operating in cycles that are composed of work extraction processes involving partial thermalizations and instantaneous adiabatic energy-level transformations. First, we review the Carnot engine for a classical two-level system in Section 9.1 and then study one such engine that incorporates work extraction processes mediated by partial thermalizations replacing the ideal isothermal processes of the Carnot cycle in Section 9.2. We then optimize the power output of such cycles for fixed time periods over different set of parameters and constraints in Section 9.2.1 and Section 9.2.2. Finally, we compare the two in Section 9.2.3.

9.1 Carnot engine: review

Let us assume that we have access to a hot bath at temperature T_h, a cold bath at temperature T_c, and a two-level system whose energy gap δ can be varied over a fixed range between δ_{min} and δ_{max}. And, let the occupation probability for the excited state be denoted by p. As done earlier, let us set the ground state energy of the system to be zero. We use the formalism of Ref. [Quan *et al.* (2007)] where a Carnot engine was studied in the quantum context but also applies to our case. Thus, a Carnot cycle is composed of four stages that can be defined using points a, b, c, d on the $p - \delta$ plot for a two-level system, Fig. 9.1. First, we have

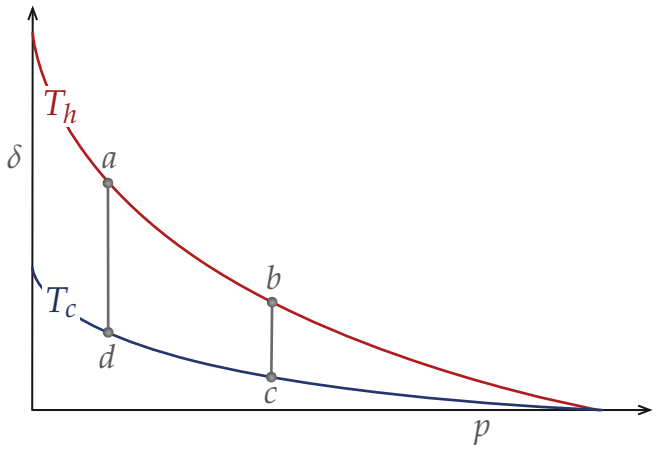


Figure 9.1: Carnot cycle for a two-level system with energy gap δ and excited state occupation probability p.

- $a \mapsto b$, an isothermal expansion: at point a, the system is in a Gibbs-thermal state at temperature T_h with an energy gap δ_a. The occupation probability for the excited state is $p_a = \frac{1}{1+e^{\delta_a/T_h}}$. During an isothermal expansion in a two-level system, the energy levels must change such that they are scaled by the same factor $k_1 < 1$, see Section B.1 for proof.

The state of the system at point b is a Gibbs state at temperature T_h with an energy gap $\delta_b = k_1\delta_a$. As has been shown in Ref. [Åberg (2013)] the work done during such a reversible isothermal process is essentially *deterministic*, and is given by

$$W_{ab} = T_h \ln \frac{Z(\delta_b)}{Z(\delta_a)}, \tag{9.1}$$

where Z is the partition function.

- Then, $b \mapsto c$, an adiabatic process: during an adiabatic process the energy levels of the system change without any accompanying change in occupation probabilities. In particular, at this stage the energy levels are changed by a factor such that the system is in the Gibbs state with respect to the cold bath at temperature T_c implying

$$\frac{\delta_b}{T_h} = \frac{\delta_c}{T_c}. \tag{9.2}$$

Thus, the energy gap of the system at point c is $\delta_c = T_h/T_c\ k_1\delta_a$. The work done in this process W_{bc} is a *random variable* as it depends on the state of the system at point b[1]. The average value of the work done during this process is

$$\overline{W}_{bc} = \frac{1}{1+e^{\delta_c/T_c}}(\delta_b - \delta_c). \tag{9.3}$$

- Next, the compression stage with $c \mapsto d$, an isothermal compression: again, during this process the energy levels are scaled by a factor $k_2 > 1$. So, the system is still in a Gibbs-thermal state with respect to the cold bath at temperature T_c at point d but with an energy gap $\delta_d = T_h/T_c\ k_1k_2\delta_a$. The work cost of this process is deterministic and is given by

$$W_{cd} = -T_c \ln \frac{Z(\delta_d)}{Z(\delta_c)}. \tag{9.4}$$

[1]This means that if the system was in the ground state then it continues to be in the ground state of the new Hamiltonian.

- Finally, we have $d \mapsto a$, an adiabatic process where the energy gap is changed such that we go back to the starting point a with energy gap δ_a and $p_d = p_a$. Therefore,

$$\frac{\delta_d}{T_c} = \frac{\delta_a}{T_h}. \tag{9.5}$$

  But, $\delta_d = T_h/T_c \; k_1 k_2 \delta_a$. This implies that the constant k_2 is not independent but must satisfy the relation $k_2 = \frac{1}{k_1}$. The average work cost of this process is

$$\overline{W}_{da} = \frac{1}{1 + e^{\delta_a / T_h}} (\delta_a - \delta_d). \tag{9.6}$$

The total work done during the Carnot cycle, denoted by the random variable W_C, is just the sum of work done at each stage and is given by

$$W_C = W_{ab} + W_{bc} - W_{cd} - W_{da}. \tag{9.7}$$

The distribution of work and expected efficiency of the Carnot engine can then be obtained as stated in the following lemma whose proof can be found in Section B.3.

Lemma 13. *The total work done during a microscopic implementation of the Carnot cycle is a random variable W_C distributed according to a four-point distribution listed in the table below.*

w_C	$\Pr[W_C = w_C]$
$(T_h - T_c) \ln Z(\delta_b)/Z(\delta_a) + 0$	$(1-p_a)(1-p_b)$
$(T_h - T_c) \ln Z(\delta_b)/Z(\delta_a) - (\delta_a - \delta_d)$	$(1-p_b)p_a$
$(T_h - T_c) \ln Z(\delta_b)/Z(\delta_a) + \delta_b - \delta_c$	$(1-p_a)p_b$
$(T_h - T_c) \ln Z(\delta_b)/Z(\delta_a) + \delta_b - \delta_c - \delta_a + \delta_d$	$p_b p_a$

The expected efficiency of the Carnot cycle is

$$\eta_C^{avg} = \left(1 - \frac{T_c}{T_h}\right). \tag{9.8}$$

Now, for the given pair of temperatures T_c and T_h the Carnot efficiency is the maximum attainable efficiency. It is independent of the points a, b, c, and d on the $p - \delta$ plot, Fig. 9.1, that define a work extraction cycle for the engine connecting the two isotherms. However, there is another quantity that becomes relevant under the constraint of being able to vary the energy gap δ only between δ_{min} and δ_{max}, the average work output. In fact, the cycle that maximizes the average work output is the Carnot cycle that encloses the largest area on the $p - \delta$ plot—it maximizes both efficiency and average work. We state this intuition in the lemma below deferring a formal proof to Section B.4 for completeness.

Lemma 14 (Optimal Carnot cycle for average work)**.** *Given a Carnot engine formed by a classical two-level system operating between a hot bath at temperature T_h and a cold bath at temperature T_c such that the energy gap of the system δ can only be varied over a fixed range between $\delta_{\min}$ and $\delta_{\max}$, the cycle (defined by the points a, b, c, and d on the $p - \delta$ plot) that maximizes the average work output of the Carnot engine is the one for which $\delta_a = \delta_{\max}$ and $\delta_c = \delta_{\min}$.*

The power output of such a cycle is zero due to the isothermal processes that require infinitely long equilibration times. But, finite-time work extraction cycles have non-zero power output and for such cycles one is generally interested in the efficiency at maximum power [Seifert (2012)]. We analyze such engines in the next section.

9.2 Finite-time heat engines

For constant time periods, maximizing power amounts to maximizing the average work output. We define a modification of the Carnot cycle that

incorporates the finite-time element—replacing isothermal processes in a Carnot cycle by work extraction processes with partial thermalizations. So, a finite-time cycle denoted by $a \mapsto b \mapsto c \mapsto d \mapsto a$ on the $p - \delta$ plot constitutes a sequence of four processes. First we have

- $a \mapsto b$, work extraction with partial thermalizations with respect to the hot bath. The coordinates of point a on the $p - \delta$ plot are $(\delta_a,\ p_a)$. The system is driven under Assumption 1 by an amount $\delta_a - \delta_{b1}$ for a time τ_1. The occupation probability for the excited state $p_b(\tau_1)$ can then be obtained using Lemma 12. Furthermore, the average work done during this process would be given by Theorem 5.

- Then, $b \mapsto c$, an adiabatic process. The energy gap is changed from δ_b to δ_c keeping the occupation probabilities fixed, i.e. $p_c = p_b(\tau_1)$. The average work done during this process would be

$$\overline{W}_{bc} = p_b(\tau_1)\big(\delta_c - \delta_b\big). \tag{9.9}$$

- Next, we have $c \mapsto d$, work extraction with partial thermalizations with respect to the cold bath. Starting from the point c with coordinates $(\delta_c,\ p_b(\tau_1))$ the system is again driven under Assumption 1 for a time τ_2 such that the energy gap increases from δ_c to δ_d. To ensure that we complete the cycle and reach point a in the end δ_d must be such that

$$p_d(\tau_2) = p_a. \tag{9.10}$$

  An expression for $p_{d_1}(\tau_2)$ and average work cost of this process can be derived along the lines of Lemma 12 and Theorem 5 as done in Section B.5.

- Finally, we close the loop with $d \mapsto a$ adiabatically. Having reached δ_d in accordance with (9.10), we complete the cycle by changing the energy gap keeping the occupation probabilities fixed. The average work cost

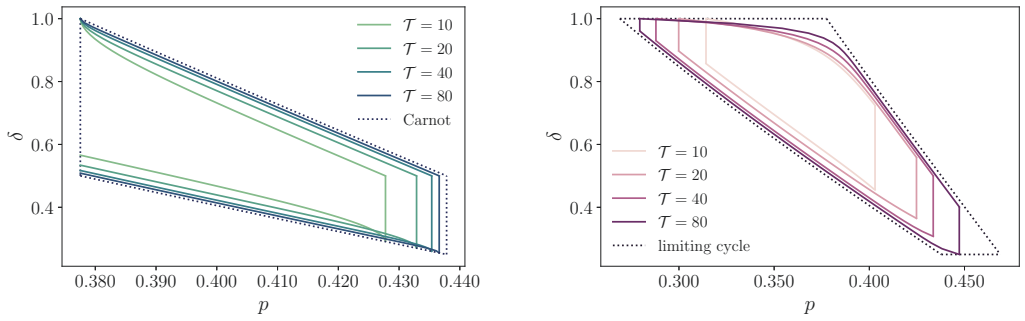


Figure 9.2: (Color online) The optimal finite-time cycles as obtained in Section 9.2. On the x-axis we have occupation probability for the excited state p. On the y-axis we have the energy gap δ. We use parameters $\delta_{max} = 1$, $\delta_{min} = 0.25$, $T_h = 2$, and $T_c = 1$. On the left we have optimal cycles as obtained in Section 9.2.1 with $\delta_a = \delta_{\max}$ and $\delta_b = 2\delta_{\min}$. On the right we have optimal cycles from Section 9.2.2.

of this process is simply

$$\overline{W}_{da} = p_a(\delta_a - \delta_d). \tag{9.11}$$

The time period of the cycle as described above would thus be $\mathcal{T} = \tau_1 + \tau_2$. Since we are interested in the efficiency at maximum power, we want to maximize the average work output of a finite-time cycle with a fixed time period $\mathcal{T} = \tau_1 + \tau_2$, which would simply be the sum of the average work done at each of the four steps described above. The parameters characterising a finite-time cycle as described above are given by the set $\{\delta_a,\ p_a,\ \delta_b,\ \delta_c,\ \tau_1\}$. As $\mathcal{T} = \tau_1 + \tau_2$, only one of them can be chosen freely—let it be τ_1. The fact that for every value of τ_2 one has to solve (9.10) for δ_d leaves no room for analytical analysis. We perform numerical optimizations instead, setting the thermalization rates for both the processes $a \mapsto b$ and $c \mapsto d$ to be unity without loss of generality. The numerical optimizations were performed on *Mathematica* [Wolfram

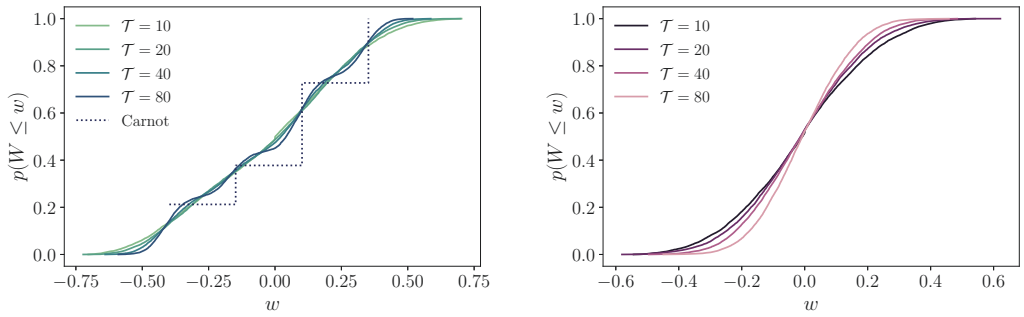


Figure 9.3: (Color online) The cumulative distribution function for the random variable W, the work extracted during different optimal cycles (different values of $\mathcal{T}$) as obtained in Section 9.2. On the x-axis we have the possible work values. The Monte Carlo simulations were performed for 10^4 samples for each of the optimum cycles. On the left is the distribution for optimal cycles as obtained in Section 9.2.1, where $\delta_a = \delta_{\max}$ and $\delta_b = 2\delta_{\min}$. On the right is the distribution for optimal cycles from Section 9.2.2.

Research, Inc.] using the *Nelder-Mead* method [Wolfram Language & System Documentation Center]. First, we perform optimizations for the special case where one can recover the Carnot cycle, Lemma 14, in the limit of large $\mathcal{T}$.

9.2.1 Optimal finite-time cycles limiting to Carnot cycle

In order to recover the Carnot cycle in the limit of large time period of a finite-time cycle, we need to fix the values of the parameters accordingly. For the first process to approach the hot isotherm, it is clear that δ_a and δ_b should be the same as in the case of the optimal Carnot cycle, Lemma 14. However, δ_c must be chosen to lie on the cold isotherm, i.e. it should

satisfy the relation

$$p_b(\tau_1) = \frac{1}{1 + e^{\delta_c / T_c}}, \tag{9.12}$$

since only then would the third leg, i.e. $c \mapsto d$ approach the cold isotherm in the limit of large $\mathcal{T}$. This implies that we are left with only one free parameter, namely τ_1. Thus, maximizing average work output for different values of $\mathcal{T}$ results in different optimal cycles which we plot on the left in Fig. 9.2. We also plot the cumulative distribution for the different optimal cycles along with that of the Carnot cycle to study the fluctuations as we approach equilibrium in Fig. 9.3 (left). Note that the Carnot cycle has a four-point work distribution, see Lemma 13. The distributions for finite-time cycles are obtained by performing Monte Carlo simulations. We find that even though the average work cycles start approaching the Carnot cycle quickly the cumulative distribution still remains smooth until we go to very large values of $\mathcal{T}$.

9.2.2 General optimal finite-time cycles

Previously we were interested in the special case that gave the Carnot cycle in the limit of large time periods. However, for the most general problem, where one has access to a hot bath at temperatures T_h and a cold one at temperature T_c and the energy gap can only be driven between $\delta_{\max}$ and $\delta_{\min}$, one should optimize all the parameters in the set $\{\delta_a,\ p_a,\ \delta_b,\ \delta_c,\ \tau_1\}$. Here, we find that the optimal cycle in the limit of large time period approaches a different cycle; one where the two isotherms are connected by two purely thermal processes. So, $d \mapsto a$ and $b \mapsto c$ would be thermalizations connecting the two isotherms at $d = a = \delta_{\max}$ and $\delta_b = \delta_c = \delta_{\min}$, respectively, the limiting cycle as shown in Fig. 9.2 on the right. This can be understood intuitively since we want to maximize work *output*—the processes where we have to perform work are not favourable. As the work output of an adiabatic process

is less than that of the corresponding isothermal process (and vice-versa for work input), the adiabatic legs are completely lost and get replaced by isothermal extensions. Even though this cycle is not relevant from the point of view of power maximization as for large time periods power is no longer a meaningful metric, it is worth noting the curious form of the cycle in contrast to the corresponding maximum efficiency cycle—the Carnot cycle. We plot the optimal cycles for different values of time periods $\mathcal{T}$ in Fig. 9.2 (right) along with the cumulative distributions in Fig. 9.3 (right).

9.2.3 Comparing finite-time optimal cycles

First, we compare the two scenarios discussed above in terms of their cumulative distributions and find that the general optimal cycles have a better quality of work—less fluctuations. For example, in Fig. 9.4 we plot the distributions for $\mathcal{T} = 10$ and observe that the cumulative distribution for the solution of the general optimum problem crosses the one obtained in Section 9.2.1 around $w = 0$ and lies below it for almost all negative values of w. This means that the probability with which one has to input work in the former case is always less than the latter. Intuitively, there is no real reason to constrain the parameter values as we did in Section 9.2.1 other than the imposed restriction of recovering the Carnot cycle in the limit of large $\mathcal{T}$. This limit is not particularly interesting from the point of view of maximizing power as it vanishes in the said limit. However, such a comparison is at the level of fluctuations only. Next, we compare P^*, the maximum power itself as a function of $\mathcal{T}$ for the two cases in Fig. 9.5 and find that the general optimal power is higher than the corresponding power from optimal cycles that approach the Carnot cycle in the limit of large time periods. This is what one would expect anyway as the latter is a restricted version of the general optimization problem, Section 9.2.2.

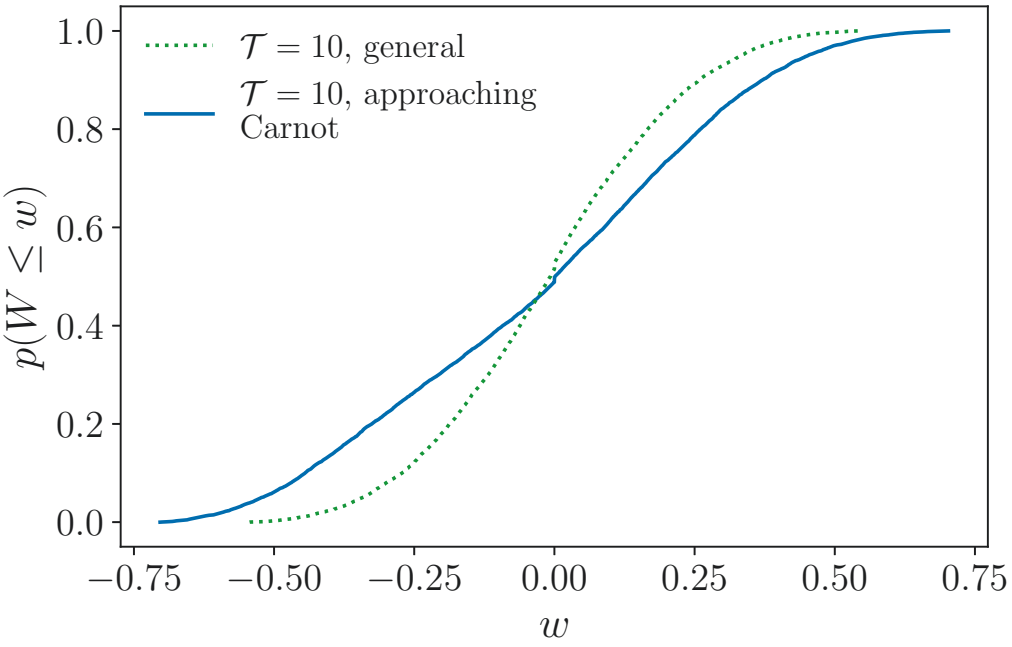


Figure 9.4: (Color online) Comparing cumulative distribution of work for optimal cycles obtained in Section 9.2.1 and Section 9.2.2. On the x-axis we have the possible work values. Negative values of w imply a net work input.

Fig. 9.4 and Fig. 9.5 together imply that the general optimal cycles are better as far as power output and fluctuations are concerned. Finally, we compare the optimal efficiencies η^* for the two scenarios as a function of $\mathcal{T}$ in Fig. 9.6 and find that the optimal cycles that approach the Carnot cycle in the limit of large time period $\mathcal{T}$ have much higher efficiencies compared to the optimal cycles for the general problem. We also compare these with the Curzon-Ahlborn efficiency $\eta_{CA} = 1 - \sqrt{T_c/T_h}$ and note the curious cross-over between $\eta^*(\mathcal{T})$ for the general problem and η_{CA}. Moreover, we observe that the optimal cycles obtained in both the cases have an assymmetric relation between the corresponding values of

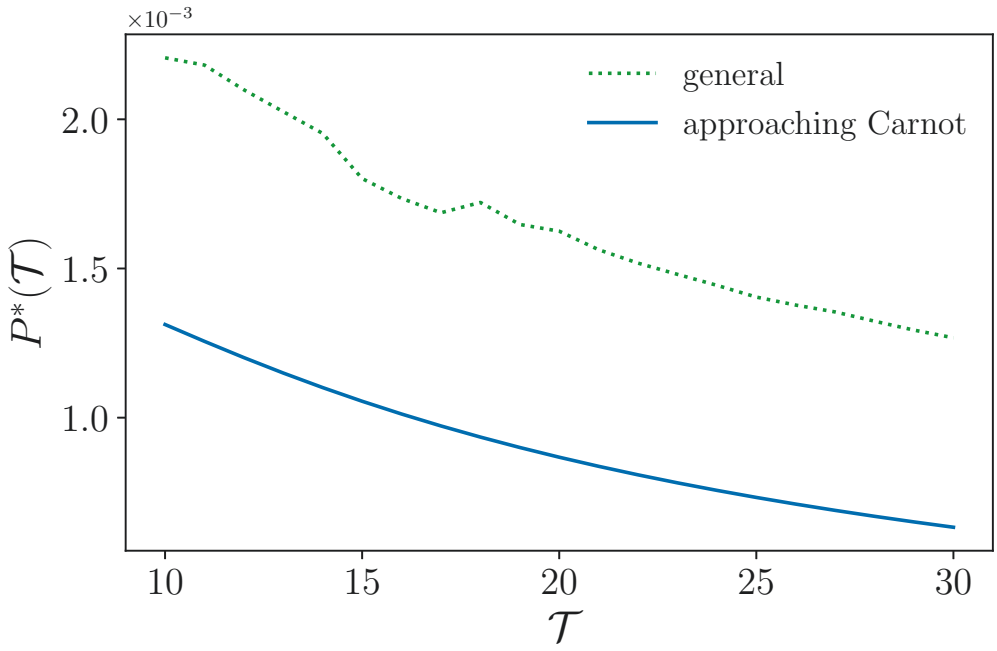


Figure 9.5: (Color online) Comparing maximum power output for optimal cycles obtained in Section 9.2.1 and Section 9.2.2. On the y-axis we have the efficiency at maximum power $P^*(\mathcal{T})$. On the x-axis we have the time period of the finite-time cycles, $\mathcal{T}$. We use parameters $T_h = 2$, $T_c = 1$, $\eta_C = 0.5$.

τ_1 and τ_2. While there is no a-priori reason to expect a symmetric partioning, namely one where $\tau_1 = \tau_2 = \mathcal{T}/2$, similar results were obtained for a heat engine using a quantum dot in Ref. [Harunari *et al.* (2021)] where the efficiencies at maximum power were found to exceed the Curzon-Ahlborn value. The Curzon-Ahlborn efficiency [Curzon and Ahlborn (1975); Novikov (1958)] was derived for a specific model of heat transfer—it is not a universal bound. However, as discussed in Ref. [Seifert (2012)], η_{CA} is close to the efficiency at maximum power for many different models. Further discussion on the topic is beyond the scope of this paper

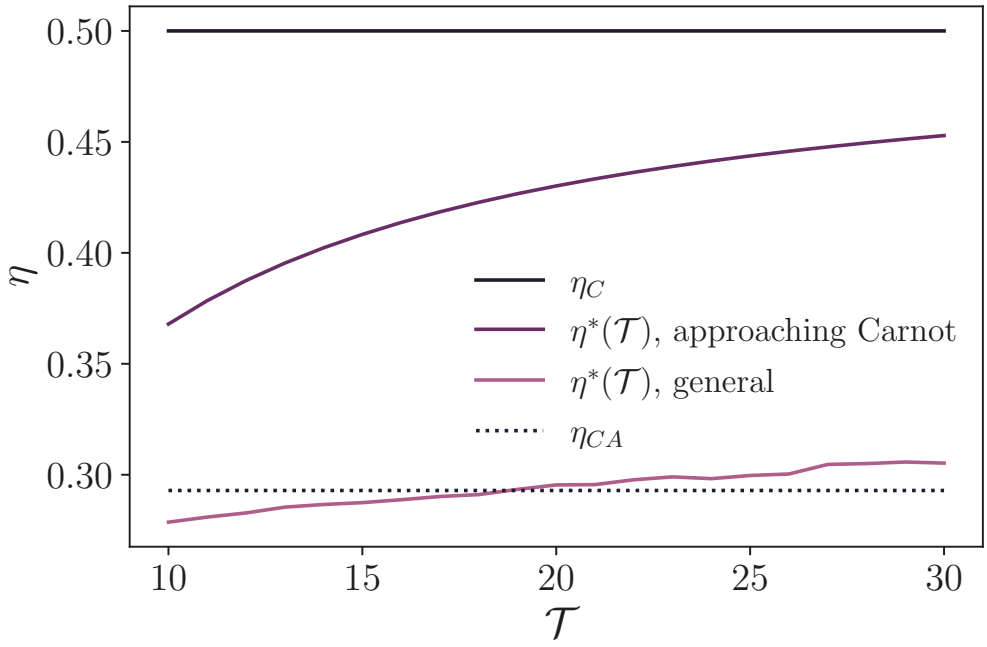


Figure 9.6: (Color online) Comparing efficiency at maximum power for optimal cycles obtained in Section 9.2.1 and Section 9.2.2. On the x-axis we have the time period of the finite-time cycles, $\mathcal{T}$. On the y-axis we have efficiency η. We use parameters $T_h = 2$, $T_c = 1$, $\eta_C = 0.5$, and $\eta_{CA} = 0.293$.

and we refer the interested reader to the aforementioned review. Our view is that the problem of maximizing power is system specific and depends upon the given set-up. To ask for universal bounds on the same requires establishing general features in the model. An attempt along the same direction was made in Ref. [Esposito *et al.* (2010)] where the authors studied a low-dissipation Carnot engine, i.e. one that was operating for a large but finite time period and obtained bounds on the efficiency at maximum power by maximizing power over the thermalization times with the hot and cold reservoirs. (Our problems as studied in

Section 9.2.1 and Section 9.2.2 are different since we only optimize over one of the two thermalization times.) They were then able to obtain the Curzon-Ahlborn efficiency as a special case when the dissipation with respect to the reservoirs was symmetric. Further generalizations to the bounds obtained in Ref. [Esposito *et al.* (2010)] and related work can be found in Refs. [Holubec and Ryabov (2016); Ma *et al.* (2018b)].

10

Conclusion & Outlook

To summarize, we pursued two themes within the single-shot quantum information theoretic framework. In Part I, we extended the work done in Ref. [Koyama *et al.* (2017)] on minimax analysis to Bregman divergences for single-shot measurements. Moreover, by re-formulating Holevo's theorem [(Holevo, 1982, pg. 171)] for the *covariant state estimation problem* in terms of estimators, we found that a *covariant* POVM is, in fact, minimax with Bregman divergence as the distance-measure. In addition to that, we found that it suffices that a measurement be covariant only under a subgroup H of covariant group G such that the unitary representation of H forms a unitary 2-design for it to be minimax. Finally, in order to understand the problem of finding a minimax POVM for arbitrary quantum states, we studied the problem for a qubit observing that a spherical 2-design defines a minimax POVM for a qubit.

In the covariant state estimation problem, we assumed that the underlying group G was compact. It is natural to ask if these results can be extended to infinite-dimensional systems, or equivalently, non-compact groups. A simple system that comes to mind when one thinks of an

infinite-dimensional system is the set of coherent states of a Harmonic oscillator. The underlying group is the translation group $\mathcal{T}$ acting on the complex plane. The projective unitary representation of which is the Weyl-Heisenberg translation operator $\{D(\alpha) \mid \alpha \in \mathbb{C}\}$. Now, the translation group is non-compact. This means that one cannot define a normalisable measure on the group. Our derivation of the main result on covariant state estimation, Theorem 3, to obtain a minimax measurement uses a Bayesian approach. Recall that a minimax measurement is the one that minimizes the worst-case risk of a minimax estimator. Thus, we are interested in the following expression:

$$\inf_{P} \inf_{\hat{\rho}} \sup_{\theta} R_P(\rho_\theta, \hat{\rho}).$$

The very first step of the proof involves re-writing the supremum over θ as a supremum over the probability distributions on Θ, i.e.

$$\inf_{P} \inf_{\hat{\rho}} \sup_{\theta} R_P(\rho_\theta, \hat{\rho}) = \inf_{P} \inf_{\hat{\rho}} \sup_{\pi} \int_{\Theta} \mathrm{d}\pi(\theta) R_P(\rho_\theta, \hat{\rho}).$$

Obviously, we cannot do so in the case of the translation group $\mathcal{T}$ that acts on the complex plane. So, our approach will not apply to the most general problem of estimating coherent states generated by the Weyl-Heisenberg translation operator $\{D(\alpha) \mid \alpha \in \mathbb{C}\}$. Indeed, a more general theorem for the case of locally compact groups [Bogomolov (1982); Hayashi (2017)] shows that covariant measurements minimize the worst-case risk (average risk cannot be defined for non-compact groups). However, the formalism considered in [Bogomolov (1982)] does not include *estimators*. It would be interesting to extend the same to our setting, and to come up with an appropriate definition of a Bayesian estimator for such cases.

Another extension would be to find minimax POVMs for arbitrary quantum states. It would be intriguing to see if some kind of a t-design comes out as a solution. However, it would require a more generalized approach than mere brute-force calculations which become tedious

in higher dimensions. One could also generalize these results to other distance-measures such as Fidelity and Renyi divergences. The authors of Ref. [Ferrie and Blume-Kohout (2016)] have derived the Bayes estimator for distance-measures based on Bhattacharya distance. Partial results [Kueng and Ferrie (2015)] are known for fidelity as the distance-measure, but the Bayes estimator remains unknown for a general state with fidelity as the distance-measure. But, these generalizations are not so straight forward either.

In Part II, changing gears, we looked at single-shot finite-time work extraction processes. We analyzed fluctuations of work in such processes for two-level systems and obtained analytic expressions for (a) average work and (b) lower bound for variance as functions of time. We also studied these processes in the context of work extraction cycles performing numerical optimizations for the power output of such cyclic processes. We found that finite-time processes are inherently prone to fluctuations that result in broad distributions of work, noting that since the Markov process that lies at the heart of the overall physical model is not a simple one, an expression for the variance of work could not be obtained. To illustrate this point, we recall Fig. 6.2. It is clear then that one can write the variance for a discrete L-step process as

$$\sigma_W^2 = \sum_x p(x)W^2(x) - \Big(\sum_x p(x)W(x)\Big)^2, \tag{10.1}$$

where x counts all the paths that correspond to a fixed amount of work $W(x)$ and $p(x)$ is the total probability of occurrence of those paths during the process. For example, there would be various paths corresponding to $W = \epsilon/2$ and one needs to count these paths and sum their contribution which is where the complexity lies. However, there is exactly one path each corresponding to $W = 0$ and $W = \epsilon$, respectively. We were able to use this fact to obtain the lower bound for variance. In fact, a similar

reasoning was used by the authors of Ref. [Marathe and Dhar (2005)] to derive the distribution of work for a similar process in the limit of slow driving which allowed them to ignore all but a few relevant paths. On this note, we would like to mention that there exist approaches [Miller *et al.* (2020); Silaev *et al.* (2014)] for deriving the distribution of work within the Lindblad master equation formalism for arbitrarily driven quantum systems interacting weakly with the bath. However, such analyses lead to generic expressions for average work and variance. Whether they can be solved to obtain closed form analytical expressions given specific driving rates and fixed thermalization times is beyond the scope of this work and constitutes a future study. Finally, we remark that one of the original motivations for this work was to observe the resource resonance phenomenon as seen in Ref.[Korzekwa *et al.* (2019)] (within the resource theory for thermodynamics) in a physical system but we could not make any relevant connections.

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Appendices

Appendix A

Part I

A.1 Quantum Bayes estimator for Bregman divergence

Theorem 7. *If the loss function is Bregman divergence, see Definition 3, then*

$$\mathbb{E}_\theta \mathbb{E}_{X|\theta}[D_f(\rho_\theta, \hat{\rho}(X)) - D_f(\rho_\theta, \hat{\rho}_B(X))] \geq 0,$$

for all states $\theta \in \Theta$ and estimators $\hat{\rho}$, where $\hat{\rho}_B$ is the Bayes estimator, see Equation(2.3)*.*

Proof.

$$\mathbb{E}_\theta \mathbb{E}_{X|\theta}[D_f(\rho_\theta, \hat{\rho}(X)) - D_f(\rho_\theta, \hat{\rho}_B(X))] =$$

$$
\begin{aligned}
& \int_{\Theta} \mathrm{d}\pi(\theta) \int_{\mathcal{X}} \mathrm{d}p(x|\theta)\, \mathrm{tr}\left[f(\rho_\theta) - f(\hat{\rho}(x)) - \right. \\
& \left. f'(\hat{\rho}(x))(\rho_\theta - \hat{\rho}(x)) - f(\rho_\theta) + f(\hat{\rho}_B(x)) + \right. \\
& \left. f'(\hat{\rho}_B(x))(\rho_\theta - \hat{\rho}_B(x)) \right] \\
= & \int_{\Theta} \mathrm{d}\pi(\theta) \int_{\mathcal{X}} \mathrm{d}p(x|\theta)\, \mathrm{tr}\left[f(\hat{\rho}_B(x)) - f(\hat{\rho}(x)) - \right. \\
& \left. f'(\hat{\rho}(x))(\rho_\theta - \hat{\rho}(x)) + f'(\hat{\rho}_B(x))(\rho_\theta - \hat{\rho}_B(x)) \right] \\
= & \int_{\mathcal{X}} \mathrm{d}p_\pi(x)\, \mathrm{tr}\left[f(\hat{\rho}_B(x)) - f(\hat{\rho}(x)) - \right. \\
& \left. f'(\hat{\rho}(x))(\hat{\rho}_B(x) - \hat{\rho}(x)) \right] + \\
& \int_{\mathcal{X}} \mathrm{d}p_\pi(x)\, \mathrm{tr}\left[f'(\hat{\rho}_B(x))(\hat{\rho}_B(x) - \hat{\rho}_B(x)) \right] \\
= & \int_{\mathcal{X}} \mathrm{d}p_\pi(x) D_f(\hat{\rho}_B(x), \hat{\rho}(x)) \geq 0. \qquad \text{(A.1)}
\end{aligned}
$$

The last inequality follows from the non-negativity of Bregman divergence. □

Corollary 4. *For all a-priori probability distributions $\pi_\Theta(\theta)$ over the parameter space Ω_Θ,*

$$r(\pi, \hat{\rho}) \geq r(\pi, \hat{\rho}_B),$$

i.e. the Bayes estimator minimizes the average risk for Bregman divergence.

A.2 Proof of Lemma 1

We first present the Radon-Nikodym theorem for operator-valued measures Maynard (1972), without proof, as stated in (Holevo, 1982, pg. 167).

Proposition 1 (Radon-Nikodym theorem for operator-valued measures)**.** *Let $(\mathcal{X}, \Sigma)$ be a measurable space and let $\{M(B);\ B \in \Sigma\}$ be an additive operator-valued function dominated by a measure $\{m(B);\ B \in \Sigma\}$ in the sense*

that

$$|\langle\phi|M(B)|\psi\rangle| \leq m(B)\|\phi\| \, \|\psi\|, \quad B \in \Sigma,$$

for all $\phi, \psi \in \mathcal{H}$. *Then, there exists an operator-valued function P(.) defined uniquely for m-almost all* $x \in \mathcal{X}$ *(i.e. for all x except for a set of zero m-measure), satisfying* $\|P(x)\| \leq 1$ *such that*

$$\langle\phi|M(B)|\psi\rangle = \int_B \langle\phi|P(x)|\psi\rangle m(dx), \quad B \in \Sigma$$

for all $\phi, \psi \in \mathcal{H}$. *If* $M(B) \geq 0$ *for all* $B \in \Sigma$, *then* $P(x) \geq 0$ *for m-almost all* $x \in \mathcal{X}$.

Lemma 1 (Existence of a POVM density)**.** *Every* $P \in \mathcal{P}$ *admits a density, i.e. for any POVM P there exists a finite measure* $\mu(dx)$ *over* $\mathcal{X}$ *such that* $\mu(\mathcal{X}) = 1$ *and*

$$P(B) = \int_B d\mu(x) M(x), \tag{2.5}$$

with $M(x) \geq 0$, *and* $\mathrm{tr}[M(x)] = d$ μ*-almost everywhere.*

Proof. Define $\mu(B) = \mathrm{tr}[P(B)]$, then

$$\langle\phi|P(B)|\phi\rangle \leq \mu(B), \quad \forall \, |\phi\rangle \in \mathcal{H}.$$

By Cauchy-Schwarz inequality,

$$|\langle\phi|P(B)|\psi\rangle| \leq \mu(B), \quad \forall |\phi\rangle, \, |\psi\rangle \in \mathcal{H}.$$

Thus, P(B) is dominated by $\mu(B)$. By the Radon-Nikodym theorem, it admits a density M(x) defined uniquely μ-almost everywhere:

$$P(B) = \int_B \mu(dx) M(x).$$

As $P(B) \geq 0, M(x) \geq 0$. Taking trace on both sides of the above equation implies $\mathrm{tr}[M(x)] = d$, μ-almost everywhere. □

A.3 Proof of l.s.c. for Bregman divergence

Before proving lower semi-continuity for D_f, we state the following lemma which will be used in the proof.

Lemma 15. *The map $\rho \mapsto \operatorname{tr} f(\rho)$ is continuous on $\Omega = [0,1]$.*

Proof. Consider a sequence of density operators $(\rho_n)_n$ that weakly converge to a density operator ρ, i.e. $\operatorname{tr}\rho_n a \to \operatorname{tr}\rho a$ for all $a \in \mathcal{B}(\mathcal{H})$, where $\mathcal{H}$ is a finite dimensional Hilbert space. By choosing $[a] = |i\rangle\langle j|$, where $|i\rangle\langle j|$ is a basis in $\mathcal{B}(\mathcal{H})$, we obtain element-wise convergence of ρ_n to ρ, which in turn implies the convergence of the corresponding eigenvalues. Now, $\operatorname{tr} f(\rho_n) = \sum_{j=1}^{rk(\rho_n)} f(\lambda_j^n)$ where $\{\lambda_j^n\}_{j=1}^{rk(\rho_n)}$ are the eigenvalues of ρ_n. But, as f is continuous on [0,1], $f(\lambda_j^n) \to f(\lambda_j)$, where $\{\lambda_j\}_{j=1}^{rk(\rho)}$ are the eigenvalues of ρ. Thus, the sum $\operatorname{tr} f(\rho_n) = \sum_{j=1}^{rk(\rho_n)} f(\lambda_j^n)$ also converges to $\operatorname{tr} f(\rho) = \sum_{j=1}^{rk(\rho)} f(\lambda_j)$, and this proves the continuity of $\rho \mapsto \operatorname{tr} f(\rho)$ on [0,1]. □

Theorem 8. *Bregman divergence $D_f(.,.)$ is lower semi-continuous.*

Proof. We generalize the proof of lower semi-continuity of relative entropy as given in Ref. [Wehrl (1978)]. To begin with, we show that there exists a representation of d_f in which the argument of trace does not contain a product of two non-commuting operators. In order to do so, let us define a quantity D_f^λ as

$$D_f^\lambda(\rho,\sigma) = \frac{1}{\lambda}\operatorname{tr}\big(\lambda f(\rho) + (1-\lambda)f(\sigma) - f(\lambda\rho + (1-\lambda)\sigma)\big),$$

where $\lambda \in (0,1)$. It is straightforward to verify that the map $\lambda \mapsto \lambda D_f^\lambda$ is concave on the interval $(0,1)$. Note that $\frac{\mathrm{d}}{\mathrm{d}\lambda}(\lambda D_f^\lambda)\big|_{\lambda=0} = D_f$. Thus, as the map $\lambda \mapsto \lambda D_f^\lambda$ is concave on (0,1), the slope at $\lambda = 0$ will always be

greater than the differences $\frac{\lambda D_f^\lambda - 0.D_f^\lambda}{\lambda}$ for all $\lambda \in (0,1)$. Assuming that $0.D_f^0 = 0$, we have

$$\lambda D_f^\lambda \leq \lambda D_f \Leftrightarrow D_f^\lambda \leq D_f, \quad \forall \lambda \in (0,1).$$

As $\lim_{\lambda \to 0} D_f^\lambda = D_f$, we have

$$\sup_\lambda D_f^\lambda(\rho, \sigma) = D_f(\rho, \sigma).$$

Let $\rho_n \Rightarrow \rho$ and $\sigma_n \Rightarrow \sigma$ be given. Then, by Lemma 15, the map $(\rho, \sigma) \mapsto D_f^\lambda(\rho, \sigma)$ is continuous. Therefore,

$$\begin{aligned} D_f(\rho, \sigma) &= \sup_\lambda D_f^\lambda(\rho, \sigma) \\ &= \sup_\lambda \lim_{n \to \infty} D_f^\lambda(\rho_n, \sigma_n) \\ &\leq \liminf_{n \to \infty} \sup_\lambda D_f^\lambda(\rho_n, \sigma_n) \\ &= \liminf_{n \to \infty} D_f(\rho_n, \sigma_n). \end{aligned}$$

But, $D_f(\rho, \sigma) \leq \liminf_{n \to \infty} D_f(\rho_n, \sigma_n)$ defines a lower semi-continuous function. □

A.4 Why the Bayes estimator is discontinuous.

For the Bayes estimator to be continuous in the prior, it should hold that for any convergent sequence $(\pi_n)_n$,

$$\lim_{n \to \infty} \hat{\rho}_B^{\pi_n}(x) = \hat{\rho}_B^{\lim_{n \to \infty} \pi_n}(x), \quad \forall x \in \mathcal{X}.$$

Below is an example that shows that the above is *not* true in general.

Example 5. *Let us assume that we are doing a σ_z measurement, thus, $\mathcal{X} = \{0, 1\}$. Now, consider a sequence of priors $(\pi_n)_n$ that converges to $\mu(\theta) =$*

$\delta(\theta-\theta_0)$ where θ_0 corresponds to $|0\rangle\langle 0|$ and let each element of the sequence be defined as below:

$$\pi_n(\theta) = \big(1-\frac{1}{n}\big)\delta(\theta-\theta_0) + \frac{1}{n}\delta(\theta-\theta_1),$$

with θ_1 corresponding to $|1\rangle\langle 1|$. Then, the Bayes estimator, see Equation (2.13)*, for each element of the sequence is*

$$\hat{\rho}_B^{\pi_n}(x) \;=\; \big(1-\frac{1}{n}\big)\frac{p(x|\theta_0)\rho_{\theta_0}}{(1-\frac{1}{n})p(x|\theta_0)+\frac{1}{n}p(x|\theta_1)} + \frac{1}{n}\frac{p(x|\theta_1)\rho_{\theta_1}}{(1-\frac{1}{n})p(x|\theta_0)+\frac{1}{n}p(x|\theta_1)},$$

which in the limiting case reduces to

$$\lim_{n\to\infty}\hat{\rho}_B^{\pi_n}(x) = \begin{cases}\rho_{\theta_0} & \text{if x=0,}\\ \rho_{\theta_1} & \text{if x=1.}\end{cases}$$

But, the Bayes estimator for the limit μ of the sequence $(\pi_n)_n$ is

$$\hat{\rho}_B^{\mu}(x) = \begin{cases}\rho_{\theta_0} & \text{if x=0,}\\ \text{not defined} & \text{if x=1.}\end{cases}$$

Since the Bayes estimator for μ is not defined at $x=1$, we can define it to be

$$\hat{\rho}_B^{\mu}(x=1) = \lim_{n\to\infty}\hat{\rho}_B^{\pi_n}(x=1).$$

However, for the Bayes estimator to be continuous in the prior the above should be true for all sequences of priors that have the same limit point. Let us consider another sequence $(\mu_n)_n$ that converges to μ with each element defined as below:

$$\mu_n(\theta) = \big(1-\frac{1}{n}\big)\delta(\theta-\theta_0) + \frac{1}{n}\delta(\theta-\theta_+),$$

where θ_+ corresponds to $|+\rangle\langle +|$. Then, the Bayes estimator for μ_n would be

$$\hat{\rho}_B^{\mu_n}(x) = \big(1-\frac{1}{n}\big)\frac{p(x|\theta_0)\rho_{\theta_0}}{(1-\frac{1}{n})p(x|\theta_0)+\frac{1}{n}p(x|\theta_+)} + \frac{1}{n}\frac{p(x|\theta_+)\rho_{\theta_+}}{(1-\frac{1}{n})p(x|\theta_0)+\frac{1}{n}p(x|\theta_+)},$$

which in the limiting case reduces to

$$\lim_{n\to\infty} \hat{\rho}_B^{\mu_n}(x) = \begin{cases} \rho_{\theta_0} & \text{if } x=0, \\ \rho_{\theta_+} & \text{if } x=1. \end{cases}$$

Now, if we again chose to define the Bayes estimator for μ at $x = 1$ as $\lim_{n\to\infty} \hat{\rho}_B^{\mu_n}(x = 1)$, we would run into a contradiction since $\lim_{n\to\infty} \hat{\rho}_B^{\mu_n}(x = 1) \neq \lim_{n\to\infty} \hat{\rho}_B^{\pi_n}(x = 1)$.

The above example establishes that the Bayes estimator does not admit a continuous extension on the null set (where it is not defined) of the given prior.

A.5 Additional lemma(s)

Lemma 16. *Given a self-adjoint operator A parametrized by u, the derivative of a function of the operator with respect to the parameter at $u = u_0$ is given by*

$$\frac{d}{du} \operatorname{tr}\left[f\Big(A(u)\Big)\right]\Big|_{u=u_0} = \operatorname{tr}\left[A'(u)\Big|_{u=u_0} f'\Big(A(u_0)\Big)\right]$$

Proof. See Ref. [Prato and Tsallis (2000)]. □

Lemma 17. *Consider a continuous function $\mathcal{F}$ defined on a compact set $\mathcal{B}$ and closed subsets $B_x \subseteq \mathcal{B}$ such that $B_1 \subseteq B_2 ... \subseteq \mathcal{B}$. Then, assuming that the sequence $(B_x)_x$ is dense in $\mathcal{B}$, the following holds:*

$$\lim_{x\to\infty} \sup_{B_x} \mathcal{F} = \sup_{\mathcal{B}} \mathcal{F}.$$

Proof. As $B_1 \subseteq B_2 ... \mathcal{B}$, it implies that

$$\lim_{x\to\infty} \sup_{B_x} \mathcal{F} \leq \sup_{\mathcal{B}} \mathcal{F}. \tag{A.2}$$

Note that $\mathcal{B}$ is a compact set and hence

$$\sup_{\mathcal{B}} \mathcal{F} = \max_{\mathcal{B}} \mathcal{F}.$$

Let $b := \arg\max_{\mathcal{B}} \mathcal{F}$. Then, as the sequence of subsets $(B_x)_x$ is dense in $\mathcal{B}$, it implies that there exists a sequence $(b_x)_x$ that converges to b such that $b_x \in B_x$. Moreover, we know that

$$\sup_{B_x} \mathcal{F} \geq F(b_x).$$

Thus,

$$\lim_{x\to\infty} \sup_{B_x} \mathcal{F} \geq \lim_{x\to\infty} F(b_x).$$

As $\mathcal{F}$ is continuous, we get

$$\lim_{x\to\infty} \sup_{B_x} \mathcal{F} \geq \mathcal{F}\big(\lim_{x\to\infty} b_x\big) = \mathcal{F}(b) = \sup_{\mathcal{B}} \mathcal{F}. \tag{A.3}$$

Equations (A.2) and (A.3) imply the result. □

Lemma 18 (Holevo (1982), Theorem 2.1)**.** *Let P_0 be a positive operator in the representation space such that $[P_0, V_g] = 0\ \forall g \in G_0$, where G_0 is the stationary subgroup of G, and satisfying:*

$$\int_G V_g P_0 V_g^\dagger d\mu(g) = \mathbb{I} \tag{A.4}$$

Then setting $P(g\theta_0) = V_g P_0 V_g^\dagger$, we get an operator-valued function of θ such that:

$$M(B) = \int_B P(\theta) d\nu(\theta), \quad B \in \mathcal{A}(\Theta) \tag{A.5}$$

is a covariant measurement with respect to $g \mapsto V_g$. Conversely, for any covariant measurement $M(d\theta)$ there is a unique operator P_0 satisfying (A.4) *such that $M(B)$ can be expressed as in* (A.5)*. P_0 is referred to as the* seed *of the covariant measurement.*

A.6 Aside on t-designs

Definition 7 (Unitary t-design)**.** *Consider the set of unitary matrices U(d) on a d-dimensional Hilbert space $\mathcal{H}$. A unitary t-design is a finite subset $\{U_i\}_{i=1}^N \subset U(d)$, such that for all states $\rho \in \mathcal{S}(\mathcal{H})$ the following holds:*

$$\frac{1}{N}\sum_{i=1}^{N} U_i^{\otimes t}\rho(U_i^\dagger)^{\otimes t} = \int_{U(d)} dU U^{\otimes t}\rho(U^\dagger)^{\otimes t},$$

where 'dU' is the Haar measure on U(d).

Definition 8 (Spherical t-design)**.** *Consider the unit sphere $\mathbb{S}^{d-1}$ in the d-dimensional Euclidean space $\mathbb{R}^d$. A spherical t-design is a finite subset $\mathcal{S} \subset \mathbb{S}^{d-1}$, such that the average value of a polynomial f of degree $\leq t$ on $\mathcal{S}$ equals its average on $\mathbb{S}^{d-1}$:*

$$\frac{1}{|\mathcal{S}|}\sum_{s_n\in\mathcal{S}} f(s_n) = \int_{\mathbb{S}^{d-1}} ds\ f(s),$$

where 'ds' is the Lebesgue measure on $\mathbb{S}^{d-1}$.

Appendix B

Part II

B.1 Quantum Isothermal processes

In the following lemma, we denote the change in the energy of a system during a thermodynamic process $a \mapsto b$ by ΔU_{ab}, the heat exchanged by Q_{ab} and the work done by W_{ab}.

Lemma 19. *A quantum isothermal expansion is such that the gaps between the energy levels of the Hamiltonian H are scaled by a factor $k < 1$.*

Proof. A-priori, there is nothing constraining the value of k other than the trivial requirement of $k > 0$. However, it is clear that if we choose $k > 1$ then we are stretching the energy levels apart while if $k < 1$ then we are compressing them together. For an isothermal process ($a \mapsto b$) to be an expansion, the following should be true

$$Q_{ab} > 0 \iff \Delta U_{ab} > W_{ab}.$$

We know that $W_{ab} = \Delta F_{ab} = T_h \ln\left(Z_a / Z_b\right)$ [Åberg (2013)], where $Z_a = \sum_i e^{-\epsilon_i / T_h}$ and $Z_b = \sum_i e^{-k\epsilon_i / T_h}$. Therefore, the following inequality must

be satisfied by any quantum isothermal expansion:

$$\sum_j \epsilon_j \left(k\frac{e^{-k\epsilon_j/T_h}}{Z_b} - \frac{e^{-\epsilon_j/T_h}}{Z_a} \right) > T_h\Big(\ln Z_a - \ln Z_b \Big). \tag{B.1}$$

Let us assume that $k > 1$, then

$$e^{-k\epsilon_i/T_h} < e^{-\epsilon_i/T_h} \tag{B.2}$$

$$\implies Z_b < Z_a. \tag{B.3}$$

Thus, (B.1) implies

$$\sum_j \epsilon_j \left(k\frac{e^{-k\epsilon_j/T_h}}{Z_b} - \frac{e^{-\epsilon_j/T_h}}{Z_a} \right) > 0,$$

which implies

$$k\frac{e^{-k\epsilon_j/T_h}}{Z_b} > \frac{e^{-\epsilon_j/T_h}}{Z_a}. \tag{B.4}$$

Now, (B.3) implies

$$\frac{e^{-k\epsilon_i/T_h}}{Z_b} > \frac{e^{-k\epsilon_i/T_h}}{Z_a}, \tag{B.5}$$

but, by (B.2), one has

$$\frac{e^{-\epsilon_i/T_h}}{Z_b} > \frac{e^{-k\epsilon_i/T_h}}{Z_b}. \tag{B.6}$$

Combining (B.5) with (B.6), we have

$$\frac{e^{-\epsilon_i/T_h}}{Z_b} > \frac{e^{-k\epsilon_i/T_h}}{Z_a}. \tag{B.7}$$

Differentiating both sides with respect to ϵ_i, we obtain

$$\frac{e^{-\epsilon_i/T_h}}{Z_b} < \frac{ke^{-k\epsilon_i/T_h}}{Z_a}.$$

But, this contradicts (B.4). So, the assumption is wrong which implies that $k < 1$ for a quantum isothermal expansion. □

B.2 Aside on special functions

Definition B.2.1 (Hypergeometric function in integral form)**.**

$$\int dx \frac{e^{px}}{1+e^{(q-rx)}} = \frac{e^{(p+r)x+q}}{p+r} \times {}_2F_1\left(1, \frac{p}{r}+1, \frac{p}{r}+2; -e^{-(q-rx)}\right), \tag{B.8}$$

where p, q, and r are rationals and the hypergeometric function is

$${}_2F_1 : (a,b,c,z) \mapsto \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{z^n}{n!}, \quad |z| \leq 1, \tag{B.9}$$

and $(x)_n$ denotes the rising factorial

$$(x)_n = \begin{cases} 1, & n = 0, \\ x(x+1)\cdots(x+n-1), & n > 0. \end{cases} \tag{B.10}$$

Definition B.2.2 (Lerch transcendent)**.**

$$\Phi_L : (z,s,a) \mapsto \sum_{n=0}^{\infty} \frac{z^n}{(n+a)^s}. \tag{B.11}$$

where $z \in \mathbb{C}$ and $Re(a) > 0$. We can then write the function $\mathcal{G}$ (Definition 6) in terms of the Lerch transcendent as

$$\mathcal{G}(t) = \frac{\kappa\tau T_h}{\epsilon} e^{-\delta(t)/T_h} \, \Phi_L(-e^{-\delta(t)/T_h}, 1, \frac{\kappa\tau T_h}{\epsilon} + 1). \tag{B.12}$$

B.3 Proof of Lemma 13

Proof. W_{ab} and W_{cd} are essentially deterministic and are given by (9.1) and (9.4) while W_{bc} and W_{da} are random variables. In Table B.1, we list all

the possible states that the system could be in at each of the four nodes a, b, c, d and thus obtain all the possible values for $W_{bc} - W_{da}$.

$a \mapsto$	$b \mapsto$	$c \mapsto$	$d \mapsto$	a	$W_{bc} - W_{da}$	$\Pr[W_{bc} - W_{da}]$
0	0	0	0	0	0	$(1-p_a)^2(1-p_b)$
0	0	0	1	1	$-(\delta_a - \delta_d)$	$(1-p_a)(1-p_b)p_a$
0	1	1	0	0	$\delta_b - \delta_c$	$(1-p_a)^2 p_b$
0	1	1	1	1	$\delta_b - \delta_c - \delta_a + \delta_d$	$(1-p_a)p_b p_a$
1	0	0	0	0	0	$p_a(1-p_a)(1-p_b)$
1	0	0	1	1	$-(\delta_a - \delta_d)$	$p_a^2(1-p_b)$
1	1	1	0	0	$\delta_b - \delta_c$	$p_a p_b(1-p_a)$
1	1	1	1	1	$\delta_b - \delta_c - \delta_a + \delta_d$	$p_a^2 p_b$

Table B.1: Occupation of the ground state is designated by 0 and that of the excited state by 1. The Carnot cycle is $a \mapsto b \mapsto c \mapsto d \mapsto a$. Starting at a with the system in the ground state as one completes the cycle the system could be in the excited state—it undergoes thermalization from $c \mapsto d$. Same colour entries under the $W_{bc} + W_{da}$ column are identical and the probabilities corresponding to those entries add up.

Thus, we can obtain an expression for the average work done by simply multiplying and adding the corresponding entries of columns W_C and $\Pr[W_C]$ to arrive at

$$\begin{aligned}
\mu_{W_C} &= (T_h - T_c)\ln\frac{Z(\delta_b)}{Z(\delta_a)} - \left(1 - \frac{T_c}{T_h}\right)\delta_a p_a + \\
&\quad \left(1 - \frac{T_c}{T_h}\right)\delta_b p_b \\
&= (T_h - T_c)\ln\frac{Z(\delta_b)}{Z(\delta_a)} - \left(1 - \frac{T_c}{T_h}\right)(\delta_a p_a - \delta_b p_b) \\
&= \left(1 - \frac{T_c}{T_h}\right)\left(T_h \ln\frac{Z(\delta_b)}{Z(\delta_a)} + \delta_b p_b - \delta_a p_a\right). \qquad \text{(B.13)}
\end{aligned}$$

We can then derive the average Carnot efficiency η_C^{avg} by dividing the average work done by the heat input (which is when the system undergoes isothermal expansion from point a to b), Q_{ab}. The heat exchanged during a process, denoted by Q, is given by the first law of Thermodynamics, i.e. $Q = \Delta U - W$, where ΔU is the change in the total energy of the system during the process while W is the corresponding work yield/cost. In our case, the process is an isothermal expansion $a \mapsto b$, so $\Delta U_{ab} = \left(\delta_b p_b - \delta_a p_a\right)$ and $W = -W_{ab}$ where W_{ab} is the deterministic work yield of the process and is given by (9.1). Thus, we have

$$Q_{ab} = \left(\delta_b p_b - \delta_a p_a\right) + T_h \ln \frac{Z(\delta_b)}{Z(\delta_a)}. \tag{B.14}$$

Since efficiency is defined as the ratio of the work output and the heat input, (B.13) and (B.14) imply (9.8). □

B.4 Proof of Lemma 14

Proof. Note that the points a, b, c, and d as in Fig. 9.1, defining a cycle of a Carnot engine, are not independent—see (9.2) and (9.5). Thus, there are only two free variables that define any particular cycle. Let us set δ_a and δ_c as the independent ones. Then, changing variables in (B.13) and plugging the expressions for the partition function Z, p_a and p_b, we obtain

$$\mu_{W_C}(\delta_a,\ \delta_c) \ = \ \Big(T_h - T_c\Big)\left(\ln\left(\frac{1+e^{-\delta_a/T_h}}{1+e^{-\delta_c/T_c}}\right) + \frac{\delta_a/T_h}{1+e^{\delta_a/T_h}} - \frac{\delta_c/T_c}{1+e^{\delta_c/T_c}}\right) \tag{B.15}$$

Introducing $x := \delta_a/T_h$ and $y := \delta_c/T_c$ reduces the equation above to

$$\mu_{W_C}(x,\ y) = \Big(T_h - T_c\Big)\left(\ln\left(\frac{1+e^{-x}}{1+e^{-y}}\right) + \frac{x}{1+e^{x}} - \frac{y}{1+e^{y}}\right). \tag{B.16}$$

Let us now look at the function

$$f : x \mapsto (1 + e^{-x})\, e^{\frac{x}{1+e^x}}. \tag{B.17}$$

Evaluating the derivative of this function we obtain

$$f'(x) = -\left(\frac{x}{1+e^x}\right) e^{\frac{x}{1+e^x}} < 0, \quad \forall\ x > 0. \tag{B.18}$$

This means that f is a monotonically decreasing function on $\mathbb{R}^+$. Hence, the minimum/maximum would be attained on the boundaries of the interval $\mathcal{I} \subset \mathbb{R}^+$. Note that (B.16) can be written in terms of f simply as

$$\mu_{W_C}(x,\ y) = \Big(T_h - T_c\Big)\Big(\ln\ f(x) - \ln\ f(y)\Big). \tag{B.19}$$

As ln is a monotonically increasing function, $\ln \circ f$ would thus be monotonically decreasing since f is monotonically decreasing. Now, as $\mu_{W_C} < 0$ where the negative sign implies work output, maximizing the average work output amounts to minimizing μ_{W_C} with respect to x and y. So, we have

$$\begin{aligned} \min_{x,\ y\in\mathcal{I}} \mu_{W_C}(x,\ y) &= \min_{x,\ y\in\mathcal{I}} \Big(T_h - T_c\Big)\Big(\ln\ f(x) - \ln\ f(y)\Big) \\ &= \Big(T_h - T_c\Big)\Big(\min_{x\in\mathcal{I}} \ln\ f(x) - \max_{y\in\mathcal{I}} \ln\ f(y)\Big). \end{aligned} \tag{B.20}$$

As $\ln \circ f$ is monotonically decreasing it implies that

$$\min_{x,\ y\in\mathcal{I}} \mu_{W_C}(x,\ y) = \Big(T_h - T_c\Big)\left(\ln\ f\Big(\max_{x\in\mathcal{I}} x\Big) - \ln\ f\Big(\min_{y\in\mathcal{I}} y\Big)\right) \tag{B.21}$$

Substituting for x and y in terms in of δ_a and δ_c and noting that

$$\max_{\delta_a} \delta_a = \delta_{\max}, \quad \text{and} \quad \min_{\delta_c} \delta_c = \delta_{\min}, \tag{B.22}$$

gives us

$$\arg\max_{\delta_a,\ \delta_c} \mu_{W_C}(\delta_a, \delta_c) = (\delta_{\max},\ \delta_{\min}). \tag{B.23}$$

□

B.5 Partial thermalization under Assumption 1 while increasing the energy gap

Definition B.5.1. *Given the energy gap $\delta(t)$ of a two-level system at time $t < \tau$, we define the function*

$$\mathcal{H} : t \mapsto \sum_{n=0}^{\infty} \frac{\left(e^{-\frac{\delta(t)}{T_c}}\right)^n}{\left(\frac{n\epsilon}{\kappa\tau T_c} + 1\right)}, \tag{B.24}$$

where $\epsilon = \delta_{\max} - \delta_{\min}$, κ is the thermalization rate, and T_c is the temperature of the ambient bath.

The function $\mathcal{H}$ is a monotone function in t. For δ monotonically increasing in t, $\mathcal{H}$ monotonically decreases. This follows by noting that $e^{-\delta}$ is also monotonically decreasing in t.

Lemma 20 (Time evolution of occupation probabilities under partial thermalization while increasing the energy gap)**.** *Given a two-level system that undergoes partial thermalization as per Assumption 1 in the presence of a bath at temperature T_c for a time τ such that its energy gap changes from δ_{min} to δ_{max}, the probability of the system to be in the excited state at any time $0 < t < \tau$ is*

$$p(t) \;=\; p_0 e^{-\kappa t} + \mathcal{H}(t) - e^{-\kappa t}\mathcal{H}(0), \tag{B.25}$$

where $\epsilon = \delta_{max} - \delta_{min}$, $p_0 = p(0)$ and $\delta(t) = \delta_{min} + \epsilon t/\tau$.

Proof. Re-writing the differential equation for general partial thermalization processes where the hot bath is replaced by the cold bath in (6.2), we have

$$\frac{\mathrm{d}p}{\mathrm{d}t} + \kappa p(t) = \kappa\gamma_c\big(\delta(t)\big), \tag{B.26}$$

which can be integrated along with the initial condition $p(0) = p_0$ to obtain

$$p(t) = p_0 e^{-\kappa t} + \kappa e^{-\kappa t} \int_0^t e^{\kappa t'} \gamma_c\big(\delta(t')\big)\, \mathrm{d}t'. \tag{B.27}$$

Given Assumption 1 and the boundary conditions $\delta(0) = \delta_{\min}$ and $\delta(\tau) = \delta_{\max}$, we have

$$\delta(t) = \delta_{\min} + \frac{\epsilon}{\tau} t, \tag{B.28}$$

where $\epsilon = \delta_{\max} - \delta_{\min}$. Plugging $\gamma_c\big(\delta(t)\big) = \frac{1}{1+e^{\delta(t)/T_c}}$ and (B.28) in (B.27), we obtain

$$p(t) = p_0 e^{-\kappa t} + \kappa e^{-\kappa t} \int_0^t \frac{e^{\kappa t'}}{1 + e^{\frac{(\delta_{\min} + \epsilon t'/\tau)}{T_c}}} \, \mathrm{d}t'. \tag{B.29}$$

Evaluating the integral above, we obtain

$$\begin{aligned}
p(t) &= p_0 e^{-\kappa t} + \kappa e^{-\kappa t} \left\{ \frac{e^{\kappa t'}}{\kappa} \, {}_2F_1\Big(1, \frac{\kappa\tau T_c}{\epsilon}, \frac{\kappa\tau T_c}{\epsilon} + 1; -e^{\frac{(\delta_{\min} + \epsilon t'/\tau)}{T_c}}\Big) \Big|_0^t \right\} \\
&= p_0 e^{-\kappa t} + \kappa e^{-\kappa t} \left\{ \frac{e^{\kappa t}}{\kappa} \, {}_2F_1\Big(1, \frac{\kappa\tau T_c}{\epsilon}, \frac{\kappa\tau T_c}{\epsilon} + 1; -e^{\frac{\delta(t)}{T_c}}\Big) - \right. \\
&\quad \left. \frac{1}{\kappa} \, {}_2F_1\Big(1, \frac{\kappa\tau T_c}{\epsilon}, \frac{\kappa\tau T_c}{\epsilon} + 1; -e^{\frac{\delta_{\min}}{T_c}}\Big) \right\} \\
&= p_0 e^{-\kappa t} + \, {}_2F_1\Big(1, \frac{\kappa\tau T_c}{\epsilon}, \frac{\kappa\tau T_c}{\epsilon} + 1; -e^{\frac{\delta(t)}{T_c}}\Big) - \\
&\quad e^{-\kappa t} \, {}_2F_1\Big(1, \frac{\kappa\tau T_c}{\epsilon}, \frac{\kappa\tau T_c}{\epsilon} + 1; -e^{\frac{\delta_{\min}}{T_c}}\Big).
\end{aligned} \tag{B.30}$$

Next, using Definition 6 we can write

$$\begin{aligned} {}_2F_1(1,a,1+a;-z) &= \sum_{n=0}^{\infty} \frac{n!(a)_n}{(1+a)_n} \frac{(-z)^n}{n!} \\ &= \sum_{n=0}^{\infty} \frac{(a)(1+a)\cdots(n-1+a)}{(1+a)(2+a)\cdots(n+a)} (-z)^n \\ &= \sum_{n=0}^{\infty} \frac{a\ (-z)^n}{(n+a)} \\ &= \sum_{n=0}^{\infty} \frac{(-z)^n}{(\frac{n}{a}+1)}. \end{aligned} \tag{B.31}$$

Using (B.31) we can write (B.30) in terms of $\mathcal{H}$ to obtain (B.25). □

Lemma 21 (Average work when increasing the energy gap)**.** *The average work done by a two-level system during a process as per Assumption 1 along with partial thermalizations in the presence of a bath at temperature T_h for a time τ such that its energy gap changes from $\delta_{\min}$ to $\delta_{\max}$ is*

$$\mu_W(\tau) = -W_{iso}^{T_c} - \frac{W_{ad}}{\kappa\tau}\left(1-e^{-\kappa\tau}\right) + \frac{\epsilon}{\kappa\tau}\left\{\mathcal{H}(\tau) - e^{-\kappa\tau}\mathcal{H}(0)\right\}, \tag{B.32}$$

where $\epsilon = \delta_{max} - \delta_{min}$, $p_0 = p(0)$, and $W_{iso}^{T_c}$ is the work output of the corresponding isothermal process, i.e. $W_{iso}^{T_c} = -T_c \log \frac{Z(\delta_{\min})}{Z(\delta_{\max})}$, where Z is the partition function $Z : \delta \mapsto 1 + e^{-\delta/T_c}$.

Proof. We start by noting that

$$\begin{aligned} \frac{\mathrm{d}p}{\mathrm{d}\delta} &= \frac{\mathrm{d}p}{\mathrm{d}t}.\frac{\mathrm{d}t}{\mathrm{d}\delta} \\ &= -\frac{\kappa\tau}{\epsilon}\Big(\gamma_h(\delta) - p\Big), \end{aligned} \tag{B.33}$$

where the last line follows from (6.2) and Assumption 1 while supressing the dependence on t. Integrating (7.11) with respect to δ from $\delta_{\min}$ to $\delta_{\max}$, we have

$$\int_{\delta_{\min}}^{\delta_{\max}} p \, \mathrm{d}\delta = \int_{\delta_{\min}}^{\delta_{\max}} \gamma_c(\delta)\mathrm{d}\delta + \frac{\epsilon}{\kappa\tau}\int_{\delta_{\min}}^{\delta_{\max}} \frac{\mathrm{d}p}{\mathrm{d}\delta}\mathrm{d}\delta. \tag{B.34}$$

Thus, (7.1) and (B.34) together imply

$$\mu_W(\tau) = \int_{\delta_{\min}}^{\delta_{\max}} \gamma_c(\delta)\mathrm{d}\delta + \frac{\epsilon}{\kappa\tau}\int_{\delta_{\min}}^{\delta_{\max}} \frac{\mathrm{d}p}{\mathrm{d}\delta}\mathrm{d}\delta. \tag{B.35}$$

The first term on the right-hand side is the negative of the work done during the corresponding isothermal process (when energy gap changes from $\delta_{\max}$ to $\delta_{\min}$). Substituting the expression for $\gamma_c(\delta)$ and evaluating the integral gives us the first term of (B.35) as

$$\int_{\delta_{\min}}^{\delta_{\max}} \gamma_c(\delta)\mathrm{d}\delta = T_c \log\frac{Z(\delta_{\min})}{Z(\delta_{\max})} = -W_{iso}^{T_c}, \tag{B.36}$$

where Z is the partition function $Z : \delta \mapsto 1 + e^{-\delta/T_c}$. Next, we evaluate the integral in the second term in (B.35) using Lemma 20. First we note that

$$\int_{\delta_{\min}}^{\delta_{\max}} \frac{\mathrm{d}p}{\mathrm{d}\delta}\,\mathrm{d}\delta \;\; = \;\; p(\delta_{\max}) - p(\delta_{\min}).$$

As $p(\delta_{\min}) = p(0) = p_0$ is given and $p(\delta_{\max}) = p(\tau)$, we use (B.25) to obtain

$$p(\delta_{\max}) - p(\delta_{\min}) \;\; = \;\; -p_0(1 - e^{-\kappa\tau}) + \mathcal{H}(\tau) - e^{-\kappa\tau}\mathcal{H}(0). \tag{B.37}$$

Plugging (B.36) and (B.37) in (B.35) along with (7.17) we obtain (B.32). □