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A Cybernetic Theory of Heat and Work

av

William Rupush

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MATEMATISKA INSTITUTIONEN, STOCKHOLMS UNIVERSITET, 106 91 STOCKHOLM

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William Rupush

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Abstract

In this thesis I will argue that the basic concepts of thermodynamics can be formalized using notions from control theory. Particular attention is paid to the distinction between heat and work, and it is argued that an implicit observability decomposition lies at the heart of the difference between the two different forms of energy flow. An explicit theory of heat and work for quantum systems is formulated based on this premise, and its implications are explored.

Notation and definitions

Throughout the thesis we'll employ the following notations and conventions.

- The symbol $\triangleq$ denotes *equality by definition*.
- W denotes *work*.
- Q denotes *heat*.
- The inner product $\langle \cdot, \cdot \rangle$ is always taken to be the *Hilbert-Schmidt inner product* defined $\langle A, B \rangle = \mathrm{Tr}\{A^\dagger B\}$ for matrices A and B, where $A^\dagger$ denotes the Hermitian adjoint of A. $||\cdot||$ is the induced Hilbert-Schmidt norm.
- Natural units are used throughout the thesis. In particular, $\hbar = k = 1$. $\hbar \approx 1.055 \times 10^{-34}$Js is *Dirac's constant*, and $k \approx 1.381 \times 10^{-23}\mathrm{m}^2\mathrm{kg\ s}^{-2}\mathrm{K}^{-1}$ is *Boltzmann's constant*.
- $[\cdot, \cdot]$ denotes the *commutator*, defined $[A, B] = AB - BA$.
- $[\cdot, \cdot]_+$ denotes the *anticommutator*, defined $[A, B]_+ = AB + BA$.
- $\otimes$ denotes the *tensor product* for operators, and *Kronecker product* for matrix representations.
- $\oplus$ denotes the *direct sum*.
- i denotes the *imaginary number* $\sqrt{-1}$.
- $U(n)$ is the *unitary group* defined

  $$U(n) \triangleq \{U \in GL(n) \mid U^\dagger = U^{-1}\},$$

  where $GL(n)$ is the general linear group.
- $u(n)$ is the Lie algebra of $U(n)$ defined

  $$u(n) \triangleq \{X \in GL(n) \mid X^\dagger = -X\},$$

- $su(n)$ is the subset of $u(n)$ defined

  $$su(n) \triangleq \{X \in u(n) \mid \mathrm{Tr}\{X\} = 0\},$$

- $sp(\frac{n}{2})$ is the *symplectic Lie algebra* defined

  $$sp(\frac{n}{2}) \triangleq \{X \in GL(n) \mid X^T J + JX = 0\},$$

  where the T superscript denotes transposition, and

  $$J \triangleq \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

- ad_A is a linear map $\mathrm{ad}_A : \mathcal{L} \to \mathcal{L}$ on a Lie algebra $\mathcal{L}$, that for a given element $A \in \mathcal{L}$ is defined $\mathrm{ad}_A B \triangleq [A, B]$.

- The *expectation value* of an observable $\hat{S}$ for a state $\hat{\rho}$ is defined $\langle \hat{S} \rangle \triangleq \mathrm{Tr}\{\hat{S}\hat{\rho}\}$. If the state is pure, i.e. $\hat{\rho} = |\psi\rangle \langle\psi|$, then we also have $\langle \hat{S} \rangle = \langle\psi| \hat{S} |\psi\rangle$. Sometimes a subscript may be added to specify the state for which the expectation value is computed, as in $\langle \hat{S} \rangle_{\hat{\rho}}$. This may arise if we are interested in calculating, say, the energy residing in the unobservable state component specifically (see section 2.2), in which case the subscript is $\hat{\rho}_u$.

- The expectation value of an observable $\hat{S}$ is termed a *microcanonical distribution* if $\langle \hat{S} \rangle \propto \mathrm{Tr}\{\hat{S}\}$.

- A bounded linear operator $T : \mathcal{H} \to \mathcal{H}$ on a Hilbert space $\mathcal{H}$ is said to be *trace-class* if $\mathrm{Tr}\{\sqrt{T^\dagger T}\} < \infty$.

- The *rank* of an operator $T : \mathcal{H} \to \mathcal{H}$ is the dimension of its image. All Hilbert spaces considered in this thesis can be taken to be finite-dimensional.

- Two Lie-subalgebras $\mathcal{L}_1$ and $\mathcal{L}_2$ of $\mathcal{L}$, are said to be *conjugate* in $\mathcal{L}$, if there exists an element $g \in \mathcal{L}$ such that $\mathcal{L}_2 = g\mathcal{L}_1 g^{-1}$.

Chapter 0

Contents

Chapter 1

Introduction

> ...any logically irreversible manipulation of information, such as the erasure of a bit or the merging of two computation paths, must be accompanied by a corresponding entropy increase in non-information-bearing degrees of freedom of the information-processing apparatus or its environment
>
> Rolf Landauer. 1961

That there is an intimate connection between control theory and thermodynamics has been known since the late nineteenth century when J. C. Maxwell considered a thought experiment wherein a sophisticated entity, later termed *Maxwell's demon*, capable of measuring the positions and velocities of molecules in a gas, and capable of precise control actuation on a microscopic scale, could potentially reduce the entropy of a system and thereby extract a larger amount of work from it than is allowed by the second law of thermodynamics, as classically concieved [1]. A substantial litterature exists where researchers, convinced of the validity of the second law, have attempted to argue that excess entropy must be produced during the operations of the demon in order for the total entropy (of the gas and demon combined) to be non-decreasing. The most widely accepted solution to the paradox is due to R. Landauer [2], which is that excess entropy is produced neither during the observation nor the actuation process, but by the end of the control cycle when the memory storage of the demon is reset to its initial state. He argued that for each bit of information erased, an amount of heat $Q \geq T \log 2$ must be produced, where T is the temperature of the storage device. While his arguments have been challenged, his conclusion is widely percieved to be an important physical law connecting information to entropy. Today the analysis of the thermodynamics of feedback control is still an active area of both theoretical and experimental research, with papers published analyzing both quantum [3] [4] [5] [6] and classical contexts [7] [8] [9] [10] [11]. In this thesis I will focus on the quantum context, although the basic argument can easily be transferred to the classical one. For a thorough review of the intersection between thermodynamics, information theory, and quantum mechanics, I refer the reader to [14].

The subject matter of this thesis is the first law of thermodynamics. The key insight of the first law is that heat is a form of energy transfer, distinct from mechanical work, and that once heat is taken into account the total energy of a system and its environment is seen to be conserved in any experimental set-up. The first law can be stated in the form $\Delta E = Q + W$, meaning that the change in the energy of a system is equal to the sum of the heat flow into (or out of) the system and the mechanical work performed on the system (or by the system on its surroundings). Despite its apparent simplicity, the exact interpretation of the aforementioned equation remains elusive, particularly in application to quantum phenomena. The problem can be stated succinctly: given a change in the energy of an arbitrary dynamical system, what are the necessary and sufficient conditions for said energy to enter the theoretical model as heat and work respectively? No rigorous treatment of this problem exists at the present moment, and practitioners are largely forced to rely on heuristics. The following paragraph from a standard textbook on the subject by C.J. Adkins is representative of how the problem is handled [13]:

"We have thus defined heat as a form of energy entirely equivalent in its effect on the total energy of a system to energy communicated by the performance of some kind of work. The distinction between heat and work is not always clear-cut in the sense that it is not always easy to decide whether a particular energy contribution should be classed as heat or work... Probably, the most convenient distinction is made in terms of whether the energy enters the system by a macroscopically ordered action or by one where order exists on the microscopic scale only. In the former case, the energy would be communicated by work and in the latter by heat. Thus, when a piston moves in a cylinder, the movement is macroscopic in the sense that the velocity of the piston is superimposed on all its molecules, and the piston does work on the gas. On the other hand, if the piston is hot, the (thermal) motions of its molecules are not correlated, energy is communicated to the gas by processes which are ordered on the microscopic scale only and we say that heat flows. That it should be impossible always to make a sharp distinction between heat and work is not surprising, for it is precisely the function of the first law to state that they are, in certain ways, equivalent."

The entire structure of classical thermodynamics is built upon the distinction between heat and work, and consists of an analysis of their relation, and in particular, the possible extent of their interconversion. Even the concept of thermodynamic entropy rests upon it. In classical considerations, the ambiguity regarding their precise definitions have not constituted a significant problem for practitioners, as it is often intuitively clear whether a certain energy contribution enters the theoretical model as heat or work. But the success of classical thermodynamics makes physicists eager to apply it to the quantum realm as well, especially in recent times as technology has matured to the point of allowing isolation and precision control of even individual atoms and molecules. But in the quantum realm our intuitions largely break down, necessitating a formal framework to mathematically determine all relevant quantities without recourse to heuristics. But so far the attempts to transfer thermodynamic science from the classical to the quantum realm has been made without sufficient clarification of what is really meant by heat and work to begin with, resulting in endless confusion and controversy. It is the contention of many researchers that the nature of the heat-work decomposition has to be clarified before quantum thermodynamics can mature to greatness, and it is considered to be among the major outstanding theoretical problems in the field. It is the goal of this work to contribute to the solution by presenting an explicit proposal using quantum control theory for how heat can be distinguished from work. For an overview of the various attempts made so far to clarify these notions in the quantum context, I refer the reader to [12]. I claim that the heat-work decomposition implicitly invokes an observability decomposition of all the dynamical degrees of freedom of the system, that this is precisely what all the heuristics classically employed conveys if interpreted carefully, and show how it can be computed for an arbitrary quantum system subjected to observation and control. More specifically, heat corresponds to energy flow into *unobservable degrees of freedom*, while work corresponds to energy flow into the *observable ones*.

A point made by Adkins in the above paragraph that I wish to stress is the following: the key feature characterizing the performance of work is that the energy is transferred by *macroscopic action*. The notion of "macroscopic" is itself somewhat fuzzy, but for all practical purposes, when dealing with classical systems, the notion is clear enough to be fruitfully used. However, problems arise when we wish to replicate the above heuristic for quantum systems small enough for the distinction between "macroscopic" and "microscopic" to be entirely irrelevant. I claim that this problem can be remedied by the simple substitution of "macroscopic action" for "observable action". This substitution preserves the original meaning of "work" in the classical context as energy transferred by motion that we can see (macroscopic motion), while also making the notions of heat and work applicable to the smallest concievable systems where all degrees of freedom are microscopic, but some of them might be observable and others not, provided we're measuring observables where the measurement result provides incomplete information about the state of the system. [1]

We will end this introduction with a concrete everyday example to illustrate an otherwise abstract proposition. Imagine a ball lying in front of you on the table. Consider changing its energy in three different ways i) you lift the ball up into the air, thereby increasing its gravitational potential energy ii) you apply a torque to it with your fingers, thereby increasing its rotational energy iii) you throw the ball out of your window, thereby increasing its linear kinetic energy. All of these three transformations are called "work" by physicists. Now consider a different kind of transformation: you rub your fingers against the ball, without perturbing its position, or its rotational and linear velocities. This transformation is called "adding heat" by physicists. Why the difference in terminology? What is the phenomenological difference between the first three energy transformations on the one hand, and the fourth? The answer provided in this thesis is this: the first three kinds result in changes readily perceptible to us, while in the last case, it looks as if the energy simply disappears. Given our human eyes as sensors, position, rotational and linear velocities, are all observable degrees of freedom, while the internal motions which result from rubbing the ball with our fingers are unobservable.

1.1 Summary

- Chapter two will familiarize the reader with the basic notions of controllability and observability for quantum systems, and some theorems needed for this thesis are presented.
- In chapter three, a few formal results regarding observability spaces are obtained, the most imporant being a novel proposition that links the basis elements of the observability space to a quantum Fisher information matrix.
- Chapter four is the main bulk of this thesis ; it contains a proposition linking unobservability to thermal equilibrium, as well as an explicit theory of heat and work for quantum systems based on the observability decomposition.
- The fifth chapter takes the discussion away from the abstract and applies the theory developed in the previous one to the concrete case of the one-dimensional quantum Ising model. It also illustrates how the time-evolution operator, under certain cases, can be decomposed into

[1] Such a set of measured observables are termed "informationally incomplete". This distinction between observable and unobservable degrees of freedom will be made explicit in section (2.2)

a product of commuting operators, one of which acts on the observable state-component, and the other on the unobservable one.

- Chapter six concludes this thesis with a summary of arguments why a cybernetic theory of heat and work should be taken seriously, as well as provides avenues for further research.

I wish to clarify what is original in this thesis and what is lifted from previous research. All of chapter two consists of a summary of previous research relevant to this work, so here the reader won't find anything original. In chapter three, Propositions 2 and 3 are original, while Theorem 1 is an application of a standard result in Lie theory to a particular case of interest. In chapter four, Proposition 4 belongs to Domenico d'Alessandro, while Corollary 1 is common knowedge among quantum thermodynamicists. They are included to stress their significance in connecting thermal equilibrium states to lack of observability. The rest of the thesis is completely original.

The main contribution is a theory of quantum thermodynamics for closed systems under semi-classical external driving. The sceptical reader who rejects the definitions presented as properly characterising heat and work flows is allowed to regard this thesis are merely a study of energy flow into, out of, and between observable and unobservable subspaces of quantum systems, under various conditions. But these characterizations of heat and work is already how many thermodynamicists intuitively view them, and that while the mathematical formalization is new, there's nothing original with regards to their conceptual content.

Chapter 2

Dynamics, Control and Observation

> Interacting with nature teaches us to live in relation with the other, not in domination over the other: You don't control the birds flying overhead, or the moon rising, or the bear walking where it would like to walk. In my appraisal, one of the overarching problems of the world today is that we see ourselves living in domination over rather than in relation with other people and with the natural world.
>
> Peter Kahn

Ignoring Peter Kahn for a while, and perhaps contributing to his angst, we will now provide the reader with a short overview of some of the most important theoretical tools developed so far for controlling nature at the quantum scale. The subject of quantum control is still in its infancy, partly due to the fact that until recently, precision control of quantum systems has been impossible due to technological limitations. As techniques have been developed for isolating quantum systems and tayloring high-frequency laser pulses with a great degree of precision, interest in quantum control has been on the rise as a consequence. In this chapter, we will present two key results obtained which provide us with necessary and sufficient conditions for when a quantum system is controllable and observable. But first, we will give a short overview of the dynamical set-up.

The mathematical objects employed for describing the most general kinds of quantum states are bounded and positive trace-class operators $\hat{\rho} : \mathcal{H} \to \mathcal{H}$ on a complex Hilbert space $\mathcal{H}$. In general these operators represent probabalistic ensembles of pure quantum states [1], so-called mixed states, and for the case of rank one operators, a single determinate pure state. These objects are called *density operators*, and are denoted $\hat{\rho}$. Their eigenvalues are interpreted as the probabilities that the system is found in a given pure state at a given time, and this interpretation requires that the constraint $\text{Tr}\{\hat{\rho}\} = 1$ holds for all time. Observables are represented by Hermitian and bounded trace-class operators $\hat{S} : \mathcal{H} \to \mathcal{H}$, with their (real-valued) eigenvalues representing the possible measurement outcomes. The expectation value for a given observable at time t is given by the equation $\langle \hat{S}(t) \rangle = \text{Tr}\{\hat{S}\hat{\rho}(t)\}$. Of all possible observables of a quantum system, a particular one known as the *Hamiltonian*, or energy operator, determines the time-evolution of the quantum state through the *Liouville-Von-Neumann equation*

$$\frac{d}{dt}\hat{\rho}(t) = -i[\hat{H}, \hat{\rho}(t)]. \tag{2.1}$$

In this thesis, we are interested in the case where the Hamiltonian is dependent on a set of complex-valued functions $u : \mathbb{R}_{\geq 0} \to \mathcal{C}$, written $\mathscr{U}$ and refered to as the *set of admissable controls*. Meaning we have $\hat{H} = \hat{H}(u)$, where the function $u \in \mathscr{U}$ can be freely chosen by the control-engineer. The solution to Eq. (2.1) is given by

$$\hat{\rho}(t) = \hat{U}_u^\dagger(t)\hat{\rho}(0)\hat{U}_u(t),$$

where the *time-evolution operator* $\hat{U}_u(t)$ (indexed by the control u) satisfies the *operator Schrödinger equation*

$$\frac{d}{dt}\hat{U}_u(t) = -i\hat{H}(u)\hat{U}_u(t), \qquad \hat{U}_u(0) = \hat{I}_{n\times n}, \tag{2.2}$$

and is always a unitary operator, meaning $\hat{U}_u^\dagger(t) = \hat{U}_u^{-1}(t)$.

Let $\hat{S} = \sum_{i=1}^n s_i\hat{S}_i$ be the spectral decomposition of the observable $\hat{S}$. When performing a measurement of $\hat{S}$, the state will (up to normalization) collapse to the post-measurement state

$$\hat{\rho}' = \hat{S}_i\hat{\rho}\hat{S}_i,$$

with probability $p_i = \text{Tr}\{\hat{S}_i\hat{\rho}\}$. In everything that follows, the output of the dynamical system will be the expectation value $y(t) = \langle \hat{S}(t) \rangle$ of an arbitrary Hermitian operator. We now have everything we need to state the definition of a *quantum control system*.

[1] A pure state is a vector $|\psi\rangle$ residing in a separable and bounded complex Hilbert space that satisfies the Schrödinger equation $i\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$, where $\hat{H}$ is the Hamiltonian.

Definition 1. (Quantum Control System) *A quantum control system is a quadruple* $\Sigma = (\mathcal{H}, \hat{H}(\cdot), \mathscr{U}, \hat{S})$, *where* $\mathcal{H}$ *is a Hilbert space,* $\hat{H}(\cdot)$ *is a Hamiltonian operator,* $\mathscr{U}$ *is a set of admissable controls on whose elements the Hamiltonian depends, and* $\hat{S}$ *is a Hermitian operator ; such that a density matrix on* $\mathcal{H}$ *satisfies Eq. (2.1).*

Having presented a brief description of the dynamical problem, we now turn to the two central notions of control theory: controllability and observability. Everything in sections 2.1, and 2.2, except for Theorem 2, can be found in [15] to which the reader is referred to for further details.

2.1 Controllability

There are various notions of controllability considered in the quantum control litterature, two prominent examples being *operator controllability* and *pure state controllability.* If a system is operator controllable, then, by suitable choices of controls $u \in \mathscr{U}$, any unitary transformation can be implemented on the system. If a system is pure state controllable then any pure state can be mapped to any other, by suitable control choices. Here we focus on the first, which is also the stronger of the two conditions. The operator controllability problem consists of determining the subset $\mathcal{R} \subseteq U(n)$ of all $n \times n$ unitary matrices that can be obtained by selection of control functions $u \in \mathscr{U}$. Namely that of determining the *reachable set*

$$\mathcal{R} \triangleq \big\{\hat{U} \in U(n) \mid \hat{U} = \hat{U}_u(t) \text{ for some } t \in \mathbb{R}_{\geq 0}, u \in \mathscr{U}, \\ \text{where } \hat{U}_u(t) \text{ satisfies Eq. (2.2)}\big\}.$$

We will now state the definition of operator controllability.

Definition 2. (Operator Controllability) *If for a dynamical system* Σ *satisfying Eq (2.1), the corresponding reachable set* $\mathcal{R}$ *is equal to the set* $U(n)$ *of* $n \times n$ *unitary matrices, or equal to the subgroup* $SU(n)$ *of* $U(n)$*, then* Σ *is said to be operator controllable.*

Remark. *The reason why* $\mathcal{R} = SU(n)$ *suffices for operator controllability even though* $\dim SU(n) = \dim U(n) - 1$*, is that control over the global phase of the system is irrelevant as it leaves no observable consequences.*

If $\hat{U}_u(t)$ is the solution to Eq (2.2) with initial condition equal to $\hat{I}_{n\times n}$, then the solution with initial condition equal to $\hat{A}$ is equal to $\hat{U}_u(t)\hat{A}$. This fact means that the set $\mathcal{R}$ is closed under concatenation of controls, and is therefore a semi-group. Moreover, as it turns out, it's a *Lie group.* Assuming $\mathscr{U}$ to be equal to the set of piece-wise constant complex valued functions, as is standard procedure in quantum control theory, it can be shown that $\mathcal{R}$ can be obtained from an object known as the *dynamical Lie algebra.* This will now be stated without proof as a theorem [2]

[2]The proof can be found in Appendix D in [15].

Theorem 1. (A Controllability Condition) *Consider a quantum system with a bilinear Hamiltonian* $\hat{H} = \hat{H}_0 + \sum_{j=1}^{m} u_j(t)\hat{H}_i$*, where* $u_j \in \mathscr{U}$ *and* $\mathscr{U}$ *is the set of piece-wise constant complex valued functions* $u_j : \mathcal{R}_{\geq 0} \to \mathbb{C}$*. Let* $\mathcal{L}$ *be the Lie algebra generated by* $i\{\hat{H}_0, \hat{H}_1, ..., \hat{H}_m\}$*, namely*

$$\mathcal{L} \triangleq \bigoplus_{j=0}^{\infty} ad^{\,j}_{i\{\hat{H}_0,\hat{H}_1,...,\hat{H}_m\}} i\{\hat{H}_0, \hat{H}_1, ..., \hat{H}_m\}.$$

Then the reachable set $\mathcal{R}$ *is given by the exponential of the dynamical Lie algebra. In equational form*

$$\mathcal{R} = e^{\mathcal{L}}.$$

Furthermore, if $\mathcal{L} = su(n)$ *or* $\mathcal{L} = u(n)$*, then the system is operator controllable.*

Remark. *Pure state controllability is a weaker condition, and here it suffices that* $\mathcal{L}$ *is either conjugate to* $sp(\frac{n}{2})$ *in* $su(n)$*, or equal to* $\mathcal{L} = span\{i\hat{I}_{n\times n}\} \oplus \tilde{\mathcal{L}}$*, where* $\tilde{\mathcal{L}}$ *is conjugate to* $sp(\frac{n}{2})$ *in* $su(n)$*.*

2.1.1 Operator Controllability of a Subspace

We will end this section with a result obtained by G. Kato et al. [16] concerning controllability when the application of controls is restricted to one part of a bipartite system. The scenario considered is a bipartite system with Hilbert space $\mathcal{H}_{\mathcal{E}} \otimes \mathcal{H}_{\Sigma}$, where the interaction between the two parts is given by the Hamiltonian $\hat{H}_I$. It is assumed that any unitary transformation can be implemented on $\mathcal{H}_{\Sigma}$, so that the full dynamical Lie algebra $\mathcal{L}$ is the one generated by $i\hat{H}_0$ and $\hat{I}_{\mathcal{E}} \otimes su(\dim(\mathcal{H}_{\Sigma}))$. They defined the *connected Lie algebra* $\mathcal{L}_c$ as the smallest ideal of $\mathcal{L}$ containing $\hat{I}_{\mathcal{E}} \otimes su(\dim(\mathcal{H}_{\Sigma}))$, and the *disconnected Lie algebra* $\mathcal{L}_d$ as the set of all elements of $\mathcal{L}$ which commutes with $\mathcal{L}_c$. Formally

$$\begin{aligned}\mathcal{L}_c &\triangleq \text{span}\{[\cdots[[g, g_1], g_2, \cdots, g_n] \mid n \in \mathbb{N}, g_i \in \mathcal{L}, g \in \hat{I}_{\mathcal{E}} \otimes \text{su}(\dim\mathcal{H}_{\Sigma})\},\\ \mathcal{L}_d &\triangleq \{g \in \text{u}(\dim\mathcal{H}_{\mathcal{E}} \cdot \dim\mathcal{H}_{\Sigma}) \mid [g, g'] = 0 \ \forall g' \in \mathcal{L}_c\}.\end{aligned}$$

In their paper they obtained several significant results regarding the structure of the total Hilbert space and these two dynamical Lie algebras. We will now state the one of interest to the subject of this work.

Theorem 2. (Control Under Limited Access) *Assume that* $dim\mathcal{H}_{\Sigma} \geq 3$*. Then the Hilbert space of the environment can be written as a direct sum of product Hilbert spaces of the form*

$$\mathcal{H} = \mathcal{H}_{\Sigma} \otimes \left(\bigoplus_{j} \mathcal{H}_{B_j} \otimes \mathcal{H}_{R_j} \right), \tag{2.3}$$

and in accordance with this decomposition, the connected and disconnected Lie algebras are given by

$$\mathcal{L}_c = \bigoplus_j \mathcal{L}_{c,j} = \bigoplus_j \{\hat{I}_{B_j}\} \otimes \mathrm{su}(\dim\, \mathcal{H}_{R_j} \cdot \dim\, \mathcal{H}_\Sigma), \tag{2.4}$$

$$\mathcal{L}_d = \bigoplus_j \mathcal{L}_{d,j} = \bigoplus_j \mathrm{u}(\dim\, \mathcal{H}_{B_j}) \otimes \{\hat{I}_{R_j} \otimes \hat{I}_\Sigma\}. \tag{2.5}$$

The interaction Hamiltonian can be written $\hat{H}_I = \hat{h}_c + \hat{h}_d$*, where* $\hat{H}_c \in \mathcal{L}_c$ *and* $\hat{H}_d \in \mathcal{L}_d$*.*

The relevance of the above theorem to this thesis is that its the first example (to the knowledge of the author) of a *controllability decomposition* for quantum systems. Here the interaction Hamiltonian is decomposed into a part which is controllable (h_c), and a part which is not (h_d) ; and the Hilbert space of the environment is decomposed into a sum of products $\mathcal{H}_{B_j} \otimes \mathcal{H}_{R_j}$, where each $\mathcal{H}_{R_j}$ is controllable and each $\mathcal{H}_{B_j}$ is not.

In chapter four we will seek to explicate the notions of heat and work, and by implication other thermodynamic notions as well, using an observability decomposition which can be defined for any quantum system without any restrictions on the availability of controls. For a full picture of the interrelation between thermodynamics and control theory the significance of controllability *per se* with regards to heat and work should explored as well. But as a controllability decomposition does not exist for general Von-Neumann Liouville systems as of yet, this thesis will primarily be centered around observability rather than controllability as the key factor differentiating heat and work.

2.2 Observability

Observability is the notion that the internal state of a system, in our case the quantum state vector or the density matrix, can be determined from measurements of its input-output relations. Since values of observables are measured with a probability distribution that depends on the state of the system, sequential measurements on an ensemble of identically prepared systems should give us information about their internal states. Such a procedure is known as *quantum state tomography.* But under what conditions can the full state be determined from such sequential measurements? Certainly, projective measurements of an arbitrary observable will not do. In this section we will present a theorem courtesy of Domenico D'Alessandro which allows us, given a measured observable and a dynamical Lie algebra, to partition all states of a quantum control system into equivalence classes of indistinguishable states, as well as find a way to determine though suitable measurements and application of controls which equivalence class any given initial state belongs to.

Consider a quantum control system Σ in the density matrix formalism, with a dynamical evolution determined by the Liouville equation

$$\frac{d\hat{\rho}}{dt} = [-\hat{H}(u(t)), \hat{\rho}], \qquad \hat{\rho}(0) = \hat{\rho}_0, \qquad y(t) = \mathrm{Tr}\{\hat{S}\hat{\rho}\},$$

and denote the solution to the above equation as $\hat{\rho}(t, u, \hat{\rho}_0)$. We now state the definition of indistinguishability, as well as of observability.

Definition 3. (Indistinguishability and Observability) *A pair of states* $(\hat{\rho}_0, \hat{\rho}_0')$ *are said to be indistinguishable, denoted by* $\hat{\rho}_0 \sim \hat{\rho}_0'$ *if for any control* $u \in \mathscr{U}$ *we have*

$$\mathrm{Tr}\{\hat{S}\hat{\rho}(t, u, \hat{\rho}_0)\} = \mathrm{Tr}\{\hat{S}\hat{\rho}(t, u, \hat{\rho}_0')\}, \qquad \forall t \in \mathcal{T}.$$

The system Σ *is said to be observable if*

$$\hat{\rho}_0 \sim \hat{\rho}_0' \iff \hat{\rho}_0 = \hat{\rho}_0'.$$

We can also use the relation $\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t)$ together with the cyclic property of the trace-operation to rewrite the indistinguishability condition as

$$\mathrm{Tr}\{\hat{U}^\dagger\hat{S}\hat{U}\hat{\rho}_0\} = \mathrm{Tr}\{\hat{U}^\dagger\hat{S}\hat{U}\hat{\rho}_0'\}, \qquad \forall \hat{U} \in e^{\mathcal{L}}.$$

Verifying that"$\sim$" is an equivalence relation is straightforward. Reflexivity follows from the uniqueness of the solutions to the Liouville equation. Symmetry and transitivity follows follows from the symmetry and transitivity of the equality relation "=". The indistinguishability relation therefore partitions the set of density operators on $\mathcal{H}$ into equivalence classes of indistinguishable states. Moreover, such classes form invariant sets under the Liouville dynamics.

In what follows we will instead of $\hat{S}$ consider the traceless matrix $\hat{S}' = \hat{S} - \frac{\mathrm{Tr}\{\hat{S}\}}{n}\hat{I}_{n\times x}$. This has the effect of shifting the output by a constant value Tr $\{\hat{S}\}$, which will have no effect on the considerations that follows. We can now present the main result on the observability of finite-dimensional quantum systems. This theorem is due to Domenico d'Alessandro, and can be found in [15]. The proof will be presented in full, since this thesis, with regards to its mathematics, is largely a set of corollaries to this highly underappreciated theorem.

Theorem 3. (Observability Decomposition) *Given a quantum control system* Σ, Σ *is observable if and only if*

$$\mathcal{V} \triangleq \bigoplus_{j=0}^{\infty} ad_{\mathcal{L}}^{j}\mathrm{span}\{i\hat{S}'\} = su(n).$$

The object $\mathcal{V}$ is called the observability space. If we decompose the density operator as $\hat{\rho} = \hat{\rho}_o + \hat{\rho}_u$, where $\hat{\rho}_o \in i\mathcal{V}$ and $\hat{\rho}_u \in i\mathcal{V}^{\perp}$, where $\mathcal{V}^{\perp}$ is the orthogonal complement of $\mathcal{V}$ in u(n), we obtain the following dynamical decomposition

$$\frac{d}{dt}\hat{\rho}_o = -i[\hat{H}(u), \hat{\rho}_o], \tag{2.6}$$

$$\frac{d}{dt}\hat{\rho}_u = -i[\hat{H}(u), \hat{\rho}_u]. \tag{2.7}$$

The output depends only on $\hat{\rho}_o$ and is given by

$$y(t) = \frac{1}{n}\mathrm{Tr}\{\hat{S}\} + \mathrm{Tr}\{\hat{S}\hat{\rho}_o\}.$$

Moreover, initial states $\hat{\rho}'_1$ and $\hat{\rho}'_2$ are indistinguishable if and only if $\hat{\rho}'_1 - \hat{\rho}'_2 \in i\mathcal{V}^{\perp}$.

Proof : We begin by decomposing the density matrix as $\hat{\rho} = \hat{\rho}_o + \hat{\rho}_u$, where $\hat{\rho}_o \in i\mathcal{V}$ and $\hat{\rho}_u \in i\mathcal{V}^{\perp}$. We then obtain a decomposition of the Liouville equation as

$$\frac{d}{dt}\hat{\rho}_o + \frac{d}{dt}\hat{\rho}_u = [-i\hat{H}(u), \hat{\rho}_o] + [-i\hat{H}(u), \hat{\rho}_u].$$

The observability space is constructed by taking repeated commutators with elements in $\mathcal{L}$, so any element initially in $i\mathcal{V}$ will stay there when commuting with $-i\hat{H}(u)$. The same holds for the orthogonal complement, so we have

$$[-i\hat{H}(u), i\mathcal{V}] \subseteq i\mathcal{V}, \qquad [-i\hat{H}(u), i\mathcal{V}^{\perp}] \subseteq i\mathcal{V}^{\perp}.$$

This implies that we can decompose the dynamics of $\hat{\rho}$ as in Eq. (2.3-4). The decomposition of the ouput $y(t)$ follows from the fact that $\hat{\rho}_o$ is tracelss, while $\hat{\rho}_u$ has trace one. To see this, we note that $\hat{\rho}_u \in i\mathcal{V}^{\perp}$ and $\hat{S}' \in i\mathcal{V}$, which implies that

$$\mathrm{Tr}\{\hat{S}'\hat{\rho}_u\} = \mathrm{Tr}\big\{(\hat{S} - \frac{\mathrm{Tr}\{\hat{S}\}}{n}\hat{I})\hat{\rho}_u\big\} = 0 \Rightarrow \mathrm{Tr}\{\hat{S}\hat{\rho}_u\} = \frac{\mathrm{Tr}\{\hat{S}\}}{n}.$$

Now consider two initial states $\hat{\rho}'_1$ and $\hat{\rho}'_2$, and decompose the corresponding solutions to Eq. (2.2) into observable and unobservable parts according to

$$\hat{\rho}(t, u, \hat{\rho}'_1) = \hat{\rho}_o(t, u, \hat{\rho}'_1) + \hat{\rho}_u(t, u, \hat{\rho}'_1),$$
$$\hat{\rho}(t, u, \hat{\rho}'_2) = \hat{\rho}_o(t, u, \hat{\rho}'_2) + \hat{\rho}_u(t, u, \hat{\rho}'_2).$$

If the output as a function of time corresponding to the two initial states are $y_1(t)$ and $y_2(t)$, we see that their difference is given by

$$y_1(t) - y_2(t) = \mathrm{Tr}\ \big\{\hat{S}(\hat{\rho}_0(t, u, \hat{\rho}'_1) - \hat{\rho}_0(t, u, \hat{\rho}'_2))\big\}.$$

The above equation implies that the outputs are identical, and hence $\hat{\rho}'_1 \sim \hat{\rho}'_2$ if $\hat{\rho}'_1 - \hat{\rho}'_2 \in i\mathcal{V}^\perp$. To prove the implication in the other direction, assume that $\hat{\rho}'_1 \sim \hat{\rho}'_2$. We then have

$$\text{Tr}\left\{\hat{U}^\dagger \hat{S}' \hat{U}(\hat{\rho}'_1 - \hat{\rho}'_2)\right\} = 0.$$

Assume that $\hat{U} = e^{\hat{R}_1^\dagger t_1}$ for $\hat{R}_1 \in \mathcal{L}$, and $t_1 \in \mathbb{R}$. Then

$$\frac{\partial}{\partial t}\text{Tr}\left\{e^{\hat{R}_1 t_1}\hat{S}' e^{\hat{R}_1^\dagger t_1}(\hat{\rho}'_1 - \hat{\rho}'_2)\right\}\Big|_{t_1=0} = \\ \text{Tr}\left\{(\hat{R}_1\hat{S}' + \hat{S}'\hat{R}_1^\dagger)(\hat{\rho}'_1 - \hat{\rho}'_2)\right\} = 0.$$

Since the elements of $\mathcal{L}$ are skew-Hermitian the above equation can be rewritten as $\text{ad}_{\hat{R}_1}(\hat{\rho}'_1 - \hat{\rho}'_2) = 0$. By induction one can prove that for any $\hat{U} = e^{\hat{R}_1^\dagger t_1} e^{\hat{R}_2^\dagger t_2} ... e^{\hat{R}_k^\dagger t_k}$ with $\hat{R}_1, ..., \hat{R}_k \in \mathcal{L}$ and $t_1, ..., t_k \in \mathbb{R}$ we have

$$\frac{\partial^k}{\partial t_1 ... \partial t_k}\text{Tr}\left\{e^{\hat{R}_1 t_1} ... e^{\hat{R}_k t_k}\hat{S}' e^{\hat{R}_1^\dagger t_1} ... e^{\hat{R}_k^\dagger t_k}(\hat{\rho}'_1 - \hat{\rho}'_2)\right\}\Big|_{t_1=...=t_k=0} = \\ \text{Tr}\left\{\text{ad}_{\hat{R}_1} ... \text{ad}_{\hat{R}_k}\hat{S}'(\hat{\rho}'_1 - \hat{\rho}'_2)\right\} = 0.$$

This shows that for any $\hat{R} \in \mathcal{V}$ we have $\text{Tr}\,\{\hat{R}(\hat{\rho}'_1 - \hat{\rho}'_2)\} = 0$, which in turn implies that $\hat{\rho}'_1 - \hat{\rho}'_2 \in i\mathcal{V}^\perp$. If we assume that $\mathcal{V} = su(n)$ then $\hat{\rho}'_1 - \hat{\rho}'_2 \in \text{span}\,\{\hat{I}\}$, which implies that the system is observable since both $\hat{\rho}'_1$ and $\hat{\rho}'_2$ have trace one. □

Remark. (Operator Controllability Implies Observability) *Since the Lie algebra su(n) is simple, and $\mathcal{V}$ is an ideal of su(n), it follows that any operator controllable system is observable for any $\hat{S}$ not proportional to the identity matrix.*

Remark. (Observability and Informational Completeness) *If $\mathcal{V} = su(n)$, then the set of all possible time-evolved observables*

$$\{\hat{U}_u^\dagger \hat{S}\hat{U}_u | u \in \mathcal{U}\},$$

is said to be ***informationally complete****, meaning sequential measurements of $\hat{S}$ on an ensemble of identically prepared systems, with application of suitable controls, can yield enough information to allow for full state determination. If $\mathcal{V} \neq su(n)$, then the above set is said to be* informationally incomplete. *If the argument presented in this thesis is correct, thermodynamics, at least as classically concieved, has no meaning when $\mathcal{V} = su(n)$; it is essentially a phenomenological theory of energy balance accounting when there are unobservables degrees of freedom, and a part of the energy is allowed to dissapear from observable dynamics, resulting in "energy degradation", or "waste". The energy which seemingly disappears is called "heat".*

Assume that we have chosen a control $u(t) \in \mathscr{U}$ with input values in $[0, T]$, for some $T \in \mathbb{R}_+$, such that the solution $\hat{U}_u$ of the operator Schrödinger equation satisfies

$$\text{span}_{\ t\in[0,T]}\{\hat{U}_u^\dagger(t)\hat{S}'\hat{U}_u(t)\} = i\mathcal{V}.$$

The output for this trajectory is given by

$$y(t) = \text{Tr}\ \{\hat{U}_u^\dagger \hat{S}'\hat{U}_u(\hat{\rho}_0 - \frac{1}{n}\hat{I}_{n\times n})\} + \text{Tr}\ \{\hat{S}\}.$$

We can now define an operator $\mathcal{W}_u : \mathscr{H}_0^{n\times n} \to \mathscr{H}_0^{n\times n}$ on traceless $n \times n$ Hermitian matrices as

$$\mathcal{W}_u(\hat{\rho}_0) \triangleq \int_0^T \hat{U}_u^\dagger(t)\hat{S}'\hat{U}_u(t)\text{Tr}\ \left\{\hat{U}_u^\dagger(t)\hat{S}'\hat{U}_u(t)\hat{\rho}_0\right\}dt.$$

We now state the essential facts about this operator, which is called the *observability gramian.*

Proposition 1. (Observability Gramian) *The range of $\mathcal{W}_u$ is equal to $i\mathcal{V}$, and the kernel is equal to $i\mathcal{V}^\perp$.*

Proof : I begin by proving that the kernel of $\mathcal{W}_u$ lies in the orthogonal complement $i\mathcal{V}^\perp$ of the observability space. Assume that $\mathcal{W}_u(\hat{\rho}_0) = 0$. Since the trace-operation is linear we can bring it under the integral sign and obtain

$$\text{Tr}\ \left\{\hat{\rho}_0\mathcal{W}_u(\hat{\rho}_0)\right\} = \int_0^T \text{Tr}\ \left\{\hat{\rho}_0\hat{U}_u^\dagger\hat{S}'\hat{U}_u\text{Tr}\ (\hat{U}_u^\dagger\hat{S}'\hat{U}_u\hat{\rho}_0)\right\}dt.$$

The inner trace is simply a scalar, and since the trace-operation is cyclic we can bring $\hat{\rho}_0$ to the right and obtain

$$\text{Tr}\ \left\{\hat{\rho}_0\mathcal{W}_u(\hat{\rho}_0)\right\} = \int_0^T \left(\text{Tr}\ \left\{\hat{U}_u^\dagger\hat{S}'\hat{U}_u\hat{\rho}_0\right\}\right)^2 dt = 0,$$

which implies that $\text{Tr}\{\hat{U}_u^\dagger\hat{S}'\hat{U}_u\hat{\rho}_0\} = 0$ almost everywhere, which implies that $\hat{\rho}_0 \in i\mathcal{V}^\perp$. Conversely, assume that $\hat{\rho}_0 \in i\mathcal{V}^\perp$. Then $\hat{U}_u^\dagger\hat{S}'\hat{U}_u\hat{\rho}_0 = 0$ and it follows immediately that $\mathcal{W}_u(\hat{\rho}_0) = 0$.

By assumption the span of $\hat{U}_u^\dagger\hat{S}'\hat{U}_u$ as t ranges over $[0, T]$ is equal to $i\mathcal{V}$, so the integrand in $\mathcal{W}_u$ lies in $i\mathcal{V}$ as well. Since $i\mathcal{V}$ is a vector space it is closed under addition, and therefore also under integration, so $\mathcal{W}_u(\hat{\rho}_0)$ lies in $i\mathcal{V}$ as well. □

Remark. (State Determination) *Noting that*

$$\int_0^T \hat{U}_u^\dagger\hat{S}'\hat{U}_u(y - \text{Tr}\{\hat{S}\})dt = \int_0^T \hat{U}_u^\dagger\hat{S}'\hat{U}_u\text{Tr}\{\hat{U}_u^\dagger\hat{S}'\hat{U}_u(\hat{\rho}_0 - \frac{1}{n}\hat{I})\}dt,$$

we can use the observability gramian to obtain an equation for the initial state $\hat{\rho}_0$ modulo elements in $i\mathcal{V}^{\perp}$

$$\hat{\rho}_0 = \frac{1}{n}\hat{I}_{n\times n} + \mathcal{W}_u^{-1}\left(\int_0^T \hat{U}_u^{\dagger}\hat{S}'\hat{U}_u(y - \mathrm{Tr}\{\hat{S}\})\right).$$

To conclude this section, we emphasize that the two key objects of analysis are the dynamical Lie algebra $\mathcal{L}$, characterizing all state transformations that can be implemented on the system, and the observability space $\mathcal{V}$, which decomposes the state into observable and unobservable components. A cybernetic theory of heat and work for quantum systems would have to explicate what the structure of these two objects imply regarding the heat-work decomposition, and by implication other thermodynamic quantities.

Chapter 3

Some Results on Observability Spaces

Analysis of the structure of the observability space $\mathcal{V}$ and its relation to the dynamical Lie algebra $\mathcal{L}$, under various conditions imposed on the measured observable $\hat{S}$, and for different algebras $\mathcal{L}$, has to date not been performed. As the pair $(\mathcal{L}, \mathcal{V})$ codifies important information regarding the controllability and observability of the system under consideration, analysis of their structure and interrelation under various measurement-and-control scenarios is bound to produce results of practical importance. And if the central proposition of this thesis is correct, namely that thermodynamics is intimately tied with notions of control and observation, it might also yield results of thermodynamic significance.

In this section, we will merely scratch the surface of the issue by presenting a simple factorization result for time-translation operators under the condition that $\hat{S} \in \mathcal{L}$, as well as computing $\mathcal{V}$ for the limited access scenario described in Section 2.2.1. But we begin this section by illustrating an application of the observability space to the practical problem of state identification, and the commonly used metric of *Fisher information* to quantify the minimum estimation errors of quantum measurements.

3.1 Observability and Fisher Information

In the theory of quantum state estimation, among the foundational results is the *Quantum Cramer-Rao inequality*, named after its classical counterpart, which states that for an r-parameter estimation problem the covariance matrix of the estimate $\tilde{\theta}$ (for the case of an unbiased estimator) satisfies the inequality

$$\mathrm{Cov}(\tilde{\theta}) \geq F^{-1},$$

where F is a symmetric $r \times r$ matrix called *the Fisher information*. Simply put, the diagonal entries of the Fisher information provides a lower bound for the variance in the estimates of each θ_i, while the off-diagonal elements bounds the correlations between them from below. The Fisher information is not unique, but can be defined in a variety of ways, and here we will focus on a particular kind of Fisher information defined using so-called *symmetric logarithmic derivative operators.* Consider a density matrix $\hat{\rho}(\theta)$ dependent on r parameters $(\theta_1, ..., \theta_r)$. One begins by defining the SLD operators $\hat{L}_k$, for $k = 1, ..., r$, by the equations

$$\frac{\partial}{\partial \theta_k}\hat{\rho}(\theta) = \frac{1}{2}[\hat{L}_{\theta_k}, \hat{\rho}]_+.$$

The matrix elements of the Fisher information are then defined by the equation

$$F_{k,j} \triangleq \frac{1}{2}\mathrm{Tr}\{\hat{\rho}[\hat{L}_{\theta_k}, \hat{L}_{\theta_j}]_+\}.$$

I will now prove a proposition showing that when $\hat{\rho}$ is a pure state, the components of F can be written as inner products of basis operators of $\mathcal{V}$.

Proposition 2. (Fisher Information as a Gramian) *If the quantum state $\hat{\rho}$ is pure, then the Fisher information can be expressed in terms of the basis matrices $\{\hat{V}_k\}_{k=1}^{dim\mathcal{V}}$ of the observability space as*

$$F_{k,j} = \frac{1}{2}\mathrm{Tr}\{[\hat{V}_k, \hat{V}_j]_+\} = \langle \hat{V}_k, \hat{V}_j \rangle.$$

Proof : Assume that $\dim(\mathcal{V}) = r$ and let ρ be written in the form

$$\hat{\rho}(\theta) = \hat{\rho}_u + \sum_{j=1}^{r} \theta_j \hat{V}_j,$$

where we have introduced the notation $\hat{V}_j$ for the basis elements of $i\mathcal{V}$, and $\theta_j \triangleq \mathrm{Tr}\{\hat{V}_j \hat{\rho}\}$. The r-parameter estimation problem is now formulated as a problem of finding the projections of $\hat{\rho}$ along every basis operator of $i\mathcal{V}$. Taking the partial derivative of $\hat{\rho}$ with respect to one of the parameters we obtain

$$\frac{\partial}{\partial \theta_j}\hat{\rho}(\theta) = \hat{V}_j = \frac{1}{2}[\hat{L}_{\theta_j}, \hat{\rho}]_+ = \frac{1}{2}(\hat{L}_{\theta_j}\hat{\rho} + \hat{\rho}\hat{L}_{\theta_j}).$$

Since the basis operators $\hat{V}_j$ are traceless, we see that the expectation values of the SLD operators vanish, i.e.

$$\langle \hat{L}_{\theta_j} \rangle = \mathrm{Tr}\{\hat{L}_{\theta_j}\hat{\rho}\} = \mathrm{Tr}\{\hat{V}_j\} = 0.$$

By employing the cyclic property of the trace, a straightforward calculation shows that

$$\mathrm{Tr}\{[\hat{V}_k, \hat{V}_j]_+\} = \mathrm{Tr}\{2\hat{L}_{\theta_k}\hat{\rho}\hat{L}_{\theta_j}\hat{\rho} + \hat{\rho}^2\hat{L}_{\theta_k}\hat{L}_{\theta_j} + \hat{\rho}^2\hat{L}_{\theta_j}\hat{L}_{\theta_k}\}.$$

If the quantum state is pure, then the density matrix is a projection with $\hat{\rho}^2 = \hat{\rho}$, and

$$\mathrm{Tr}\{2\hat{L}_{\theta_k}\hat{\rho}\hat{L}_{\theta_j}\hat{\rho}\} = 2\langle\hat{L}_{\theta_k}\rangle\langle\hat{L}_{\theta_j}\rangle = 0.$$

To see why the first equation in the above holds, write it out using the bra-ket notation as

$$\mathrm{Tr}\{2\hat{L}_{\theta_k}\hat{\rho}\hat{L}_{\theta_j}\hat{\rho}\} = \mathrm{Tr}\{2\hat{L}_{\theta_k}\,|\psi\rangle\,\langle\psi|\,\hat{L}_{\theta_j}\,|\psi\rangle\,\langle\psi|\}.$$

Note that

$$\langle\psi|\,\hat{L}_{\theta_j}\,|\psi\rangle = \langle\hat{L}_{\theta_j}\rangle$$

is a scalar, and can therefore be pulled out of the trace. The identity now follows.

Writing out the Fisher information explicitly

$$F_{k,j} = \frac{1}{2}\mathrm{Tr}\{\hat{\rho}\hat{L}_{\theta_k}\hat{L}_{\theta_j} + \hat{\rho}\hat{L}_{\theta_j}\hat{L}_{\theta_k}\},$$

we now see that under the assumption of purity,

$$F_{k,j} = \frac{1}{2}\mathrm{Tr}\{[\hat{V}_k, \hat{V}_j]_+\}.$$

By the cyclic property of the trace, and the hermiticity of the matrices $\{\hat{V}_k\}$, this is equal to $\langle\hat{V}_k, \hat{V}_j\rangle$. □

We see that the Fisher information for pure states takes the form of a "gramian" formed from the basis operators of $\mathcal{V}$

$$F_{\theta_k,\theta_j} = \begin{pmatrix} \langle\hat{V}_1,\hat{V}_1\rangle & \langle\hat{V}_1,\hat{V}_2\rangle & \dots & \langle\hat{V}_1,\hat{V}_r\rangle \\ \langle\hat{V}_2,\hat{V}_1\rangle & \langle\hat{V}_2,\hat{V}_2\rangle & \dots & \langle\hat{V}_2,\hat{V}_r\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle\hat{V}_r,\hat{V}_1\rangle & \langle\hat{V}_r,\hat{V}_2\rangle & \dots & \langle\hat{V}_r,\hat{V}_r\rangle \end{pmatrix}.$$

An exactly analogous argument as in the above proof shows that in the case of single-parameter estimation of a pure quantum state we have $F_\theta = ||\hat{V}||^2$. We will now leave the subject of state estimation, but the Fisher information will occur later in this thesis when we consider heat and work flows for pure states.

3.2 Factorization of Time-Translation Operators

Within the context of thermodynamics, typical observables under measurement are ones associated with the energy. For this reason it is of particular interest to study the implications on the structure of $(\mathcal{L}, \mathcal{V})$ in the case where $i\hat{S} \in \mathcal{L}$. This means that we are either measuring the energy of the system under isolation, an interaction energy between system and control field, a commutator of drift or control Hamiltonians, or any combination of the aforementioned. We begin with the following theorem, which states that any $\hat{U} \in e^{\mathcal{L}}$ can be factorized into two commuting parts, one of which leaves the output $y(t) = \mathrm{Tr}\{\hat{S}\hat{\rho}\}$ invariant. [1]

Theorem 4. (Factorization of Time-Translation Operators) *Suppose we are measuring $i\hat{S} \in \mathcal{L}$, and that $\mathcal{V} \neq \mathcal{L}$. Then $e^{\mathcal{V}}$ and $e^{\mathcal{L}\cap\mathcal{V}^\perp}$ are both normal subgroups of $e^{\mathcal{L}}$, and any element $\hat{U} \in e^{\mathcal{L}}$ has a unique decomposition of the form $\hat{U} = \hat{U}_o\hat{U}_u$, where $\hat{U}_o \in e^{\mathcal{V}}$ and $\hat{U}_u \in e^{\mathcal{L}\cap\mathcal{V}^\perp}$, such that $[\hat{U}_o, \hat{U}_u] = 0$. Moreover, we have the following isomorphisms*

$$e^{\mathcal{L}}/e^{\mathcal{L}\cap\mathcal{V}^\perp} \simeq e^{\mathcal{V}}, \qquad e^{\mathcal{L}}/e^{\mathcal{V}} \simeq e^{\mathcal{L}\cap\mathcal{V}^\perp}.$$

Proof : Since $i\hat{S} \in \mathcal{L}$, and $\mathcal{L}$ is closed under commutatation, it holds that $\mathcal{V} \subseteq \mathcal{L}$. Assuming the inclusion to be strict, the commutation relation $[\mathcal{L}, \mathcal{V}] \subseteq \mathcal{V}$ implies that $\mathcal{V}$ is a non-trivial ideal of $\mathcal{L}$. Furthermore, an ideal of a Lie algebra is a subalgebra closed under the Lie bracket, and is therefore itself a Lie algebra. By a standard result, since $\mathcal{V}$ is an ideal of $\mathcal{L}$, the associated Lie group $e^{\mathcal{V}}$ is a normal subgroup of $e^{\mathcal{L}}$ (this fact is proven in for example [.]). The quotient group $e^{\mathcal{L}}/e^{\mathcal{V}}$, consisting of all left (or right) cosets $e^g e^{\mathcal{V}} = \{e^g e^v | v \in \mathcal{V}\}$, where $g \in \mathcal{L}$, is a Lie group of dimension

$$\dim(e^{\mathcal{L}}/e^{\mathcal{V}}) = \dim(e^{\mathcal{L}}) - \dim(e^{\mathcal{V}}).$$

The orthogonal complement of $\mathcal{V}$ in $\mathcal{L}$ with respect to the Killing form

$$\langle g, g' \rangle_K \triangleq \mathrm{Tr}\ (\ \mathrm{ad}_g\ \mathrm{ad}_{g'}),$$

namely the set

$$\mathcal{V}^\perp_{\mathcal{L},K} \triangleq \{g \in \mathcal{L} \mid \langle g, g' \rangle_K = 0\ \forall g' \in \mathcal{L}\},$$

is also an ideal. To see this, we employ the associativity of the Killing form. If $v_u \in \mathcal{V}^\perp_{\mathcal{L},K}$, then $\langle v_u, v \rangle_K = 0$ for all $v \in \mathcal{V}$. Since $\mathcal{V}$ is an ideal, for any $g \in \mathcal{L}$ we have $[g, v] \in \mathcal{V}$. We now obtain

$$\langle [v_u, g], v \rangle_K = \langle v_u, [g, v] \rangle_K = 0 \Longrightarrow [\mathcal{L}, \mathcal{V}^\perp_{\mathcal{L},K}] \subseteq \mathcal{V}^\perp_{\mathcal{L},K}.$$

Assuming the Killing form is proportional to the Hilbert-Schmidt inner product [2], every element of $\mathcal{V}^\perp_{\mathcal{L},K}$ is also an element of $\mathcal{V}^\perp$, and we therefore have

[1] This is a standard result in the theory of Lie algebras merely specialized to this particular case, but as I couldn't find a proof I decided to include an attempt (partly) of my own.

[2] This is very often the case, and perhaps (?) always the case for subalgebras of $su(n)$, which is what we're dealing with here.

$\mathcal{V}^{\perp}_{\mathcal{L},K} = \mathcal{L} \cap \mathcal{V}^{\perp}$. We can now conclude, as before, that the Lie group $e^{\mathcal{L}\cap\mathcal{V}^{\perp}}$ is a normal subgroup of $e^{\mathcal{L}}$, and the quotient $e^{\mathcal{L}}/e^{\mathcal{L}\cap\mathcal{V}^{\perp}}$ is a Lie group. Now decompose $\mathcal{L}$ into a direct sum as

$$\mathcal{L} = \mathcal{V} \oplus (\mathcal{L} \cap \mathcal{V}^{\perp}).$$

The above implies that any element $\hat{U} \in e^{\mathcal{L}}$ can be decomposed uniquely as $\hat{U} = \hat{U}_o\hat{U}_u$, where $\hat{U}_o \in e^{\mathcal{V}}$ and $\hat{U}_u \in e^{\mathcal{L}\cap\mathcal{V}^{\perp}}$. A proof of this can be found in [15].

To see that $[\mathcal{V}, \mathcal{L} \cap \mathcal{V}^{\perp}] = 0$, we first note that $\mathcal{V} \cap \mathcal{V}^{\perp} = \emptyset$. Now, since $\mathcal{V}$ is an ideal of $\mathcal{L}$ and $\mathcal{L} \cap \mathcal{V}^{\perp} \subset \mathcal{L}$, we have $[\mathcal{V}, \mathcal{L} \cap \mathcal{V}^{\perp}] \subseteq \mathcal{V}$. Similarly since $\mathcal{L} \cap \mathcal{V}^{\perp}$ is an ideal of $\mathcal{L}$ and $\mathcal{V} \subset \mathcal{L}$, we have $[\mathcal{V}, \mathcal{L} \cap \mathcal{V}^{\perp}] \subseteq \mathcal{L} \cap \mathcal{V}^{\perp}$. As the intersection between the two sets are empty, the commutator must vanish. We now have everything we need to prove the isomorphisms. Consider the function $\phi : e^{\mathcal{L}} \to e^{\mathcal{V}}$ defined $\phi \triangleq \pi \circ f$ where

$$f : e^{\mathcal{L}} \to e^{\mathcal{V}} \times e^{\mathcal{L}\cap\mathcal{V}^{\perp}} \ ; \ \hat{U} \mapsto (\hat{U}_o, \hat{U}_u),$$
$$\pi : e^{\mathcal{V}} \times e^{\mathcal{L}\cap\mathcal{V}^{\perp}} \to e^{\mathcal{V}} \ ; \ (\hat{U}_o, \hat{U}_u) \mapsto \hat{U}_o.$$

Employing factorization $\hat{U} = \hat{U}_o\hat{U}_u$ and the commutation relation $[\mathcal{V}, \mathcal{L} \cap \mathcal{V}^{\perp}] = 0$ we obtain

$$f(\hat{U}_1\hat{U}_2) = f(\hat{U}_{1,o}\hat{U}_{1,u}\hat{U}_{2,o}\hat{U}_{2,u}) = f(\hat{U}_{1,o}\hat{U}_{2,o}\hat{U}_{1,u}\hat{U}_{2,u}) = (\hat{U}_{1,o}\hat{U}_{2,o}, \hat{U}_{1,u}\hat{U}_{2,u}).$$

Applying the projection π to the above yields

$$\phi(\hat{U}_1\hat{U}_2) = \hat{U}_{1,o}\hat{U}_{2,o} = \phi(\hat{U}_1)\phi(\hat{U}_2),$$

from which we can conclude that ϕ is a homomorphism. Moreover, since $\mathcal{V} \subset \mathcal{L}$, it is also surjective, and it is easy to see that $\ker \phi = e^{\mathcal{L}\cap\mathcal{V}^{\perp}}$. The first isomorphism theorem for groups now implies that

$$e^{\mathcal{L}}/e^{\mathcal{L}\cap\mathcal{V}^{\perp}} \simeq e^{\mathcal{V}}.$$

An exactly analogous argument shows that

$$e^{\mathcal{L}}/e^{\mathcal{V}} \simeq e^{\mathcal{L}\cap\mathcal{V}^{\perp}},$$

and this completes the proof. □

Remark. The commutator relation $[\mathcal{V}, \mathcal{L} \cap \mathcal{V}^{\perp}] = 0$ gives an interpretation of elements in $\mathcal{L} \cap \mathcal{V}^{\perp}$ as those elements of $\mathcal{L}$ generating time-translations $\hat{U}$ that leave the output invariant. To see this, note that for any matrices A and B we have

$$[A, e^B] = \sum_{i=1}^{\infty} \frac{[A, B^i]}{i!},$$

from which it follows that if $g \in \mathcal{L} \cap \mathcal{V}^{\perp}$ then $[e^g, \hat{S}] = 0$, and consequently for $\hat{U} = e^g$ we have $\hat{U}^{\dagger}\hat{S}\hat{U} = \hat{U}^{\dagger}\hat{U}\hat{S} = \hat{S}$.

3.3 Access Restricted to an Operator Controllable Subspace

We will now compute the observability space for the bipartite scenario considered in section (2.2.1), using the results of G. Kato et al. as a springboard.

Proposition 3. (Observability Under Limited Access) *Assuming the scenario described in section (2.2.1), if* $\hat{S} = \hat{I}_{\mathcal{E}} \otimes \hat{S}_{\Sigma}$ *is a non-trivial local observable on* Σ*, then* $\mathcal{V} = \mathcal{L}_c$.

Proof : We decompose the identity operator on the environment according to the Hilbert space decomposition Eq. (2.3) as

$$\hat{I}_{\mathcal{E}} = \bigoplus_j \hat{I}_{B_j} \otimes \hat{I}_{R_j}.$$

We first consider the contribution to $\mathcal{V}$ by the disconnected Lie algebra. Let $\hat{g} \in \mathcal{L}_d$. Taking the commutator with $\hat{S}$ we obtain, with the notation $\hat{g}_{B_j} \in \mathrm{u}(\dim \mathcal{H}_{B_j})$ for an arbitrary element acting on the subspace $\mathcal{H}_{B_j}$,

$$[\hat{g}, \hat{S}] = [\hat{g}, \hat{I}_{\mathcal{E}} \otimes \hat{S}_{\Sigma}] = \left[\bigoplus_j \hat{g}_{B_j} \otimes \hat{I}_{R_j} \otimes \hat{I}_{\Sigma}, \left(\bigoplus_j \hat{I}_{B_j} \otimes \hat{I}_{R_j} \right) \otimes \hat{S}_{\Sigma} \right] =$$
$$\bigoplus_j \left[\hat{g}_{B_j} \otimes \hat{I}_{R_j} \otimes \hat{I}_{\Sigma}, \hat{I}_{B_j} \otimes \hat{I}_{R_j} \otimes \hat{S}_{\Sigma} \right].$$

In transitioning to the second line we used the fact that tensor products distribute over direct sums, and applied the definition of Lie brackets for direct sums of Lie algebras. Since we are dealing exclusively with matrix subalgebras of su(n), we can apply the formula obtained in [24] for commutators of tensor products of matrices, in which case the above becomes

$$\bigoplus_j \frac{1}{2} \Big(\left[\hat{g}_{B_j}, \hat{I}_{B_j} \right] \otimes \left\{ \hat{I}_{R_j} \otimes \hat{I}_{\Sigma}, \hat{I}_{R_j} \otimes \hat{S}_{\Sigma} \right\} + \left\{ \hat{g}_{B_j}, \hat{I}_{B_j} \right\} \otimes \left[\hat{I}_{R_j} \otimes \hat{I}_{\Sigma}, \hat{I}_{R_j} \otimes \hat{S}_{\Sigma} \right] \Big).$$

Noting that the commutator of an arbitrary matrix with the identity vanishes, we see that $[\hat{g}, \hat{S}] = 0$. We conclude that the observation space is generated solely by taking commutators with elements from $\mathcal{L}_c$, i.e.

$$\mathcal{V} = \bigoplus_{i=1}^{\infty} \mathrm{ad}^i_{\mathcal{L}} \mathrm{span}\{ i\hat{I}_{\mathcal{E}} \otimes \hat{S}_{\Sigma} \} = \bigoplus_{i=1}^{\infty} \mathrm{ad}^i_{\mathcal{L}_c} \mathrm{span}\{ i\hat{I}_{\mathcal{E}} \otimes \hat{S}_{\Sigma} \}.$$

If instead $\hat{g} \in \mathcal{L}_c$, with $\hat{g}_{R_j,\Sigma} \in \mathrm{su}(\dim \mathcal{H}_{R_j} \otimes \mathcal{H}_{\Sigma})$ being an arbitrary element acting on the subspace $\mathcal{H}_{R_j} \otimes \mathcal{H}_\Sigma$, an analogous calculation yields the result

$$[\hat{g}, \hat{S}] = \bigoplus_j \left[\hat{I}_{B_j} \otimes \hat{g}_{R_j,\Sigma}, \hat{I}_{B_j} \otimes \hat{I}_{R_j} \otimes \hat{S}_\Sigma\right] =$$

$$\bigoplus_j \frac{1}{2}\Big([\hat{I}_{B_j}, \hat{I}_{B_j}] \otimes \{\hat{g}_{R_j,\Sigma}, \hat{I}_{R_j} \otimes \hat{S}_\Sigma\} + \{\hat{I}_{B_j}, \hat{I}_{B_j}\} \otimes [\hat{g}_{R_j,\Sigma}, \hat{I}_{R_j} \otimes \hat{S}_\Sigma] \Big) =$$

$$\bigoplus_j \hat{I}_{B_j} \otimes [\hat{g}_{R_j,\Sigma}, \hat{I}_{R_j} \otimes \hat{S}_\Sigma],$$

which implies that $[\mathcal{L}_c, \hat{S}] \subseteq \mathcal{L}_c$. Since $\hat{S}$ is an element of $\hat{I}_\mathcal{E} \otimes \mathrm{su}(\mathrm{dim}\mathcal{H}_\Sigma)$, it is also an element of $\mathcal{L}_c$ which contains the former. We conclude that $\mathcal{V}$ is an ideal of $\mathcal{L}_c$. To proceed from here, note that $\mathcal{L}_c$ is a direct sum of simple ideals $\mathcal{L}_{c,j}$, and is therefore semi-simple. Since $\hat{S} \cap \mathcal{L}_{c,j} \neq \emptyset$ for every j, the only possible ideal is the maximal ideal, namely $\mathcal{L}_c$ itself. $\square$.

Chapter 4

Quantum Thermodynamics

> Every mathematician knows it is impossible to understand an elementary course in thermodynamics.
>
> V.I. Arnold

Thermodynamics holds the peculiar position in the pantheon of physical theories of simultaneously being among the most fruitful with regards to its practical applications, while also having the most obscure and incomprehensible foundational concepts. I believe this confusion to be partly due to many physicists interpreting thermodynamics as purely a *physical theory*. Namely, that it speaks of what happens in nature itself, without reference to anything parochial and human. The author contends that it is equally a theory of *engineering*, and is deeply intervowen with cybernetic notions. It is perhaps even tied to economic notions, as work is sometimes referred to as energy which is *useful*, or even more explicitly, as energy of *economic value*. That this is the case should not be surprising to the historian of science, as its early practitioners were principally interested in maximizing the performance of heat engines for industrial purposes. Control theory contains the tools to make these concepts explicit, and if we follow this path then hopefully mathematicians might someday understand an introductory text in thermodynamics.

This chapter will begin with a section illustrating a link between observability and thermal equilibrium. It will then move on to the main part of this thesis in which a cybernetic theory of heat and work is developed.

4.1 Microcanonical Thermal Equilibrium

Some physical systems, when left to themselves, will eventually reach a stationary state at which no further changes are instrumentally perceptible, which can be characterized as a state of maximum entropy. Such a state is called *thermal equilibrium*. Experimentally observed properties of equilibrium states include time-translational invariance, robustness against small perturbations, as well as being for all practical purposes characterized by a number of parameters very small compared to the dimensionality of the complete classical or quantum model. Equilibrium states that exchange neither heat nor particles with their surroundings are called *microcanonical*. It is a well known fact that at microcanonical equilibrium, the observable output is given by the trace of the corresponding Hermitian operator, normalized by the dimensionality of the state space. This is taken as a necessary condition for a system to be at microcanonical equilibrium.

In this section I will present an immediate corollary of the observability decomposition which proves that an observable output satisfies the microcanonical condition if and only if the state lies in the orthogonal complement of the observation space corresponding to the measured observable. The proof used here is contained in the proofs of Theorem 3, and in the derivation of properties of the observability gramian.

Proposition 4. (The Equilibrium State is Unobservable) *Consider a quantum control system* $\Sigma = (\mathcal{H}, \hat{H}(\cdot), \mathscr{U}, \hat{S})$. *Then* $\hat{\rho} \in i\mathcal{V}^{\perp}$ *is a necessary and sufficient condition for a microcanonical distribution of* $\hat{S}$. *Furthermore, the microcanonical distribution is stable under any control action* $u \in \mathscr{U}$.

Proof : To prove sufficiency, assume that $\hat{\rho} \in i\mathcal{V}^{\perp}$, in which case $\mathcal{W}_u(\hat{\rho}) = 0$. This implies that $\mathrm{Tr}\ \{\hat{\rho}\mathcal{W}_u(\hat{\rho})\} = 0$. Noting that the trace operation is linear, we can bring it under the integral sign and obtain

$$\mathrm{Tr}\ \{\hat{\rho}\mathcal{W}_u(\hat{\rho})\} = \mathrm{Tr}\left\{ \int_0^T \hat{\rho}_0 \hat{U}_u^\dagger \hat{S}' \hat{U}_u \mathrm{Tr}\ \{\hat{U}_u^\dagger \hat{S}' \hat{U}_u \hat{\rho}_0\} dt \right\} = \int_0^T \mathrm{Tr}\ \{\hat{U}_u^\dagger \hat{S}' \hat{U}_u \hat{\rho}_0\}^2 dt = 0.$$

For the above equation to hold, the integrand must vanish almost everywhere. This yields

$$\mathrm{Tr}\ \{\hat{U}_u^\dagger \hat{S}' \hat{U}_u \hat{\rho}_0\} = \mathrm{Tr}\ \{\hat{U}_u^\dagger (\hat{S} - \frac{\mathrm{Tr}\{\hat{S}\}}{n} \hat{I}_{n\times n}) \hat{U}_u \hat{\rho}_0\} =$$
$$\mathrm{Tr}\ \{\hat{U}_u^\dagger \hat{S} U_u \hat{\rho}_0\} - \frac{\mathrm{Tr}\{\hat{S}\}}{n} = 0 \implies y(t) = \mathrm{Tr}\{\hat{S}\hat{\rho}(t)\} = \frac{\mathrm{Tr}\{\hat{S}\}}{n} = \langle \hat{S} \rangle_{\mathrm{mic}},$$

for almost all $t \in [0, T]$. We can conclude that a microcanonical distribution for $\hat{S}$ will be present if $\hat{\rho} \in i\mathcal{V}^{\perp}$. To prove necessity, we simply note that the trace within the integrand of $\mathcal{W}_u(\hat{\rho})$ will vanish whenever $y(t) = \langle \hat{S} \rangle_{\mathrm{mic}}$.

Since $i\mathcal{V}$ is defined as the smallest subspace of $\mathrm{su}(n)$ containing $\{i\hat{S}'\}$ which is invariant under all commutators with elements in the dynamical Lie algebra $\mathcal{L}$, it is clearly invariant. From the invariance of $i\mathcal{V}$ it follows that for any element $\mathcal{F} \in i\mathcal{V}^{\perp}$ and $\mathcal{A} \in i\mathcal{V}$ we have

$$\mathrm{Tr}\{[-i\hat{H}(u), \mathcal{F}]\mathcal{A}\} = \mathrm{Tr}\{[-i\hat{H}(u), \mathcal{A}]\mathcal{F}\} = 0,$$

so $[-i\hat{H}(u), i\mathcal{V}^{\perp}] \subseteq i\mathcal{V}^{\perp}$ for any control action $u \in \mathscr{U}$. □

The above proposition proves that unobservability of the state is necessary for a system to be at microcanonical equilibrium. It follows directly from the work of D'Alessandro, but is included here to stress that it suggests a strong connection between observability and thermal equilibrium, which should be explored in greater detail. Note that the condition that $\hat{\rho} \in i\mathcal{V}^{\perp}$, for an observability space $\mathcal{V}$ constructed from an observable $\hat{S}$, says nothing of how other observables would behave for the same quantum state, merely that this particular observable is "thermalized". A paper arguing that one should consider a notion of thermalization pertaining to particular observables rather than the state itself can be found in [17]. A main point of their argument is that thermalization of the actual state is not a notion that can be probed experimentally, but thermalization of particular observables can.

Remark. (Quantum Thermalization) The traditional measure of thermalization is the Von-Neumann entropy $S = -\mathrm{Tr}\{\hat{\rho}\log\hat{\rho}\}$, which as its form indicates, is a function of only the state itself, and not any specific observable. A property of the Von-Neumann entropy is that it is invariant under unitary transformations. An implication of this, if this entropy is taken as a proper measure of thermalization, is that a closed system can never thermalize. But experiments have shown that closed systems can indeed thermalize. This is known as the *quantum thermalization problem*; closed quantum systems should not be able to thermalize, but in reality they do. So perhaps one should look for alternative measures of thermalization, and arguments have been put forward that the Von-Neumann entropy does not correspond to entropy as thermodynamicists speak of it [18]. Proposition 4 suggests that one might use methods of quantum control to tackle this problem.

Another corollary of the observability decomposition, is that the only universally unobservable state is the maximally mixed state, or equivalently, the (canonical) [1] thermal equilibrium state at infinite temperature. That is, this is the only state which is unobservable regardless of measured observable and availability of controls.

Corollary 1. (Only $\hat{I}$ is Universally Unobservable) Assume that the quantum control system Σ is operator controllable and observable. Then

[1] An equilibrium state is termed canonical if it is allowed to exchange heat with an environment at a specified temperature.

the only element of $i\mathcal{V}^{\perp}$ is given by

$$\hat{\rho}_u = \frac{1}{n}\hat{I} = \frac{1}{n}\lim_{\beta\to 0}e^{-\beta\hat{H}}.\Box$$

Proof : The proof that the canonical equilibrium state at infinite temperature is proportional to the identity matrix can be found in many refereces, and it goes as follows. One writes the equilibrium density matrix $e^{-\beta\hat{H}}$ in the basis of energy eigenstates $|E_1\rangle, ..., |E_n\rangle$, by using the completeness relation $\sum_{k=1}^{n}|E_k\rangle\langle E_k| = \hat{I}$, and taking the limit as $\beta\to 0$ to obtain

$$\lim_{\beta\to 0}e^{-\beta\hat{H}} = \lim_{\beta\to 0}\sum_{j=1}^{n}\sum_{k=1}^{n}|E_k\rangle\langle E_k| e^{-\beta\hat{H}}|E_j\rangle\langle E_j| =$$

$$\lim_{\beta\to 0}\sum_{k=1}^{n}e^{-\beta E_k}|E_k\rangle\langle E_k| = \lim_{\beta\to 0}\ \mathrm{diag}\big(e^{-\beta E_1}, e^{-\beta E_2}, ..., e^{-\beta E_n}\big) = \hat{I}.$$

The main point of this section is that thermal equilibrium states can be characterized as states of "non-observability", in some sense of the term. For microcanonical equilibrium we explicitly have $\hat{\rho}\in i\mathcal{V}^{\perp}$.

4.2 Heat and Work

Before proceeding to provide the central definitions of this thesis, we will consider the most common way of defining heat and work for quantum systems found in research papers on quantum thermodynamics. Traditionally, one simply takes the time-derivative of the total energy to obtain

$$\frac{d}{dt}\langle\hat{H}\rangle_{\hat{\rho}} = \left\langle\frac{d\hat{H}}{dt}, \hat{\rho}\right\rangle + \left\langle\hat{H}, \frac{d\hat{\rho}}{dt}\right\rangle,$$

and identifies the first term with work, and the second with heat. This definition arises time and time again in research papers, but when it does, the author often includes a caveat that these identifications are unsatisfactory and even leads to unphysical results, but due to the lack of alternatives it is taken as a tentative solution to the problem. The identification is usually motivated by claiming that the Hamiltonian is under our direct control, and therefore changes resulting from it constitutes some form of work, while the state is generally uncontrollable and therefore energy changes relating to changes in state can be called heat. It is worth noting that even here control-theoretic notions are used to justify the distinction. For a more detailed discussion of this way of defining heat and work, and its problems, the reader is referred to [19]. One point I wish to stress is that internal heat and work flows are impossible to define in this way, since for a closed system both terms must be identically zero, and therefore this definition cannot be employed when analyzing thermalization of closed systems.

4.2.1 Operational Definitions of Heat and Work

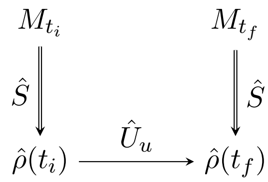

Figure 4.1: Operational determination of heat and work, schema.

Before presenting a *formal* definition of heat and work we will first provide an *operational* definition, which illustrates the experimental determination of these quantities, given a quantum control system Σ. By Theorem 3 the total energy can be decomposed as follows $\langle \hat{H} \rangle_{\hat{\rho}} = \mathcal{O}[\hat{\rho}_o] + \mathcal{U}[\hat{\rho}_u]$, where we have defined $\langle \hat{H} \rangle_{\hat{\rho}_o} \triangleq \mathcal{O}[\hat{\rho}_o]$ and $\langle \hat{H} \rangle_{\hat{\rho}_u} \triangleq \mathcal{U}[\hat{\rho}_u]$. This decomposition implies that any observation performed on Σ can at best determine a part of the total energy, namely $\mathcal{O}$. Consider the three-step process, shown in Figure 4.1 :

- 1 : Perform a projective measurement of $\hat{S}$ to determine the component $\hat{\rho}_o(t_i)$ of the density matrix along $i\mathcal{V}$. This gives us an initial observable energy $\mathcal{O}_{t_i} = \mathcal{O}[\hat{\rho}_o(t_i)]$.
- 2 : Apply a semi-classical control $u_{[t_i,t_f]} \in \mathscr{U}$ resulting in a *known* change $\Delta E[u_{[t_i,t_f]}]$ in the energy of Σ.
- 3 : Repeat step 1 to obtain a final observable energy $\mathcal{O}_{t_f} = \mathcal{O}[\hat{\rho}_o(t_f)]$.

The energy spent by applying the control is in general not equal to the difference between the observable energies at t_i and t_f, as an arbitrary control will couple to unobservable degrees of freedom. We define *heat* to be equal to this deficit, and *work* to be the change in observable energies, i.e.

$$Q \triangleq \Delta E[u_{[t_i,t_f]}] + \mathcal{O}_{t_i} - \mathcal{O}_{t_f},$$
$$W \triangleq \mathcal{O}_{t_f} - \mathcal{O}_{t_i}.$$

The claim is that the operational definition of "heat" is that quantity of energy that *we know a priori* must have been transfered to the system, even though we cannot see it, in order for energy conservation to hold. These quantities can be determined experimentally provided that two conditions are satisfied; firstly the functional dependence of $\mathcal{O}$ on $\hat{\rho}_o$ must be known, since $\mathcal{O}$ is not measured directly but computed from $\hat{\rho}_o$ which in turn is constructed from a direct measurement of $\hat{S}$; second, we must be able to keep track of the energy ΔE that we spend for Q to be determinable from the energy balance equation. If satisfied, the above procedure provides a way to determine a plausible candidate for Q under semi-classical external driving, without having to invoke an environment to be traced out. Note that there are two ways in which the energy change constituting Q can be supplied: it can arise due to a change in the Hamiltonian, meaning from energy that *we* supply, or from an interconversion of $\mathcal{O}$ to $\mathcal{U}$ occuring uncontrollably inside the system. The distinction between internal and external heat flow will be made explicit shortly.

4.2.2 Formal Definitions of Heat and Work

The following definitions form the foundation stones on which the rest of the theory is built. They will not only distinguish between heat and work, but also between internal and external heat and work flows. The internal flows preserve the total energy of the system, are driven by internal state changes, and are therefore present also in the absence of external controls. The external heat and work flows, on the other hand, are driven by changes in the Hamiltonian, and are - in general - energy non-conserving interactions with the control apparatus. Before providing the central definitions of this thesis, we will introduce some notation. Given bases $\{\hat{V}_i\}_{i=1}^{\dim\mathcal{V}}$ and $\{\hat{V}_i^{\perp}\}_{i=1}^{\dim\mathcal{V}^{\perp}}$ for $\mathcal{V}$ and $\mathcal{V}^{\perp}$ respectively, we introduce the components of the Hamiltonian along the two spaces

$$\hat{H}_V \triangleq \sum_{j=1}^{\dim\mathcal{V}} \langle \hat{H}, \hat{V}_j \rangle \frac{\hat{V}_j}{||\hat{V}_j||}, \qquad \hat{H}_{V^{\perp}} \triangleq \sum_{j=1}^{\dim\mathcal{V}^{\perp}} \langle \hat{H}, \hat{V}_j^{\perp} \rangle \frac{\hat{V}_j^{\perp}}{||\hat{V}_j^{\perp}||}.$$

Definition 4. (Heat and Work) *Consider a quantum control system Σ of finite dimension n, with a dynamical Lie algebra $\mathcal{L}$ and an observability space $\mathcal{V}$. An arbitrary control $u \in \mathscr{U}$ will induce a time-varying total energy $\langle \hat{H}(t) \rangle$. Decompose the density matrix as $\hat{\rho}(t) = \hat{\rho}_o(t) + \hat{\rho}_u(t)$, where $\hat{\rho}_o(t) \in i\mathcal{V}$ and $\hat{\rho}_u(t) \in i\mathcal{V}^{\perp}$. We then define the work and heat flows as*

$$\frac{dW}{dt} \triangleq \frac{d}{dt}\mathcal{O} = \left\langle \frac{d\hat{H}_V(t)}{dt}, \hat{\rho}_o(t) \right\rangle + \left\langle \hat{H}_V(t), \frac{d\hat{\rho}_o(t)}{dt} \right\rangle,$$
$$\frac{dQ}{dt} \triangleq \frac{d}{dt}\mathcal{U} = \left\langle \frac{d\hat{H}_{V^{\perp}}(t)}{dt}, \hat{\rho}_u(t) \right\rangle + \left\langle \hat{H}_{V^{\perp}}(t), \frac{d\hat{\rho}_u(t)}{dt} \right\rangle.$$

We further make the distinction between internal and external work and heat flows depending on whether the energy flow occurs through a change in the state or the Hamiltonian. Formally the individual terms are given by the inexact derivatives

$$\frac{đW_I}{đt} \triangleq \left\langle \hat{H}_V(t), \frac{d\hat{\rho}_o(t)}{dt} \right\rangle, \qquad \frac{đW_E}{đt} \triangleq \left\langle \frac{d\hat{H}_V(t)}{dt}, \hat{\rho}_o(t) \right\rangle,$$
$$\frac{đQ_I}{đt} \triangleq \left\langle \hat{H}_{V^{\perp}}(t), \frac{d\hat{\rho}_u(t)}{dt} \right\rangle, \qquad \frac{đQ_E}{đt} \triangleq \left\langle \frac{d\hat{H}_{V^{\perp}}(t)}{dt}, \hat{\rho}_u(t) \right\rangle.$$

What follows is a proposition giving a set of sufficient algebraic conditions for when $\mathcal{O}$, and hence also $\mathcal{U}$, is a constant of motion in the absence of controls. The proof is elementary, but the result is potentially significant as it provides a new tool for thinking about thermalization of closed systems ; a system can in a meaningful sense be said to "thermalize" if over time energy is transferred from $\mathcal{O}$ to $\mathcal{U}$, until the measured output is nearly microcanonical. [2]

Proposition 5. (Conditions for the Time-Invariance of $\mathcal{U}$ and $\mathcal{O}$) *Each of the following is a sufficient conditions for the observable energy to be a constant of motion in the absence of controls*

$$[\hat{H}_V, \hat{H}_{V^\perp}] = 0, \qquad [\hat{H}_V, \hat{H}_{V^\perp}] \in \mathcal{V}^\perp, \qquad [\hat{H}_V, \hat{H}_{V^\perp}] \in \mathcal{V},$$
$$\hat{H}_V \in \mathcal{L}, \qquad \hat{H}_{V^\perp} \in \mathcal{L}.$$

Proof : In the absence of controls, only the internal work flow will be (possibly) non-zero, and it is given by

$$\frac{đW_I}{đt} = \left\langle \hat{H}_V, \frac{d\hat{\rho}_o(t)}{dt} \right\rangle = -i\big\langle \hat{H}_V, [\hat{H}, \hat{\rho}_o]\big\rangle = -i\big\langle [\hat{H}_V, \hat{H}], \hat{\rho}_o\big\rangle =$$
$$-i\big\langle [\hat{H}_V, \hat{H}_{V^\perp}], \hat{\rho}_o\big\rangle.$$

In the last line we decomposed the total Hamiltonian as $\hat{H} = \hat{H}_V + \hat{H}_{V^\perp}$ and noted that $[\hat{H}_V, \hat{H}_V] = 0$. We can now make a few observations. Clearly the above vanishes if $[\hat{H}_V, \hat{H}_{V^\perp}] = 0$. The internal work flow is also equal to zero provided that $[\hat{H}_V, \hat{H}_{V^\perp}] \in \mathcal{V}^\perp$, and this condition is guaranteed to be satisfied if $\hat{H}_V \in \mathcal{L}$ since $[\mathcal{L}, \mathcal{V}^\perp] \subseteq \mathcal{V}^\perp$. The remaining conditions for the constancy of $\mathcal{O}$ is obtained by noting that energy conservation gives us the equation

$$\frac{đW_I}{đt} = -\frac{đQ_I}{đt} = i\big\langle [\hat{H}_{V^\perp}, \hat{H}_V], \hat{\rho}_u\big\rangle,$$

and then going through a similar argument as before. □

While sufficient, neither of these conditions are necessary. If $\mathcal{O}$ is a constant of motion, that implies that either $[\hat{H}_V, \hat{H}_{V^\perp}] = 0$ or $[\hat{H}_V, \hat{H}_{V^\perp}] \perp \hat{\rho}_o$. But for $[\hat{H}_V, \hat{H}_{V^\perp}] \in \mathcal{V}^\perp$ to hold it is required that $[\hat{H}_V, \hat{H}_{V^\perp}] \perp \hat{\rho}'_o$ for *every* $\hat{\rho}'_o \in i\mathcal{V}$. Nevertheless, if one is interested in engineering a control system without thermalization the above condition will suffice.

[2] The reason why "nearly" was included in the last sentence is because if $\mathrm{Tr}\{\hat{S}\hat{\rho}_o\} \neq 0$ at some point in time, it will never be identically zero, due to the inclusions $[\mathcal{L}, \mathcal{V}^\perp] \subseteq \mathcal{V}^\perp$ and $[\mathcal{L}, \mathcal{V}] \subseteq \mathcal{V}$. However, there is nothing, generally speaking, which prevents $\mathrm{Tr}\{\hat{S}\hat{\rho}_o\}$ from decreasing in its value over time. If it does, and finally fluctuates around some small value, then that value can be taken to be the scale of "thermal fluctuations"; this can be interpreted as meaning that information about the initial state never fully disappears as the system thermalizes, but remains encoded in the fluctuations of $\mathrm{Tr}\{\hat{S}\hat{\rho}_o\}$ near the microcanonical value.

4.2.3 Energetics of Quantum Measurements

In this section, we will consider if and when the unobservable energy $\mathcal{U}$ changes under selective and non-selective measurements respectively. The observable $\hat{S}$ has a spectral decomposition into projectors $\hat{S}_j$ onto the eigenspaces corresponding to the eigenvalues s_j, constrained to satisfy a completeness relation

$$\hat{S} = \sum_{j=1}^{m} s_j \hat{S}_j, \qquad \sum_{j=1}^{m} \hat{S}_j = \hat{I}.$$

We can pick any $k \in \{1, ..., m\}$ and decompose the projector sum as

$$\sum_{j=1}^{m} \hat{S}_j = \sum_{j=1, j\neq k}^{m} \hat{S}_j + \left(\hat{I} - \sum_{j=1, j\neq k}^{m} \hat{S}_j\right) = \hat{S}^{\neg k} + \big(\hat{I} - \hat{S}^{\neg k}\big),$$

where we have introduced the symbol $\hat{S}^{\neg k}$ for the sum excluding the k-th term. Assuming a selective measurement yielding the result s_k, the post-measurement state is given by

$$\mathcal{M}(\hat{\rho}) = (\hat{I} - \hat{S}^{\neg k})\hat{\rho}(\hat{I} - \hat{S}^{\neg k}) = \hat{\rho} - [\hat{S}^{\neg k}, \hat{\rho}] + \hat{S}^{\neg k}\hat{\rho}\hat{S}^{\neg k}.$$

We now apply the observability decomposition $\hat{\rho} = \hat{\rho}_o + \hat{\rho}_u$. Since $\hat{S}^{\neg k} \in i\mathcal{V}$, we have $\hat{S}^{\neg k}\hat{\rho}_u\hat{S}^{\neg k} = \langle \hat{S}^{\neg k}, \hat{\rho}_u \rangle \hat{S}^{\neg k} = 0$. The two separate components are therefore modified by the measurement according to

$$\mathcal{M}(\hat{\rho}_o) = \hat{\rho}_o - [\hat{S}^{\neg k}, \hat{\rho}_o] + \hat{S}^{\neg k}\hat{\rho}_o\hat{S}^{\neg k}, \qquad \mathcal{M}(\hat{\rho}_u) = \hat{\rho}_u - [\hat{S}^{\neg k}, \hat{\rho}_u].$$

The changes in observable and unobservable energies therefore satisfy

$$\Delta\mathcal{O} = \big\langle \hat{H}_V, \hat{S}^{\neg k}\hat{\rho}_o\hat{S}^{\neg k} - [\hat{S}^{\neg k}, \hat{\rho}_o] \big\rangle,$$
$$\Delta\mathcal{U} = -\big\langle \hat{H}_{V^\perp}, [\hat{S}^{\neg k}, \hat{\rho}_o] \big\rangle = -\big\langle [\hat{S}^{\neg k}, \hat{H}_{V^\perp}], \hat{\rho}_u \big\rangle.$$

The second line implies that $\Delta\mathcal{U} = 0$ if $[\hat{S}^{\neg k}, \hat{H}_{V^\perp}] = 0$ or $[\hat{S}^{\neg k}, \hat{H}_{V^\perp}] \in \mathcal{V}$. If $\hat{H}_{V^\perp} \in \mathcal{L}$, this is sufficient for the second condition to hold, since $[\mathcal{L}, \mathcal{V}] \subseteq \mathcal{V}$.

Now consider the case where the measurement is non-selective; meaning the measurement is performed, but the result is discarded. In this case the post-measurement state is a statistical ensemble of all possible results, obtained from the selective case by summing over all ks. We then have for the unobservable component, up to normalization, that

$$\mathcal{M}(\hat{\rho}_u) = \sum_{k=1}^{m} \left(\hat{\rho}_u - [\hat{S}^{\neg k}, \hat{\rho}_u]\right) = m\hat{\rho}_u - \left[\sum_{k=1}^{m} \hat{S}^{\neg k}, \hat{\rho}_u\right] =$$
$$m\hat{\rho}_u - (m-1)[\hat{I}, \hat{\rho}_u] = m\hat{\rho}_u.$$

After normalization this equals $\hat{\rho}_u$, so the unobservable component, and hence its energy, is unaffected. We will now summarize the results of this section in a proposition.

Proposition 6. (Invariance of the Unobservable Energy Under Measurements) *For any quantum control system Σ, the unobservable energy $\mathcal{U}$ is invariant under non-selective measurements, and invariant under selective measurements provided that $\hat{H}_{V^\perp} \in \mathcal{L}$.*

4.2.4 Maximum Extractable Heat

Any inner product can be used to define (abstract or concrete) angles, and the Hilbert-Schmidt inner product is no exception. The following angle can be taken as quantifying the extent to which the systems energy is unobservable (or "degraded")

$$\tau(t) \triangleq \arccos\left\{\frac{\mathcal{U}}{||\hat{H}_{V^\perp}||||\hat{\rho}_u||}\right\},$$

and we can always write $\mathcal{U} = ||\hat{H}_{V^\perp}||||\hat{\rho}_u|| \cos\tau$. Of all terms in this equation, the Hamiltonian norm $||\hat{H}_{V^\perp}||$ is the only one under our direct control. The state norm $||\hat{\rho}_u||$ is a constant regardless of applied controls (see remark), and the angle τ depends partly on $\hat{H}_{V^\perp}$, which is under our control, and partly on $\hat{\rho}_u$, which is not.

Remark. The norm $||\hat{\rho}_u||$ always remains constant over time, as a consequence of the time-evolution being unitary. This can be seen be employing the cyclic property of the trace

$$||\hat{\rho}_u(t)|| = \sqrt{\text{Tr}\{\hat{\rho}_u(t)\hat{\rho}_u(t)\}} = \sqrt{\text{Tr}\{\hat{U}_t\hat{\rho}_u(0)\hat{U}_t^\dagger\hat{U}_t\hat{\rho}_u(0)\hat{U}_t^\dagger\}} = \sqrt{\text{Tr}\{\hat{U}_t\hat{\rho}_u(0)\hat{\rho}_u(0)\hat{U}_t^\dagger\}} = \sqrt{\text{Tr}\{\hat{\rho}_u(0)\hat{\rho}_u(0)\}}.$$

Therefore, in what follows, keep in mind that $\frac{d}{dt}||\hat{\rho}_u|| = 0$.

Now consider the quantity

$$S \triangleq ||\hat{\rho}_u|| \cos\tau = \frac{\mathcal{U}}{||\hat{H}_{V^\perp}||}. \tag{4.1}$$

The reason why this quantity is denoted S is that it seems to play a similar role in this theory as that of entropy in classical thermodynamics. In what follows we will refer to it as the entropy, and at the end of the chapter, present a summary of the arguments for why this is justified. Among other things, it is closely related to the maximum heat extractable at a given time. This statement is made explicit in the following proposition.

Proposition 7. (Maximum Extractable Heat) *Consider two quantum systems Σ_1 and Σ_2, subject to the same control system, with equal unobservable energies $\mathcal{U}_1 = \mathcal{U}_2$ but with $S_1 < S_2$. Then the maximum heat extractable from Σ_1 is higher than that from Σ_2, provided there exists a lowest attainable norm $||\hat{H}^0_{V^\perp}||$ for both systems.*

Proof : The equality $\mathcal{U}_1 = \mathcal{U}_2$ implies that

$$\frac{||\hat{\rho}_u^1|| \cos \tau^1}{||\hat{\rho}_u^2|| \cos \tau^2} = \frac{||\hat{H}_{V^\perp}^2||}{||\hat{H}_{V^\perp}^1||},$$

and furthermore, the inequality $S_1 < S_2$ implies that $||\hat{H}_{V^\perp}^1|| > ||\hat{H}_{V^\perp}^2||$. The maximum extractable heat is in both cases obtained by controlling the Hamiltonian norm down to its lowest attainable value $||\hat{H}_{V^\perp}^0||$. The heats extracted are determined by

$$Q_{\max}^1 = ||\hat{\rho}_u^1|| \cos \tau^1 \big(||\hat{H}_{V^\perp}^0|| - ||\hat{H}_{V^\perp}^1||\big),$$
$$Q_{\max}^2 = ||\hat{\rho}_u^2|| \cos \tau^2 \big(||\hat{H}_{V^\perp}^0|| - ||\hat{H}_{V^\perp}^2||\big).$$

Their ratio is

$$\frac{Q_{\max}^1}{Q_{\max}^2} = \frac{||\hat{\rho}_u^1|| \cos \tau^1 \big(||\hat{H}_{V^\perp}^0|| - ||\hat{H}_{V^\perp}^1||\big)}{||\hat{\rho}_u^2|| \cos \tau^2 \big(||\hat{H}_{V^\perp}^0|| - ||\hat{H}_{V^\perp}^2||\big)} =$$
$$\frac{||\hat{H}_{V^\perp}^2||}{||\hat{H}_{V^\perp}^1||} \frac{||\hat{H}_{V^\perp}^0|| - ||\hat{H}_{V^\perp}^1||}{||\hat{H}_{V^\perp}^0|| - ||\hat{H}_{V^\perp}^2||}.$$

If there is no lowest attainable bound to the norm of the Hamiltonian, this ratio is equal to unity, but as long as $||\hat{H}_{V^\perp}^0|| \neq 0$ it will always be > 1, and so $Q_{\max}^1 > Q_{\max}^2$. □

We'll now present a proposition showing how the quantity S depends on the degree of overlap between the basis elements of $\mathcal{V}^\perp$.

Proposition 8. (The Entropy and the Basis Elements of $\mathcal{V}$) *Assume that the basis elements of $\mathcal{V}^\perp$ are normalized. If they're "maximally mixed" in the sense that $\langle \hat{V}_k^\perp, \hat{V}_j^\perp \rangle \approx 1 \ \forall kj$, then $S \approx ||\hat{\rho}_u||$. If instead they satisfy $\langle \hat{V}_k^\perp, \hat{V}_j^\perp \rangle = \delta_{kj}$, then*

$$S = \frac{1}{||\hat{H}_{V^\perp}||} \sum_{k=1}^{dim\mathcal{V}^\perp} \langle \hat{H}_{V^\perp}, \hat{V}_k^\perp \rangle \langle \hat{\rho}_u, \hat{V}_k^\perp \rangle.$$

Proof : We begin by expanding both $\hat{H}_{V^\perp}$ and $\hat{\rho}_u$ in the basis of $\mathcal{V}^\perp$,

$$\mathcal{U} = \sum_{k=1}^{\dim\mathcal{V}^\perp} \sum_{j=1}^{\dim\mathcal{V}^\perp} \langle \hat{H}_{V^\perp}, \hat{V}_k^\perp \rangle \langle \hat{\rho}_u, \hat{V}_j^\perp \rangle \frac{\langle \hat{V}_k^\perp, \hat{V}_j^\perp \rangle}{||\hat{V}_k^\perp|| ||\hat{V}_j^\perp||}.$$

This is also equal to $\mathcal{U} = ||\hat{\rho}_u|| ||\hat{H}_{V^\perp}|| \cos \tau$. By the triangle-inequality for norms we have

$$||\hat{H}_{V^\perp}|| \leq \sum_{k=1}^{\dim\mathcal{V}^\perp} \langle \hat{H}_{V^\perp}, \hat{V}_k^\perp \rangle, \qquad ||\hat{\rho}_u|| \leq \sum_{j=1}^{\dim\mathcal{V}^\perp} \langle \hat{\rho}_u, \hat{V}_j^\perp \rangle. \tag{4.2}$$

This gives a lower bound for the cosine

$$\cos\tau \geq \frac{\sum_{k=1}^{\dim\mathcal{V}^\perp}\sum_{j=1}^{\dim\mathcal{V}^\perp}\langle\hat{H}_{V^\perp},\hat{V}_k^\perp\rangle\langle\hat{\rho}_u,\hat{V}_j^\perp\rangle\frac{\langle\hat{V}_k^\perp,\hat{V}_j^\perp\rangle}{||\hat{V}_k^\perp||||\hat{V}_j^\perp||}}{\sum_{p=1}^{\dim\mathcal{V}^\perp}\sum_{l=1}^{\dim\mathcal{V}^\perp}\langle\hat{H}_{V^\perp},\hat{V}_p^\perp\rangle\langle\hat{\rho}_u,\hat{V}_l^\perp\rangle}.$$

Assuming the basis elements are normalized, we obtain $\cos\tau \gtrapprox 1$ for the case where $\langle\hat{V}_k^\perp,\hat{V}_j^\perp\rangle \approx 1$. In the ortho-normal case the inequalities (4.1) are saturated and we have

$$S = \frac{1}{||\hat{H}_{V^\perp}||}\sum_{k=1}^{\dim\mathcal{V}^\perp}\langle\hat{H}_{V^\perp},\hat{V}_k^\perp\rangle\langle\hat{\rho}_u,\hat{V}_k^\perp\rangle.$$

□

From the previous proposition it is evident that the quantity S is larger when there is much overlap between the basis elements of $\mathcal{V}^\perp$ as opposed to when they are orthogonal. In the Heisenberg picture the time-evolution of the system resides solely in the basis elements, so this proposition can be taken as suggesting a link between increasing values of S and mixing between the basis elements. It also follows from Eq (...) that if the basis is ortho-normal *and* $\cos\tau = 1$ then $\sum_{i\neq j}\theta_j h_i = 0$.

4.2.5 Availability of Work

The concept of entropy was intially introduced to quantify the extent of energy degradation, in the sense that the energy available for performing work satisfies the equation $A = E - TS$, where T is the temperature (with $[T] = \mathrm{K}$) and S the entropy (with $[S] = \mathrm{J/K}$), and their product the degraded part of the total energy. We make the identifications $A = \mathcal{O}$ and $TS = \mathcal{U}$. But how can we write $\mathcal{U}$ as a product of two terms to be identified with temperature and entropy respectively? We have the following clue from classical thermodynamics: if the energy of the system remains constant, but the entropy increases due to some internal irreversible process, then the loss of available work satisfies $-dA = TdS$. In our case we have for an isolated system

$$-d\mathcal{O} = ||\hat{H}_{V^\perp}||d(||\hat{\rho}_u||\cos\tau).$$

The term within the differential is the quantity S defined in the previous section. This suggests that in the framework presented in this thesis, the norm $||\hat{H}_{V^\perp}||$ plays the role of a temperature function, an identification that has some intuitive appeal, as this would imply that temperature is the magnitude of the component of the energy operator along the unobservable degrees of freedom. If this identification is correct would have to be determined by showing that it in fact equals T for a variety of known paradigmatic cases. Whether this is so is outside of the scope of this thesis, but it stands as an intriguing possibility. However, it also accords with the definition $S = \frac{\mathcal{U}}{||\hat{H}_{V^\perp}||}$, as in classical thermodynamics, a given amount of thermal energy has a lower entropy if it exists at a higher temperature as compared to the same amount at a lower temperature.

4.2.6 Integrating Factors for the Heat Flows

Another way of ascertaining possible candidates for the temperature and entropy functions comes from the search for integrating factors for the (inexact) external heat flow. In classical thermodynamics, the existence of the entropy is equivalent to the integrability of the external heat flow, namely the existence of an integrating factor T^{-1} for $đQ_E$, such that $dS = T^{-1}đQ_E$ is the exact differential of a state function S. The integrating factor is identified with the inverse temperature, and the resulting state function with the entropy. The above equality holds only in the absence of internal heat production, and in general $dS \geq T^{-1}đQ_E$. This is known as *Clausius' theorem.* In this section we'll show that an analogous statement can be made using Definition 4 for the heat flows. It is worth noting that the integrating factor for $đQ_E$ is not unique in classical thermodynamics, so there exists a variety of definitions for temperature and entropy. For a discussion of these issues, see [20].

We begin by defining additional generalized angles using the Hilbert-Schmidt inner-product, similarly to how we defined τ. Besides τ we also define the angles

$$\phi(t) \triangleq \arccos\left\{\frac{\langle \dot{\hat{H}}_{V^\perp}, \hat{\rho}_u \rangle}{||\dot{\hat{H}}_{V^\perp}||||\hat{\rho}_u||}\right\}, \qquad \psi(t) \triangleq \arccos\left\{\frac{\langle \dot{\hat{H}}_{V^\perp}, \hat{H}_{V^\perp} \rangle}{||\dot{\hat{H}}_{V^\perp}||||\hat{H}_{V^\perp}||}\right\}.$$

With these definitions in place, we can formulate the analogue of Clausius' theorem for our theory of heat and work.

Theorem 5. (Analogue of Clausius' Theorem) *The time-derivative of S is related to the internal and external heat flows by the equation*

$$\dot{S} = \frac{1}{||\hat{H}_{V^\perp}||}\frac{đQ_I}{đt} + \left(\frac{1}{||\hat{H}_{V^\perp}||} - \frac{1}{2}\frac{\cos\tau\cos\psi}{\cos\phi}\right)\frac{đQ_E}{đt}.$$

Proof : Consider the external heat flow

$$\frac{đQ_E}{đt} = ||\dot{\hat{H}}_{V^\perp}||||\hat{\rho}_u||\cos\phi.$$

We now make use of the identity

$$\frac{d}{dt}||\hat{H}_{V^\perp}|| = \frac{1}{2}\langle \dot{\hat{H}}_{V^\perp}, \hat{H}_{V^\perp} \rangle = \frac{1}{2}||\dot{\hat{H}}_{V^\perp}||||\hat{H}_{V^\perp}||\cos\psi \tag{4.3}$$

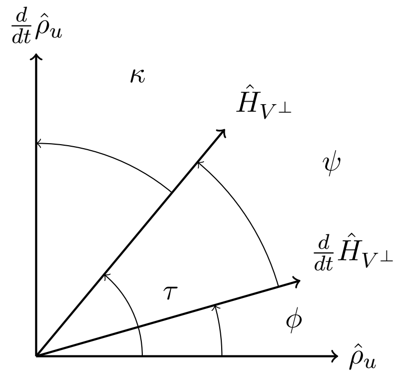

Figure 4.2: Diagram showing how the various Hilbert-Schmidt angles are defined.

to eliminate the factor $||\dot{\hat{H}}_{V^\perp}||$ from the external heat flow and obtain

$$\frac{đQ_E}{đt} = 2\frac{||\hat{\rho}_u||}{||\hat{H}_{V^\perp}||}\frac{\cos\phi}{\cos\psi}\frac{d}{dt}||\hat{H}_{V^\perp}||,$$

or equivalently

$$\frac{d}{dt}\log||\hat{H}_{V^\perp}|| = \frac{1}{2}\frac{1}{||\hat{\rho}_u||}\frac{\cos\psi}{\cos\phi}\frac{đQ_E}{đt}.$$

We now see that the external heat flow has an integrating factor making it the total derivative of $\log||\hat{H}_{V^\perp}||$. However, we are looking for an entropy candidate that also depends on the internal heat flow. The time-derivative of S is given by

$$\dot{S} = \frac{1}{||\hat{H}_{V^\perp}||^2}\left(\dot{\mathcal{U}}||\hat{H}_{V^\perp}|| - \mathcal{U}\frac{d}{dt}||\hat{H}_{V^\perp}||\right) = \frac{\dot{\mathcal{U}}}{||\hat{H}_{V^\perp}||} - S\frac{d}{dt}\log||\hat{H}_{V^\perp}|| =$$
$$\frac{1}{||\hat{H}_{V^\perp}||}\left(\frac{đQ_E}{đt} + \frac{đQ_I}{đt}\right) - \frac{1}{2}\frac{\cos\tau\cos\psi}{\cos\phi}\frac{đQ_E}{đt},$$

Gathering terms we arrive at the final result. □

We see that $||\hat{H}_{V^\perp}||^{-1}$ is an integrating factor for the internal heat flow (in the absence of external flows), and approximately an integrating factor for the external heat flow as well (in the absence of internal flows) when either the fractional change $||\hat{H}_{V^\perp}||^{-1}\frac{d}{dt}||\hat{H}_{V^\perp}||$ (the "isothermal" case), or S, is small.

4.2.7 A Simple Heat Engine

A perennial problem of thermodynamics is the analysis of machines converting thermal into mechanical energy, and vice versa, and of the efficiency of

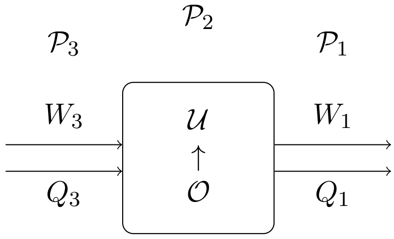

Figure 4.3: Diagram of the process $\mathcal{P}_3 \circ \mathcal{P}_2 \circ \mathcal{P}_1$, from right to left. The box represents the quantum system at hand.

such interconversions. In this section we will design a simple engine that converts heat into work, and derive an equation for its efficiency. We take a *machine state* to be any tuple that specifies uniquely the observable and unobservable energies, which we can represent in the form

$$\mathcal{U} = ||\hat{H}_{V^\perp}||||\hat{\rho}_u|| \cos\tau,$$
$$\mathcal{O} = ||\hat{H}_V||||\hat{\rho}_o|| \cos o.$$

Here we define a machine state to be a quadruple $(||\hat{H}_{V^\perp}||, ||\hat{H}_V||, S, \tilde{o})$, where S is defined as in Eq (4.1) and $\tilde{o} \triangleq ||\hat{\rho}_o|| \cos o$. The total heat and work transfers for any process is given by the integrals of the differential flows

$$\int_{t_i}^{t_f} \frac{d}{dt}\Big\{||\hat{H}_{V^\perp}(t)||S(t)\Big\}dt + \int_{t_i}^{t_f} \frac{d}{dt}\Big\{||\hat{H}_V(t)||\tilde{o}(t)\Big\}dt = \Delta E,$$

where ΔE is the total energy exchange with the control apparatus during the process. Now consider a three-step process $\mathcal{P} = \mathcal{P}_3 \circ \mathcal{P}_2 \circ \mathcal{P}_1$ consisting of the mappings

$$\mathcal{P}_1 : (||\hat{H}^i_{V^\perp}||, ||\hat{H}^i_V||, S^i, \tilde{o}^i) \longmapsto (||\hat{H}^f_{V^\perp}||, ||\hat{H}^f_V||, S^i, \tilde{o}^i),$$
$$\mathcal{P}_2 : (||\hat{H}^f_{V^\perp}||, ||\hat{H}^f_V||, S^i, \tilde{o}^i) \longmapsto (||\hat{H}^f_{V^\perp}||, ||\hat{H}^f_V||, S^f, \tilde{o}^f),$$
$$\mathcal{P}_3 : (||\hat{H}^f_{V^\perp}||, ||\hat{H}^f_V||, S^f, \tilde{o}^f) \longmapsto (||\hat{H}^i_{V^\perp}||, ||\hat{H}^i_V||, S^f, \tilde{o}^f).$$

Steps one and three represent energy exchanges with the control apparatus, while step two involves a transfer of energy between $\mathcal{U}$ and $\mathcal{O}$ while preserving the total. What this process accomplishes is a transformation of external heat flow into external work flow, at the cost of internal heat production during $\mathcal{P}_2$. We start with the map $\hat{H}^i \mapsto \hat{H}^f$, then allow the system to thermalize, and end the process by applying the inverse map $\hat{H}^f \mapsto \hat{H}^i$.

We assume that $||\hat{H}^f_{V^\perp}|| \leq ||\hat{H}^i_{V^\perp}||$ and $||\hat{H}^f_V|| \leq ||\hat{H}^i_V||$, so that in the initial step heat and work are extracted from the system, and inserted in the final step. The heat and work transfers during the three processes are

$$Q_1 = S^i\big(||\hat{H}^f_{V^\perp}|| - ||\hat{H}^i_{V^\perp}||\big), \qquad W_1 = \tilde{o}^i\big(||\hat{H}^f_V|| - ||\hat{H}^i_V||\big),$$
$$Q_2 = ||\hat{H}^f_{V^\perp}||\big(S^f - S^i\big), \qquad W_2 = ||\hat{H}^f_V||\big(\tilde{o}^f - \tilde{o}^i\big),$$
$$Q_3 = -S^f\big(||\hat{H}^f_{V^\perp}|| - ||\hat{H}^i_{V^\perp}||\big), \qquad W_3 = -\tilde{o}^f\big(||\hat{H}^f_V|| - ||\hat{H}^i_V||\big).$$

They satisfy the energy balance equations

$$\Delta E_1 = W_1 + Q_1, \qquad Q_2 = -W_2, \qquad \Delta E_3 = W_3 + Q_3.$$

The thermal efficiency is defined as the ratio of the net work extracted, in this case $|W_3| - |W_1|$ [3], to the net heat supplied, here $|Q_3| - |Q_1|$. Using the above heat, work, and energy balance equations, and some elementary algebraic manipulations, we arrive at the efficiency

$$\eta' = \frac{|W_3| - |W_1|}{|Q_3| - |Q_1|} = \frac{1 - \frac{||\hat{H}^i_V||}{||\hat{H}^f_V||}}{1 - \frac{||\hat{H}^i_{V^\perp}||}{||\hat{H}^f_{V^\perp}||}}.$$

This quantity depends on the two term ΔE_1 and ΔE_3. Here we are interested in the efficiency of *full conversion* relative to the internal heat production Q_2, so we'll set $\Delta E_1 = -\Delta E_3$. That is, there is no net energy supplied or gained, only interconversion between W and Q. The energy balance equations for steps 1 and 3 then imply that $\eta' = 1$. For the efficiency we are interested in, namely the work obtained relative to the internal heat production Q_2, we have

$$\eta = \frac{|W_3| - |W_1|}{|Q_2|} = \frac{||\hat{H}^f_V|| - ||\hat{H}^i_V||}{||\hat{H}^f_{V^\perp}||}\,\frac{\tilde{o}^f - \tilde{o}^i}{S^f - S^i}.$$

We now exploit the energy balance equation for $\mathcal{P}_2$ to obtain

$$\frac{\tilde{o}^f - \tilde{o}^i}{S^f - S^i} = \frac{||\hat{H}^f_{V^\perp}||}{||\hat{H}^f_V||},$$

which implies that $\eta = 1 - \frac{||\hat{H}^i_V||}{||\hat{H}^f_V||}$. Now note that $\eta' = 1$ to arrive at the final result

$$\eta = 1 - \frac{||\hat{H}^i_{V^\perp}||}{||\hat{H}^f_{V^\perp}||}.$$

[3] The absolute-value functions come from sign conventions. In the above, energy is counted as positive if it enters the system, and negative if it leaves it. But when calculating the efficiency, we count work that we *put in* as negative, and work that we *recieve* as positive.

In conclusion, external heat flows can be converted into external work flows, provided we have a repository of low S that pays the price in terms of internal heat production. The efficiency of that conversion increases as we decrease the ratio of Hamiltonian norms that the repository is subject to during the process. However, we have not proven that the above process *optimizes* the heat-work conversion; there could possibly be another process that achives a higher efficiency.

This result is strongly reminiscent of the Carnot efficiency $\eta = 1 - \frac{T_c}{T_h}$, which states that the efficiency is made better provided we work between larger temperature differences.

4.2.8 Work Flows for Pure States

A feature of work flows for pure states is the explicit appearance of the Fisher information. Consider the expansion of the components $\hat{H}_V$ and $\hat{\rho}_o$ in $\mathcal{V}$ in the basis $\{\hat{V}_k\}_{k=1}^{\dim\mathcal{V}}$

$$\hat{H}_V = \sum_{k=1}^{\dim\mathcal{V}} h_k \hat{V}_k, \qquad \hat{\rho}_o = \sum_{j=1}^{\dim\mathcal{V}} \theta_j \hat{V}_j,$$

where $h_k \triangleq \langle \hat{H}, \hat{V}_k \rangle$ and $\theta_j \triangleq \langle \hat{\rho}, \hat{V}_j \rangle$. Using the bilinearity and conjugate symmetry of the inner-product we can write the observable energy in the form

$$\mathcal{O} = \langle \hat{H}_V, \hat{\rho}_o \rangle = \left\langle \sum_{k=1}^{\dim\mathcal{V}} h_k \hat{V}_k, \sum_{j=1}^{\dim\mathcal{V}} \theta_j \hat{V}_j \right\rangle = \sum_{k=1}^{\dim\mathcal{V}} \sum_{j=1}^{\dim\mathcal{V}} h_k^* \theta_j \langle \hat{V}_k, \hat{V}_j \rangle.$$

For pure quantum states the inner products satisfy $\langle \hat{V}_k, \hat{V}_j \rangle = F_{kj}$. Introducing the matrix $\Theta_{kj} \triangleq h_k^* \theta_j$, we can write $\mathcal{O} = \langle \Theta, F \rangle$. Noting that the norm of its time-derivative is $||\dot{\Theta}|| = \sum_{ij} |h_k|^2 |\dot{\theta}_j|^2$ we obtain an upper bound for the rate of change of S for a closed pure system

$$|\dot{S}| \leq \sum_{kj} |h_k|^2 |\dot{\theta}_j|^2 \frac{||F||}{||\hat{H}_{V^\perp}||}.$$

The Fisher information has previously been shown to bound the entropy change for a variety of systems [21] [22], so this can be taken to be another suggestion that S is indeed related to the thermodynamic entropy.

Considering the observable energy as a function of the θ-parameters $\mathcal{O} = \mathcal{O}(\theta_1, \theta_2, ..., \theta_{\dim\mathcal{V}})$ we have the partial derivatives

$$\frac{\partial \mathcal{O}}{\partial \theta_k} = \sum_{j=1}^{\dim\mathcal{V}} h_j F_{kj}.$$

The Fisher information is closely related to thermal response functions [23], so its appearance here is not suprising.

4.2.9 Structural Constraints on Heat and Work Flows

We will now investigate how the heat-work decomposition, and energy flows in observable and unobservable subspaces, are constrained by algebraic properties of the dynamical and observation algebras. To give us enough mathematical structure to work with we'll assume the thermodynamically pertinent case where the measured observable is an element of the dynamical Lie algebra, in which case the observation algebra is an ideal. We begin by considering the case where $\mathcal{L}$ is simple.

Simple Lie Algebras

Since $\mathcal{V} \subseteq \mathcal{L}$ is an invariant subalgebra, the simplicity of $\mathcal{L}$ gives us only two possibilities : either $\mathcal{V} = \mathcal{L}$ or $\mathcal{V} = 0$. In the latter case, since $\hat{\rho}_o = 0$, all energy changes appear as heat transfers : $\frac{d}{dt}\langle \hat{H} \rangle_{\hat{\rho}} = \dot{Q}$. In the first case, we note that $\hat{H}_{V^\perp} = 0$, and so $\frac{d}{dt}\langle \hat{H} \rangle_{\hat{\rho}} = \dot{W}$. To obtain a non-trivial decomposition, we need to move on to more complicated dynamical algebras than simple ones. We will now consider semi-simple Lie algebras.

Semi-simple Lie Algebras

Let $\mathcal{L}$ be a semi-simple Lie algebra with a decomposition into simple ideals $\mathcal{L} = l_1 \oplus ... \oplus l_{k'}$ where $[l_k, l_j] = 0$ for $k \neq j$. Any ideal, in this particular case $\mathcal{V}$, is a direct sum of some of the simple ideals in the above decomposition. So we will re-label the above ideals and write

$$\mathcal{L} = v_1 \oplus ... \oplus v_m \oplus l_1 \oplus ... \oplus l_{m'} = \mathcal{V} \oplus l,$$

where $\mathcal{V} \triangleq v_1 \oplus ... \oplus v_m$ and $l \triangleq l_1 \oplus ... \oplus l_{m'}$. Using this decomposition we can factorize any given time-evolution operator $\hat{U}_t \in e^{\mathcal{L}}$ as $\hat{U}_t = \hat{V}_t \hat{L}_t$, where $\hat{V}_t \in e^{\mathcal{V}}$ and $\hat{L}_t \in e^{l}$. A given time-evolved state is then given by

$$\hat{\rho}(t) = \hat{V}_t \hat{L}_t \hat{\rho}_o \hat{L}_t^\dagger \hat{V}_t^\dagger + \hat{V}_t \hat{L}_t \hat{\rho}_u \hat{L}_t^\dagger \hat{V}_t^\dagger.$$

The evolution operators $\hat{V}_t$ and $\hat{L}_t$ can in turn be factorized into products of operators from the normal subgroups of $e^{\mathcal{V}}$ and e^{l} corresponding to each ideal in the direct sums of $\mathcal{V}$ and l respectively. The first term can be simplified using the fact that $[\hat{V}_t, \hat{L}_t] = [\hat{\rho}_o, \hat{L}_t] = 0$. The second term can not be simplified in the same way at this point, since $[\hat{\rho}_u, \hat{V}_t] \neq 0$ in general. If we decompose the Hamiltonian as $\hat{H} = \hat{H}_V + \hat{H}_L$, where $\hat{H}_V \in \mathcal{V}$ and $\hat{H}_L \in L$, we can write the energy at time t as

$$\langle \hat{H}(t) \rangle_{\hat{\rho}} = \big\langle \hat{H}_V, \hat{V}_t \hat{\rho}_o \hat{V}_t^\dagger \big\rangle + \big\langle \hat{H}_L, \hat{V}_t \hat{L}_t \hat{\rho}_u \hat{L}_t^\dagger \hat{V}_t^\dagger \big\rangle.$$

The cyclic property of the trace, together with the vanishing commutator $[\hat{H}_L, \hat{V}_t] = 0$ means that the operator $\hat{V}_t$ can be eliminated from the second term. We obtain the energy equation

$$\langle \hat{H}(t)\rangle_{\hat{\rho}} = \big\langle \hat{H}_V, \hat{V}_t \hat{\rho}_o \hat{V}_t^\dagger \big\rangle + \big\langle \hat{H}_L, \hat{L}_t \hat{\rho}_u \hat{L}_t^\dagger \big\rangle.$$

We can reveal further structure by factorizing the evolution operators, and decomposing $\hat{\rho}_o$ into a sum of elements from the ideals:

$$\hat{V}_t \hat{\rho}_o \hat{V}_t^\dagger = \hat{V}_{t,1}\hat{V}_{t,2}\ldots\hat{V}_{t,m}\big(\hat{\rho}_{o,1} + \hat{\rho}_{o,2} + \cdots + \hat{\rho}_{o,m}\big)\hat{V}_{t,m}^\dagger \ldots \hat{V}_{t,2}^\dagger \hat{V}_{t,1}^\dagger = \sum_{k=1}^{m} \hat{V}_{t,k}\hat{\rho}_{o,k}\hat{V}_{t,k}^\dagger.$$

The last line follows from the commutators $[\hat{V}_{t,k}, \hat{V}_{t,j}] = 0, \forall ij$ and $[\hat{V}_{t,k}, \hat{\rho}_{o,j}] = 0$ for $k \neq j$. We now decompose $\hat{H}_V$ as well

$$\mathcal{O} = \sum_{k=1}^{m}\sum_{j=1}^{m} \big\langle \hat{H}_{V,j}, \hat{V}_{t,k}\hat{\rho}_{o,k}\hat{V}_{t,k}^\dagger \big\rangle.$$

One final simplification can be made. When $k \neq j$ the evolution operator $\hat{V}_{t,k}$ can be commuted past $\hat{H}_{V,j}$ to its left, after which we can use the cyclic property of the trace to bring it to the right of $\hat{V}_{t,k}^\dagger$, eliminating them both by unitarity. We now obtain the final form of the observable energy

$$\mathcal{O} = \sum_{k,j=1\ k\neq j}^{m} \big\langle \hat{H}_{V,j}, \hat{\rho}_{o,k} \big\rangle + \sum_{p=1}^{m} \big\langle \hat{H}_{V,p}, \hat{V}_{t,p}\hat{\rho}_{o,p}\hat{V}_{t,p}^\dagger \big\rangle.$$

This reveals an interesting feature: the cross terms are constant as the state undergoes time-evolution, and can only be changed by modifying the Hamiltonian. The same procedure can be performed for the unobservable energy with a couple of differences. As before, we cannot commute anything past $\hat{\rho}_u$, and the simplifications only occur inside the inner product by the cyclic property of the trace ; also the state $\hat{\rho}_u$ itself does not admit any decompositions in general. We then get

$$\mathcal{U} = \sum_{k=1}^{m'} \big\langle \hat{H}_{L,k}, \hat{L}_{t,k}\hat{\rho}_u \hat{L}_{t,k}^\dagger \big\rangle.$$

This concludes our analysis of the semi-simple case, and we will now move on to solvable Lie algebras.

Solvable Lie Algebras

Let $\mathcal{L}$ be solvable, in which case $\mathcal{V} \subseteq \mathcal{L}$ is a solvable ideal. As will be seen, the main feature here is that as far as the energy is concerned, the observability space can be taken to be one-dimensional. The dynamical Lie algebra has the decomposition $\mathcal{L} = \mathcal{V} \oplus (\mathcal{V}^\perp)_\mathcal{L}$, where $(\mathcal{V}^\perp)_\mathcal{L}$ is an arbitrary complement in $\mathcal{L}$ which furthermore satisfies the isomorphism $(\mathcal{V}^\perp)_\mathcal{L} \simeq \mathcal{L}/\mathcal{V}$. Anticipating application of Cartan's solvability criterion, we write the observability space in the form

$$\mathcal{V} = \text{span}\{i\hat{S}'\} \oplus \big([\mathcal{L}, \mathcal{L}] \cap \mathcal{V}\big),$$

and write the observable state-component as $\hat{\rho}_o(t) = f(t)\hat{S}' + \hat{\sigma}_o(t)$, where $\hat{\sigma}_o(t) \in [\mathcal{L}, \mathcal{L}] \cap \mathcal{V}$ and $f : \mathbb{R}_{\geq 0} \to \mathbb{C}$. As before, we decompose the Hamiltonian operator as $\hat{H} = \hat{H}_V + \hat{H}_L$ where $\hat{H}_V \in \mathcal{V}$ and $\hat{H}_L \in (\mathcal{V}^\perp)_\mathcal{L}$. A given time-evolution operator decomposes as $\hat{U}_t = \hat{V}_t\hat{L}_t$, where $\hat{V} \in e^{\mathcal{V}}$ and $\hat{L}_t$ is a product of elements of $e^{(\mathcal{V}^\perp)_\mathcal{L}}$. If, moreover, $(\mathcal{V}^\perp)_\mathcal{L}$ is a subalgebra of $\mathcal{L}$ then $\hat{L}_t \in e^{(\mathcal{V}^\perp)_\mathcal{L}}$. The energy at time t is given by

$$\langle \hat{H} \rangle_{\hat{\rho}} = \langle \hat{H}_V, \hat{\rho}_o \rangle + \langle \hat{H}_L, \hat{\rho}_u \rangle.$$

Since $\hat{H}_V \in \mathcal{L}$, and $\hat{\sigma}(t) \in [\mathcal{L}, \mathcal{L}]$, the Cartan solvability criterion implies that $\langle \hat{H}_V, \hat{\sigma}_o \rangle = 0$. This gives us the observable energy

$$\mathcal{O} = f(t)\langle \hat{H}_V, \hat{S}' \rangle.$$

We note that $\hat{H}_V$, being an element of $\mathcal{V}$, will be proportional to $\hat{S}'$. If we are considering a pure quantum state, we can use Proposition 2 and write the observable energy as

$$\mathcal{O} = \tilde{f}(t)F,$$

where the proportionality constant of $\hat{H}_V$ has been absorbed into $\tilde{f}$, and $F \in \mathbb{R}$ is the Fisher information. We now state this result as a proposition.

Proposition 9. (Observable Energy is Proportional to the Fisher Information) *If for a given quantum control system Σ we have $\hat{S} \in \mathcal{L}$, and if the state is pure and $\mathcal{L}$ is solvable, then $\mathcal{O} \propto F$.*

Further structure can be ascertained by using the Lie-Kochin triangularization theorem, which states that the entire image $\pi(e^{\mathcal{L}})$ is simultaneously upper triangularizable when $\mathcal{L}$ is solvable. This implies that with respect to a suitable basis, every operator $U_t \in e^{\mathcal{L}}$ is upper-triangular. Since they are also unitary, they in fact have to be diagonal in this basis.

4.2.10 Temperature and Entropy

We will now summarize the arguments for identifying $||\hat{H}_{V^\perp}||$ as the temperature, and S as the entropy. These arguments, of course, hinges upon the identifications of the heat and work flows being acceptable.

- $||\hat{H}_{V^\perp}||$ is an integrating factor for the internal heat flow (individually), and an approximate integrating factor for the external one, making the heat flows the total derivative of S. That is, they appear to be related to each other and the heat flows in a way similar to the classical variables in Clausius' theorem.

- In classical thermodynamics the temperature is often defined as

$$\left(\frac{\partial S}{\partial E}\right)_V = \frac{1}{T},$$

where the partial derivative is taken with respect to energy, as the volume is held constant. If instead of holding the volume constant, we choose to hold $\mathcal{O}$ constant, or some observable parameter on which $\mathcal{O}$ solely depends, then

$$\left(\frac{\partial S}{\partial E}\right)_{\mathcal{O}} = \frac{1}{||\hat{H}_{V^\perp}||}.$$

- The function $\cos\tau$ provides an intuitive formalization of the informal notion of "energy degradation", as it quantifies the extent to which the systems energy resides in the unobservable subspace. The energy $\mathcal{U}$ is taken to be "degraded", since lack of knowledge about $\hat{\rho}_u$ makes it difficult, although theoretically possible using a lucky guess, to design an appropriate control function to extract the energy residing therein. It is also bounded, and if $\dim\mathcal{V}^\perp >> \dim\mathcal{V}$, and there is sufficient interaction between the observable and unobservable degrees of freedom, it can be expected to increase on average.

- Aside from being related to state underdetermination, S is proportional to something with units of energy, making it a candidate for a truly *thermodynamic* entropy (with units of J/K), and not just an information-theoretic one (with units of bits). The conceptualization of temperature as the magnitude of the component of the energy operator along the unobservable subspace also has some intuitive appeal. This would mean that temperature is a quantity which sets the scale for the unobservable energy, but is not identical to it. Explicitly, we have $\mathcal{U} = TS$.

- For pure states, the rate of change of S is bounded from above by something proportional to the Fisher information.

Chapter 5

Applications

We will now illustrate the concepts developed in the previous chapter by deploying them for an analysis of the Ising model, as well as showing how Theorem 4 can be used to factorize the time-translation operator and simplify the resulting equations by applying it to the limited access scenario described in section (2.2.1). We begin with the Ising model. This particular model is chosen partly for its computational tractability, but also since it is commonly used to illustrate thermodynamic concepts and every physicist is familiar with it.

5.1 A Concrete Example : The Ising Model

We will now see how the heat-work decomposition is performed in practice, and show explicitly how it depends on the availability of control resources. First, we consider two spin-1/2 particles with Ising interaction, with a constant magnetic field along the z-axis, and arbitrary fields applied along the x and y axes as controls. As a further control, we're able to tune the interaction strength γ between the two spins. We then have the operator Schrödinger equation

$$\frac{d}{dt}\hat{U} = -i\left\{\gamma(t)\hat{\sigma}_z \otimes \hat{\sigma}_z + \sum_{l=x,y} \hat{\sigma}_l \otimes \hat{I}u_l(t) + \sum_{l=x,y} \hat{I} \otimes \hat{\sigma}_l u_l(t)\right\}\hat{U},$$

where the Pauli matrices are defined as follows

$$\hat{\sigma}_x \triangleq \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y \triangleq \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z \triangleq \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and $\hat{I}$ is the 2×2 identity matrix. We assume that the control fields couple identically to both spins, implying that any transformation actuated on one acts the same on the other. We now proceed to compute the dynamical Lie algebra. We start off with the following basis elements

$$\hat{B}_1 \triangleq i\hat{\sigma}_z \otimes \hat{\sigma}_z,$$
$$\hat{B}_{2,3,4} \triangleq i\hat{I} \otimes \hat{\sigma}_{x,y,z} + i\hat{\sigma}_{x,y,z} \otimes \hat{I}.$$

The commutators of depth one gives us two additional basis elements

$$\hat{B}_5 \triangleq \mathrm{ad}_{\hat{B}_1}(\hat{B}_2) = -i\hat{\sigma}_z \otimes \hat{\sigma}_y - i\hat{\sigma}_y \otimes \hat{\sigma}_z,$$
$$\hat{B}_6 \triangleq \mathrm{ad}_{\hat{B}_1}(\hat{B}_3) = i\hat{\sigma}_z \otimes \hat{\sigma}_x + i\hat{\sigma}_x \otimes \hat{\sigma}_z.$$

The depth-two commutators are

$$\hat{B}_7 \triangleq \mathrm{ad}_{\hat{B}_2}(\hat{B}_6) = i\hat{\sigma}_x \otimes \hat{\sigma}_y + i\hat{\sigma}_y \otimes \hat{\sigma}_x,$$
$$\hat{B}_8 \triangleq \mathrm{ad}_{\hat{B}_2}(\hat{B}_5) = 2i\hat{\sigma}_z \otimes \hat{\sigma}_z - 2i\hat{\sigma}_y \otimes \hat{\sigma}_y.$$

The only depth-three commutator that generates a new basis element is

$$\hat{B}_9 \triangleq \mathrm{ad}_{\hat{B}_1}(\hat{B}_8) = -2i\hat{\sigma}_x \otimes \hat{\sigma}_x.$$

No other commutators generate new linearly independent elements. We conclude that the dynamical Lie algebra is given by

$$i\mathcal{L} = \mathrm{span}\{\hat{\sigma}_{x,y,z} \otimes \hat{\sigma}_{x,y,z}, \hat{\sigma}_{x,y,z} \otimes \hat{I} + \hat{I} \otimes \hat{\sigma}_{x,y,x}, \hat{\sigma}_z \otimes \hat{\sigma}_y + \hat{\sigma}_y \otimes \hat{\sigma}_z$$
$$\hat{\sigma}_z \otimes \hat{\sigma}_x + \hat{\sigma}_x \otimes \hat{\sigma}_z, \hat{\sigma}_x \otimes \hat{\sigma}_y + \hat{\sigma}_y \otimes \hat{\sigma}_x\},$$

and $\dim(\mathcal{L}) = 9$. The lack of operator controllability comes from the fact that the fields couple identically to both spins, which results in a dynamical Lie group generated by the magnetic fields given by

$$\{\hat{X} \otimes \hat{X} : \hat{X} \in SU(2)\}.$$

If the coupling constants were different for the two spins the magnetic fields would instead be able to effect any transformation from the set

$$\{\hat{X}_1 \otimes \hat{X}_2 : \hat{X}_1, \hat{X}_2 \in SU(2)\},$$

and the full dynamical Lie algebra would be given by $su(4)$. The measured observable is the total magnetization along the z-axis, i.e. $\hat{S} = \hat{I} \otimes \hat{\sigma}_z + \hat{\sigma}_z \otimes \hat{I}$. The observation space

$$\mathcal{V} = \bigoplus_{j=0}^{\infty} \mathrm{ad}^j_{\mathcal{L}} \mathrm{span}\{i\hat{I} \otimes \hat{\sigma}_z + i\hat{\sigma}_z \otimes \hat{I}\},$$

is the ideal of $\mathcal{L}$ generated by the element $\hat{S} \in \mathcal{L}$. As it turns out, $\mathcal{V} = \mathcal{L}$, and so $\langle \hat{H} \rangle_{\hat{\rho}} = \mathcal{O}$ with $\mathcal{U} = 0$. With these control resources all energy residing in the system is observable "high grade" energy with the "entropic" part of the energy vanishing. We will now see how the situation changes when we reduce the control resources at our disposal.

Now consider the same scenario, but with our control options restricted to modulating the interaction strength between the two spins, and to applying a magnetic field along the x-axis to *one* of the spins only. We then have the Schrödinger equation

$$\frac{d}{dt}\hat{U} = -i\Big\{\gamma(t)\hat{\sigma}_z \otimes \hat{\sigma}_z + \hat{I} \otimes \hat{\sigma}_x u(t)\Big\}\hat{U}.$$

The dynamical Lie algebra is given by

$$\mathcal{L} = \text{span}\big\{i\hat{\sigma}_z \otimes \hat{\sigma}_z, i\hat{I} \otimes \hat{\sigma}_x, i\hat{\sigma}_z \otimes \hat{\sigma}_y\big\},$$

and $\dim(\mathcal{L}) = 3$. We measure the same observable as before. All Lie brackets of $i\hat{S}$ taken with a single generator of $\mathcal{L}$ are listed below

$$\begin{aligned} \text{ad}_{i\hat{\sigma}_z\otimes\hat{\sigma}_z}(i\hat{S}) &= 0, & \text{ad}_{i\hat{I}\otimes\hat{\sigma}_x}(i\hat{S}) &= i\hat{I} \otimes \hat{\sigma}_y, \\ \text{ad}^2_{i\hat{I}\otimes\hat{\sigma}_x}(i\hat{S}) &= -i\hat{I} \otimes \hat{\sigma}_z, & \text{ad}^3_{i\hat{I}\otimes\hat{\sigma}_x}(i\hat{S}) &= -\text{ad}_{i\hat{I}\otimes\hat{\sigma}_x}(i\hat{S}), \\ \text{ad}_{i\hat{\sigma}_z\otimes\hat{\sigma}_y}(i\hat{S}) &= -i\hat{\sigma}_z \otimes \hat{\sigma}_x, & \text{ad}^2_{i\hat{\sigma}_z\otimes\hat{\sigma}_y}(i\hat{S}) &= \text{ad}^2_{i\hat{I}\otimes\hat{\sigma}_x}(i\hat{S}). \end{aligned}$$

The Lie brackets with mixed generators all vanish. We conclude that the observation space is given by

$$i\mathcal{V} = \text{span}\{\hat{\sigma}_z \otimes \hat{I}, \hat{I} \otimes \hat{\sigma}_x, \hat{I} \otimes \hat{\sigma}_z, \hat{\sigma}_z \otimes \hat{\sigma}_x\},$$

and $\dim(\mathcal{V}) = 4$. Its orthogonal complement (in $su(4)$) is

$$i\mathcal{V}^{\perp} = \text{span}\{\hat{\sigma}_{x,y,z} \otimes \hat{\sigma}_{x,y,z}, \hat{\sigma}_{x,y} \otimes \hat{I}, \hat{I} \otimes \hat{\sigma}_y, \hat{\sigma}_{x,y} \otimes \hat{\sigma}_{y,x}, \hat{\sigma}_{y,z} \otimes \hat{\sigma}_{z,y}, \hat{\sigma}_x \otimes \hat{\sigma}_z\},$$

and $\dim(\mathcal{V}^{\perp}) = 11$. We now obtain a non-trivial decomposition of the energy into observable and unobservable parts

$$\begin{aligned} \mathcal{O} &= u(t)\text{Tr}\big\{\hat{I} \otimes \hat{\sigma}_x \hat{\rho}_o\big\}, \\ \mathcal{U} &= \gamma(t)\text{Tr}\big\{\hat{\sigma}_z \otimes \hat{\sigma}_z \hat{\rho}_u\big\}. \end{aligned}$$

The magnetic moment along the x-axis for the spin on which we apply the control field is the repository of observable energy. The unobservable energy resides in the Ising interaction between the two spins. The external work and heat flows resulting from a change in the Hamiltonian are

$$\begin{aligned} \frac{đW_E}{đt} &= \dot{u}(t)\text{Tr}\big\{\hat{I} \otimes \hat{\sigma}_x \hat{\rho}_o\big\}, \\ \frac{đQ_E}{đt} &= \dot{\gamma}(t)\text{Tr}\big\{\hat{\sigma}_z \otimes \hat{\sigma}_z \hat{\rho}_u\big\}. \end{aligned}$$

To compute the internal work flow we first expand $\hat{\rho}_o$ in the basis of $\mathcal{V}$. With the basis elements labeled as follows

$$\hat{V}_1 \triangleq \hat{I} \otimes \hat{\sigma}_z, \qquad \hat{V}_2 \triangleq \hat{I} \otimes \hat{\sigma}_x, \qquad \hat{V}_3 \triangleq \hat{\sigma}_z \otimes \hat{I}, \qquad \hat{V}_4 \triangleq \hat{\sigma}_z \otimes \hat{\sigma}_x,$$

the observable state-component can be written as

$$\hat{\rho}_o = \sum_{j=1}^{4} \langle \hat{\rho}(t=0), \hat{V}_j \rangle \hat{V}_j.$$

The time derivative of $\hat{\rho}_o$ is given by the Liouville-Von-Neumann equation

$$\frac{d}{dt}\hat{\rho}_o = -i[\hat{H}, \hat{\rho}_o] = -i \sum_{j=1}^{4} \langle \hat{\rho}(t=0), \hat{V}_j \rangle [\hat{H}, \hat{V}_j].$$

Computing the commutators inside the sum yields

$$[\hat{H}, \hat{V}_1] = -iu(t)\hat{I} \otimes \hat{\sigma}_y \in i\mathcal{V}^{\perp}, \qquad [\hat{H}, \hat{V}_2] = i\gamma(t)\hat{\sigma}_z \otimes \hat{\sigma}_y \in i\mathcal{V}^{\perp},$$
$$[\hat{H}, \hat{V}_3] = 0, \qquad [\hat{H}, \hat{V}_4] = i\gamma(t)\hat{I} \otimes \hat{\sigma}_y \in i\mathcal{V}^{\perp}.$$

As all three non-zero commutators are Hilbert-Schmidt orthogonal to $\hat{H}_V$, we can conclude that

$$\frac{đW_I}{đt} = \langle \hat{H}_V, \frac{d}{dt}\hat{\rho}_o \rangle = 0,$$

and consequently the internal heat flow must satisfy $đQ_I = 0$ as well, by conservation of energy. Evidently the observable and unobservable energies are constants of motion in this setting in the absence of explicit time-dependence in the Hamiltonian; thus we can state that when isolated the system will not thermalize.

The component of the Hamiltonian along the normalized bases of $i\mathcal{V}^{\perp}$, its time-derivative, and its norm are [1]

$$\hat{H}_{V^{\perp}} = \frac{\gamma(t)}{4}\hat{\sigma}_z \otimes \hat{\sigma}_z, \qquad \dot{\hat{H}}_{V^{\perp}} = \frac{\dot{\gamma}(t)}{4}\hat{\sigma}_z \otimes \hat{\sigma}_z, \qquad ||\hat{H}_{V^{\perp}}|| = \gamma(t).$$

We see that the temperature is given by the interaction strength γ; an intuitive result, since the interaction energy is unobservable. Eq. (4.1) then gives us $\cos\psi = 2/\gamma(t)$, which yields the entropy change

$$\dot{S} = \mathrm{Tr}\{\hat{\sigma}_z \otimes \hat{\sigma}_z \hat{\rho}_u\} \left(1 - \frac{\cos\tau}{\cos\phi}\right) \frac{d}{dt} \log\gamma(t).$$

[1] We see that $\hat{H}_{V^{\perp}} \in \mathcal{L}$, a fact that could also be used to conclude that $\frac{đW_I}{dt} = 0$, by Proposition 5.

Further unpacking of this equation would require knowledge of the exact value of $\hat{\rho}_u$.

The basis elements of the observation space are Hilbert-Schmidt orthogonal and satisfy $\hat{V}_i\hat{V}_j = \delta_{ij}\hat{I}\otimes\hat{I}$ and therefore $\langle\hat{V}_i, \hat{V}_j\rangle = 4\delta_{ij}$. Assuming the state is pure, Proposition 2 tells us that the Fisher information is given by $F = 4\hat{I}_{4\times 4}$, and thus the response of the observable energy to changes in (observable) parameter variations is

$$\frac{\partial\mathcal{O}}{\partial\theta_i} = \sum_{j=1}^{4} h_j F_{ij} = \sum_{j=1}^{4} 4h_j\delta_{ij} = 4h_i = 16u(t)\delta_{i2},$$

where the last equality follows from the fact that $h_2 = 4u(t)$ is the only non-zero component of the Hamiltonian along the basis elements of $i\mathcal{V}$.

Finally, we can note that since $\hat{H}_{V^\perp} \in \mathcal{L}$ both selective and non-selective measurements of $\hat{S}$ leave $\mathcal{U}$ invariant, by the results of section (4.2.3).

5.2 Heat and Work Flows in Bipartite Systems

We will now consider heat and work flows in the bipartite scenario described in section (2.2.1). As the output y we pick any local observable $\hat{S} = \hat{I}_{\mathcal{E}} \otimes \hat{S}_\Sigma$ on Σ. Decomposing the interaction Hamiltonian into connected and disconnected components we can write the total Hamiltonian as

$$\hat{H} = \hat{I}_{\mathcal{E}} \otimes \hat{H}_\Sigma + \hat{H}_{\mathcal{E}} \otimes \hat{I}_\Sigma + \hat{h}_d + \hat{h}_c.$$

Since $\hat{I}_{\mathcal{E}} \otimes \hat{S}_\Sigma$ is a local observable on Σ, the results of Proposition 3 applies, and we have

$$\mathcal{V} = \mathcal{L}_c, \qquad \mathcal{L}\cap\mathcal{L}_d \subseteq \mathcal{V}^\perp.$$

By Theorem 4 the time-evolution operator $\hat{U}$ can be decomposed as $\hat{U} = \hat{U}_c\hat{U}_d$, where $\hat{U}_c \in e^{\mathcal{L}_c}$ and $\hat{U}_d \in e^{\mathcal{L}_d}$, where $[\hat{U}_c, \hat{U}_c] = 0$. Consider the time-evolved density matrix under the observability decomposition $\hat{\rho} = \hat{\rho}_o + \hat{\rho}_u \in i\mathcal{V} \oplus i\mathcal{V}^\perp$

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}\hat{U}^\dagger(t) = \hat{U}_c(t)\hat{U}_d(t)(\hat{\rho}_o + \hat{\rho}_u)\hat{U}_d^\dagger(t)\hat{U}_c^\dagger(t).$$

The participating elements in the above equation satisfy the following set membership relations

$$\hat{\rho}_o \in i\mathcal{V}, \qquad \hat{\rho}_u \in i\mathcal{V}^\perp, \qquad \hat{U}_c \in e^{\mathcal{V}}, \qquad \hat{U}_d \in e^{\mathcal{V}^\perp\cap\mathcal{L}_d}.$$

Since $[\mathcal{L}_c, \mathcal{L}_d] = 0$, we have the following vanishing commutators

$$[\hat{\rho}_o, \hat{U}_d] = [\hat{\rho}_u, \hat{U}_c] = 0.$$

This allows a decomposition of the time-evolved density matrix into two terms, one observable and governed by the connected Lie algebra, and the other unobservable and governed by the disconnected Lie algebra. Explicitly

$$\hat{\rho}(t) = \hat{U}_c(t)\hat{\rho}_o\hat{U}_c^\dagger(t) + \hat{U}_d(t)\hat{\rho}_u\hat{U}_d^\dagger(t).$$

The energy of Σ is the sum of its local energy $\hat{I}_\mathcal{E} \otimes \hat{H}_\Sigma$ and the interaction energy $\hat{h}_c + \hat{h}_d$; we call this the *local energy.* Consider the time-evolution of its expectation value

$$\langle \hat{H}_{\text{loc}}(t)\rangle = \text{Tr}\big\{\hat{U}_c(t)\hat{\rho}_o\hat{U}_c^\dagger(t)(\hat{I}_\mathcal{E} \otimes \hat{H}_\Sigma + \hat{h}_c + \hat{h}_d)\big\} + \\ \text{Tr}\big\{\hat{U}_d(t)\hat{\rho}_o\hat{U}_d^\dagger(t)(\hat{I}_\mathcal{E} \otimes \hat{H}_\Sigma + \hat{h}_c + \hat{h}_d)\big\}.$$

We have the following implications

$$[\mathcal{L},\mathcal{V}] \subseteq \mathcal{V} \Longrightarrow \hat{U}_c(t)\hat{\rho}_o\hat{U}_c^\dagger(t) \in i\mathcal{V},$$
$$[\mathcal{L},\mathcal{V}^\perp] \subseteq \mathcal{V}^\perp \Longrightarrow \hat{U}_d(t)\hat{\rho}_u\hat{U}_d^\dagger(t) \in i\mathcal{V}^\perp.$$

As $\hat{I}_\mathcal{E} \otimes \hat{H}_\Sigma + \hat{h}_c \in \mathcal{V}$ and $\hat{h}_d \in \mathcal{V}^\perp \cap \mathcal{L}_d$, we have

$$\text{Tr}\big\{\hat{U}_c(t)\hat{\rho}_o\hat{U}_c^\dagger(t)\hat{h}_d\big\} = \text{Tr}\big\{\hat{U}_d(t)\hat{\rho}_o\hat{U}_d^\dagger(t)(\hat{I}_\mathcal{E} \otimes \hat{H}_\Sigma + \hat{h}_c)\big\} = 0.$$

The expectation value of $\hat{H}_{\text{loc}}$ now assumes the form

$$\langle \hat{H}_{\text{loc}}(t)\rangle = \text{Tr}\big\{\hat{U}_c(t)\hat{\rho}_o\hat{U}_c^\dagger(t)(\hat{I}_\mathcal{E} \otimes \hat{H}_\Sigma + \hat{h}_c)\big\} + \text{Tr}\big\{\hat{U}_d(t)\hat{\rho}_u\hat{U}_d^\dagger(t)\hat{h}_d\big\} = \\ \langle \hat{H}_{\text{loc}}(t)\rangle_{\hat{\rho}_o} + \langle \hat{H}_{\text{loc}}(t)\rangle_{\hat{\rho}_u}.$$

Here we have a decomposition of the total energy into one part which is both observable and controllable, and one part which is both unobservable and uncontrollable. In the absence of controls the work and heat flows are

$$\frac{dW_I}{dt} \triangleq \frac{d}{dt}\langle \hat{H}_{\text{loc}}(t)\rangle_{\hat{\rho}_o} = \text{Tr}\bigg\{\big(\frac{d}{dt}\hat{\rho}_o(t)\big)(\hat{I}_\mathcal{E} \otimes \hat{H}_\Sigma + \hat{h}_c)\bigg\},$$

and

$$\frac{dQ_I}{dt} \triangleq \frac{d}{dt}\langle \hat{H}_{\text{loc}}(t)\rangle_{\hat{\rho}_u} = \text{Tr}\bigg\{\big(\frac{d}{dt}\hat{\rho}_u(t)\big)\hat{h}_d\bigg\}.$$

The density matrices are governed by the Liouville-Von-Neumann equations

$$\frac{d}{dt}\hat{\rho}_o = -i\big[\hat{I}_\mathcal{E} \otimes \hat{H}_\Sigma + \hat{h}_c, \hat{\rho}_o\big], \qquad \frac{d}{dt}\hat{\rho}_u = -i\big[\hat{h}_d, \hat{\rho}_u\big].$$

If we apply external controls to Σ, the heat flow remains unchanged as the term $\hat{h}_d$ cannot be modified in this set-up. The work flow, however, acquires an additional term

$$\frac{dW}{dt} = \text{Tr}\bigg\{\big(\frac{d}{dt}\hat{\rho}_o(t)\big)(\hat{I}_\mathcal{E} \otimes \hat{H}_\Sigma(u))\bigg\} + \text{Tr}\bigg\{\hat{\rho}_o(t)\big(\hat{I}_\mathcal{E} \otimes \frac{d}{dt}\hat{H}_\Sigma(u) + \frac{d}{dt}\hat{h}_c\big)\bigg\}.$$

We can also consider the case where an external and uncontrollable perturbation $\hat{H}_p$ affects the combined system $\mathcal{H}_\mathcal{E} \otimes \mathcal{H}_\Sigma$. In the general case energy will be deposited into every subspace of the system. In the absence of controls on Σ the work and heat flows are

$$\frac{dW}{dt} = \mathrm{Tr}\Big\{ \big(\frac{d}{dt}\hat{\rho}_o(t)\big)(\hat{I}_\mathcal{E} \otimes \hat{H}_\Sigma + \hat{h}_c) \Big\} + \mathrm{Tr}\Big\{ \hat{\rho}_o(t)\big[\hat{H}_p, \hat{I}_\mathcal{E} \otimes \hat{H}_\Sigma + \hat{h}_c\big] \Big\},$$

$$\frac{dQ}{dt} = \mathrm{Tr}\Big\{ \big(\frac{d}{dt}\hat{\rho}_u(t)\big)\hat{h}_d \Big\} + \mathrm{Tr}\Big\{ \hat{\rho}_u(t)\big[\hat{H}_p, \hat{h}_d\big] \Big\}.$$

The dynamics on the subspaces $\mathcal{V}$ and $\mathcal{V}^\perp$ are governed by the equations

$$\frac{d}{dt}\hat{\rho}_o = -i\big[\hat{I}_\mathcal{E} \otimes \hat{H}_\Sigma + \hat{h}_c + \hat{H}_p, \hat{\rho}_o\big], \qquad \frac{d}{dt}\hat{\rho}_u = -i\big[\hat{h}_d + \hat{H}_p, \hat{\rho}_u\big].$$

Remark. It is worth investigating whether the observation space and its orthogonal complement are invariant under external uncontrollable (and Hermitian) perturbations $\hat{H}_p$, i.e whether

$$\big[\hat{H}_p, \mathcal{V}\big] \subseteq \mathcal{V}, \qquad \big[\hat{H}_p, \mathcal{V}^\perp\big] \subseteq \mathcal{V}^\perp.$$

If in general they were not, characterizing what perturbations cause transitions between the two subspaces would be of importance for analyzes of quantum thermalization, as it would illustrate effective thermalization brought about by unitary dynamics.

Chapter 6

Conclusions

We will now summarize the main arguments for why a cybernetic theory of heat and work should be considered.

- When identifying energy contributions as either heat or work in both the research litterature, and in standard textbooks on the subject, references are invariably made to the cybernetic notions of controllability and observability. Two common claims are that work is energy effected through parameters that are under our direct control, and that work is energy that corresponds to changes in parameters we can directly observe.

- Entropy is commonly understood with reference to state underdetermination, and that a higher entropy corresponds to a case where the observables we have access to gives less information about the internal state of the system. This is clearly connected to the cybernetic concept of observability.

- The fundamental laws of physics are time-reversible, while thermodynamic laws are irreversible. This is known as *Loschmidt's paradox*. One resolution of the paradox is that nature is fundamentally time-reversible, but that irreversibility is a practical reality due to control limitations. When Boltzmann heard of Loschmidt's objection to his theory, that theoretically the time-evolution could be reversed by reversing the sign of the Hamiltonian, he answered : *"Then try it!"*. The response would seem to imply that he suspects that irreversibility is a control-theoretic issue rather than a fundamental one.

- The standard resolution to the paradox of Maxwell's demon is that gathering information about every constituent particle of the system, storing it, and erasing it at the end of the process, would generate more entropy than the amount reduced by the demons control actuation. But *theoretically*, the demon could just guess the correct control function without gathering information at all. This again would seem to suggest that the second law, in some sense, is a statement about practical possibilities rather than fundamental limitations.

- As shown in Proposition 4, unobservability of the state is a necessary and sufficient condition for the measured observable to be given by a microcanonical distribution. This establishes a clear link between thermal equilibrium and unobservability. Considering thermalization within this framework also sidesteps the quantum thermalization problem, and allows one to compute meaningful "heat" and "work" quantities for closed systems under external driving.

This thesis has provided an attempt, for the first time (to the knowledge of the author), to explicate the notions of heat and work using an observability decomposition. Heuristic remarks to the same effect has been made countless times in the research litterature, but no explicit attempt has been made at formalization, perhaps due to lack of contact between the quantum thermodynamics and quantum control communities.

Exploring this avenue further for general Liouville Von-Neumann systems is difficult due to the poverty of control and observability results obtained thus far (Theorems 1 & 2 & 3 are the primary results available). Further implications of this theory can probably be found with the few results available, for example by analyzing their implications for a wider variety of algebras $(\mathcal{L}, \mathcal{V})$ and trying to ascertain what structures lead to thermalization. Further work should also consist in applying the theory to more model systems other than the Ising model considered in Section (5.1), again, attemping to find what algebraic structures $(\mathcal{L}, \mathcal{V})$ lead to thermalization (the Ising model considered here doesn't thermalize). A more restricted project would be to explore the theory further within the context of *linear dynamical quantum systems*, where a wealth of control and observability results already exist [25], including a full Kalman decomposition [26]. A problem of particular interest would be to relate the maximum work extractable from a system (with and without feedback) to its controllability and observability properties, and to an entropy-like function similar to the one defined in Eq. (4.1).

As a final remark, I hope that this thesis has shed some light on the meaning of thermodynamic concepts, or at least offered some food for thought.

Chapter 6

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