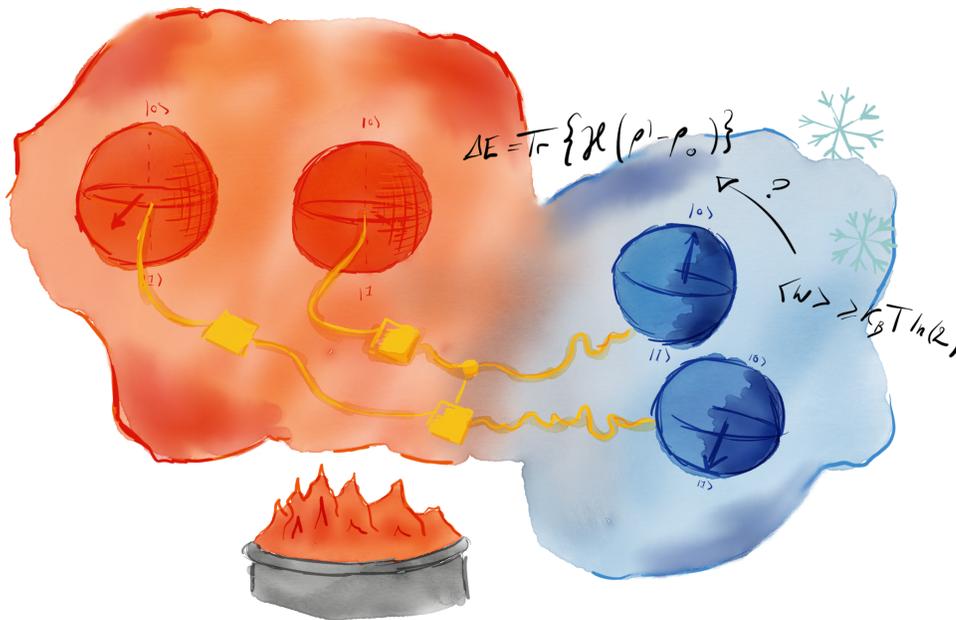

Quantum Thermodynamics and Information

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Abstract

This review hopes to remind one of the foundational concepts of modern thermodynamics, introduce nonequilibrium thermodynamics and describe how both lead to quantum thermodynamics. It then builds on this framework to review recent work [1, 2, 3, 4] developing connections between quantum information and quantum thermodynamics, namely in the establishment of Landauer type bounds. It's written for someone who like me knows more quantum information than they do thermodynamics. Whilst the essentials are presented for completeness, to brush up on quantum information check out [5, 6, 7, 8]. This review borrows heavily from the recently published and excellent book by Cambell & Deffner [9]. If it's not cited directly at points, assume

it's at least inspiring the presentation.

I should take this opportunity to thank Dr Campbell for pointing me in this direction to improve on and provide a better context for entropy bounds I obtained for the DQC1 trace estimation algorithm [10], in a recent conversation.

There's a liberal use of colour coding with boxes. Gray boxes are foundational things one should already know, Red boxes are important things, Violet boxes require material that will be presented later on for a full appreciation.

This review also misses some essential aspects of modern quantum thermodynamics - namely resource theoretic approaches and thermomajorisation.

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1 Modern Thermodynamics 101

Thermodynamics is a phenomenological¹ language developed in the 18th and 19th centuries by people that were thinking about pistons and steam engines. Despite the limited picture this leads one to draw mentally, it results in a robust conceptual framework for dealing with the transfer of heat and energy between systems in a way which transcends the setting for which this tool-set was intended. In this section, we will introduce the main ideas of thermodynamics as axiomatic guideposts and build off of them to more modern ideas. To be clear, thermodynamics can be treated as a purely mathematical structure, emerging from a set of axioms following the approach of [11]. Here, ideas like "equilibrium states" are done away with and zeroth laws are shown to be redundant [12] whilst other laws which we take to be axioms are derived from postulates. In the interest of pragmatism we will be much looser in the use of the term axiom than in [11, 12] which will allow us to draw more directly from current work.

Thermodynamic Priors

- ◇ **System** - In thermodynamics a system is something often chosen as a matter of context or taste but in general it is a subset of the universe wherein activity is thermodynamically consistent. Such as a fluid under some piston head, water in a cup, qubit coupled to a spin chain or the universe at large. Systems can be *open* if they are interacting with some environment or *closed* if they are impervious to external interactions.
- ◇ **Work** - is a change in internal energy due to some process carried out on the system or by the system and so is related to a process we have *control* over.
- ◇ **Temperature** - this a quantity one can associate to systems at which quantifies the thermodynamic energy of the system.
- ◇ **Heat** - This is a term used as short hand for energy of a thermodynamic nature. That is, energy to which a temperature may be associated. Often this term is used for energy being transferred between an environment or external system and the system of interest.
- ◇ **Equilibrium** is a relation between systems characterising if there are thermodynamic differences between the two systems, typically characterised by heat transfer. If there is no heat being transferred then the systems are said to be in equilibrium.

¹Statistical mechanics offers an alternate a view which is more *ground up*, starting from investigating microscopic degrees of freedom. We won't emphasise this formalism as it does not lend itself to quantum thermodynamics. This being said, we will review the main results as statistical mechanics is often a tool used to make arguments in quantum thermodynamics and provides a context for a great deal of the language used.

1.1 Axiomatic Guideposts

Phenomenological Axioms - The Zeroth Law

Thermal equilibrium is transitive - if two systems are in thermal equilibrium with a third system, then they are in equilibrium with each other.

This law whilst having clear phenomenological motivation and experiential relevance has been shown to be redundant in some formulations [12]. We may see it to be of relevance because it exemplifies the relational nature of equilibrium which in more modern contexts can be lost as a property of a state.

Phenomenological Axioms - The First Law

A change in the thermodynamic energy of a system is due to work carried out on the system or by the system and heat transferred between the system and environment.

$$\Delta E = \Delta W + \Delta Q \quad (1)$$

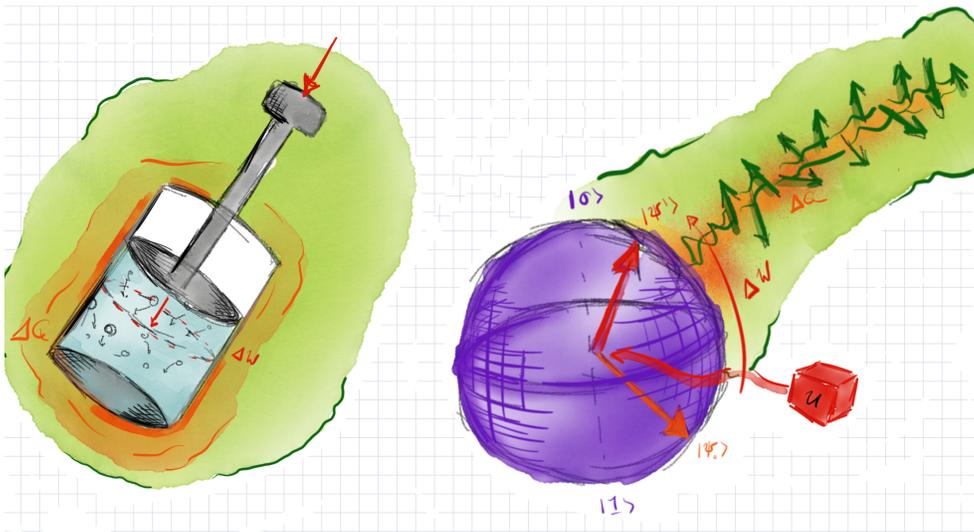


Figure 1: Two very different thermodynamic contexts.

This is effectively a restatement of conservation of energy, it also applies to nonequilibrium systems [13] which we will discuss in greater depth shortly. In fact, we can compare the first law as it appears in two contexts as in Fig. 1. On the left, the classical piston. Its environment is the air surrounding the piston, which depending on the temperature gradient between it and the piston will result in heat transfer (ΔQ). We then have the ability to carry out work (ΔW) on the piston by compressing the air inside it for example, in doing so increasing the internal energy (ΔE). On the right, consider a qubit coupled to a spin chain. The spin chain is its environment which, depending on the purity

of either system, might lead the establishment of correlations which affect the energy of the qubit on average (ΔQ). Work (ΔW) can also be carried out on the qubit through some unitary operation which physically might correspond ex: to varying a magnetic field, depending on your architecture.

In the context of equilibrium thermodynamics, where we consider changes from one equilibrium state to another, the first law is also an exact differential in phase space. This means that a change in energy is independent of the path taken in phase space and that a change in state can be identified directly with a change in energy. Grounding this once more with pistons and recalling some undergraduate thermodynamics [14, 15], each state can be describe by an equation

$$f(V, P, T) = 0 \quad (2)$$

which defines a smooth manifold. Work and Heat are *inexact* differential forms

$$dE = dW + dQ \quad (3)$$

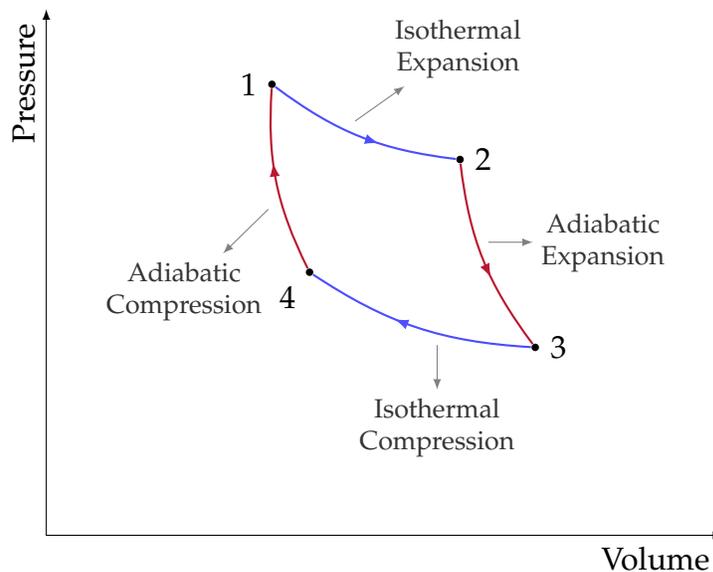
meaning they are path dependent and can be integrated over some process which takes you from one equilibrium state to another on this manifold

$$W = - \int_{v_0}^{v_1} P dV \quad (4)$$

We will deal with heat in the next section.

The power of the first law in a classical context is then this expressibility of extensive parameters, which leads one to ask whether this is possible in a quantum context. This is the work of stochastic thermodynamics which we will introduce shortly.

Figure 2: State diagram for a Carnot Cycle



Carnot Cycles

In the early 19th century French engineer Nicolas Léonard Sadi Carnot developed the Carnot engine and its corresponding cycle which have now become a language for discussing ideas of efficiency and temperature in equilibrium thermodynamics. The setup involves two thermal reservoirs coupled to two different ends of a piston filled with an ideal gas, one at T_1 and the other at T_2 such that $T_1 > T_2$. The process is reversible and features 4 steps as in figure 2.

- 1 → 2 **Isothermal expansion** - Heat from the T_1 reservoir is absorbed by the ideal gas in the piston to expand at constant temperature whilst it does work on the environment.
- 2 → 3 **Adiabatic expansion** - The temperature gradient has been equalised but the pressure in the piston decreases further resulting in the system doing work on the environment making it cool down to T_2 .
- 3 → 4 **Isothermal compression** - Pressure increases as work is performed on the system and heat is transferred to the reservoir at T_2 to maintain the temperature of the piston.
- 4 → 1 **Adiabatic compression** - Pressure continues to increase in the ideal gas but this time heat is not transferred out of the system allowing to reach T_1 .

We may also define the efficiency associated to this process as

$$\eta = \frac{W}{Q_1} \quad (5)$$

where work carried out by the system is the area enclosed by the cycle and Q_1 is the heat transferred to the system by the hotter reservoir. *What get out over what you put in.* Making use of the first law, the efficiency can be restated as

$$\eta = 1 - \frac{Q_2}{Q_1} \quad (6)$$

Carnot's Theorem

No engine operating between two reservoirs can be more efficient than a Carnot engine operating between those two reservoirs.

Corollary - All Carnot engines operating between the same two reservoirs have the same efficiency.

As a result of this theorem we can now define temperature in terms of efficiency [14]

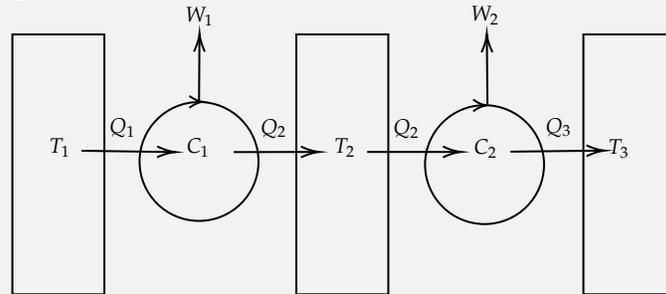
$$\eta_C = \frac{T_1 - T_2}{T_1} = 1 - \frac{T_2}{T_1} \quad (7)$$

which gives the following for Carnot engines comparing with eq. 6

$$\frac{Q_1}{Q_2} = \frac{T_1}{T_2}. \quad (8)$$

Formalising Temperature

Much like the Hamiltonian is one phenomenological model which gives us a way to formalise the *naturalistic* notion of energy, Carnot cycles offer a powerful way to formalise the *sense experience* notion of temperature.



Consider two Carnot engines joined by a common reservoir. Directly from (8) we have that

$$\frac{T_1}{T_2} = \frac{Q_1}{Q_2} \qquad \frac{T_2}{T_3} = \frac{Q_2}{Q_3} \qquad (9)$$

respectively. Multiplying the the two equations we have an equality from the total composite process

$$\frac{T_1}{T_3} = \frac{Q_1}{Q_3}. \qquad (10)$$

It is clear that this process can be extended to reach any arbitrary temperature allowing us to formally define temperature and an associated scale which is equivalent to the Ideal gas temperature scale [14]. In this sense, temperature can be seen as a feature that determines the efficiency of a Carnot cycle. A characteristic of a well-defined thermodynamic process, not just a phenomenological model.

1.1.1 Understanding Entropy through a Thermodynamic Lens

We can directly relate a thermodynamic understanding of work (4) with the way it is used in classical mechanics as the scalar product of force and distance, it is unclear how such a relationship can be achieved for heat.

We may postulate that small heat transfers may be decomposed into Carnot cycles such that

$$\frac{T_1}{T_2} = \frac{dQ_1}{dQ_2} \implies \frac{dQ_1}{T_1} = \frac{dQ_2}{T_2} \qquad (11)$$

and so for a reversible process involving such cycles

$$\oint \frac{dQ}{T_R} = 0 \qquad (12)$$

where T_R denotes the temperature of the reservoir. If the process is irreversible, although still cyclic and heat is flowing into the system then this equality is weakened to

$$\oint \frac{dQ}{T_R} \leq 0 \quad (13)$$

since Carnot cycles are at the maximum (the inequality is reversed if the heat flow is reversed). This is known as **Clausius' Inequality**. We may use this quantity to define an extrinsic state function which Clausius called *entropy* (S) such that

$$\Delta S_{A \rightarrow B} \geq \int_A^B \frac{dQ}{T} \quad (14)$$

which in turn solves our inexact differential issue giving $dQ = TdS$ for cyclic, reversible, entropy preserving processes. From this definition, entropy is seen as the quantifier for what ruins Carnot efficiency and introduces the idea of *disorder*. Whilst this definition can seem like a primitive understanding of entropy with knowledge of Boltzmann, Shannon, von Neumann and even quantum correlations, one ought to still acknowledge it as the most foundational definition of entropy.

Phenomenological Axioms - The Second Law

The entropy of the universe is a non-decreasing function of time,

$$\Delta S \geq 0. \quad (15)$$

There are a couple of ways that this can be reformulated. Taking this formulation of entropy we've introduced due to Carnot and Clausius we see that the second law is telling us that in general the Universe is not made of Carnot cycles and so entropy must always be on the rise with each thermodynamic process that occurs in the Universe. After the 1st law was formulated, Kelvin and Planck formulated the 2nd law in similar terms as the notion that *no process is possible whose sole result is the extraction of energy from a heat bath, and the conversion of all that energy into work*.

1.2 Statistical Mechanics 101

An alternate picture of equilibrium thermodynamics is given to us by statistical mechanics.

The Ergodic Hypothesis

Over sufficiently long time, the time for which a system occupies a state (*microstate*) in phase space with the same energy is proportional to the volume of this region in phase space. Alternatively, the occupation of each microstate is equiprobable over sufficiently long time.

Ok, so what's statistical mechanics all about? It's essentially a theory of probability. Our phase space is no longer concerning itself with quantities the system at large possesses, like Pressure or Volume, no. Now, our phase space concerns itself with the position and momentum of individual

constituents forming our system. In the case of an ideal gas, it will be the positions and moment of the constituent particles creating a 6 dimensional vector space as our phase space.

1.2.1 Understanding Entropy through a Statistical Lens

By the ergodic hypothesis ² it is clear that a thermodynamic system wishes to maximise the number of microstates (Ω) it covers over time. From the second law of thermodynamics, we know also that over time, entropy is always increasing and so we seek to relate these two quantities on phenomenological grounds. Since entropy is extrinsic meaning $S = \sum_i S_i$ and $\Omega = \prod_i \Omega_i$ then they may only be related via a logarithmic expression giving the celebrated Boltzmann relation

$$S = k_B \log \Omega \quad (16)$$

where k_B is the dimensionless Boltzmann's constant.

This definition of entropy clarifies the relationship with *disorder* as the more states a system can occupy the greater the entropy and intuitively more options gives rise to more disorder. It also begins to point towards a relationship with the information content of a system which we will explore shortly.

Fairly recently, Deffner and Zurek [18] reformulated the basic notions of statistical mechanics, including (16), starting from entanglement resulting in a less phenomenological basis for this model.

The Third Law (Nernst's Theorem)

In classical systems, the change in entropy vanishes as the temperature approaches absolute zero

$$\lim_{T \rightarrow 0} \Delta S = 0. \quad (17)$$

Taking the view provided by (16), we should have that at $T = 0$, $\Omega = 1$, the ground state for some perfectly crystalline material, giving $S = k_B \ln(1) = 0$, making sense of this law. This being said in a quantum context, where ground state degeneracy is an *everyday* phenomenon this law can be violated and should be adapted [19].

1.2.2 Formalism

In most cases, Ω is a bit naïve. It is not enough to count states. One has to concern themselves with the likelihood that the system is in one of these states. That is, the probability distribution across these states referred to as a *statistical ensemble*. You're probably thinking back to the ergodic hypothesis and asking how probability distributions make sense in the context of equiprobability. They do because closed systems are formed of a system of interest and a reservoir in statistical mechanics so

²The ergodic hypothesis, also known as Boltzmann's hypothesis was at the time, strikingly deep intuition on the part of Boltzmann. Later, this hypothesis was furnished by independent work of Birkhoff and von Neumann [16, 17].

Canonical Formalism	Grand Canonical Formalism
$\mathcal{P}_j = \frac{\Omega_R(E_T - E_j)}{\Omega_T(E_T)}$	$\mathcal{P}_j = \frac{\Omega_R(E_T - E_j, N_T - N_j)}{\Omega_T(E_T, N_T)}$
$F = U - TS$	$\Phi = U - TS - \mu N$
$\mathcal{Z}_C = e^{-\beta F} = \sum_j e^{-\beta E_j}$	$\mathcal{Z}_G = e^{-\beta \Phi} = \sum_j e^{-\beta(E_j - \mu N_j)}$

Table 1: A summary of the main tools of statistical mechanics. Throughout, $_T$ refers to total.

the probability that one can occupy a given state is dependent on the state of the reservoir, adding a context on top of the equiprobability. Using this structure³ we're able to achieve a thermodynamic understanding systems by calculating partial derivatives of some Legendre transform of the energy (F or Φ).

The Partition Function & Legendre Transforms

To derive the partition function we begin with the probability of the system being in the state j which is characterised by a fraction of the no. of states the reservoir can occupy provided the system of interest is in a state of energy E_j out of all total states. Notice that states in the canonical formalism are determined by energy.

$$\mathcal{P}_j = \frac{\Omega_R(E_T - E_j)}{\Omega_T(E_T)} \quad (18)$$

Next, we make use of the Boltzmann relation (16) giving

$$\mathcal{P}_j = \frac{\exp(k^{-1}S_R(E_T - E_j))}{\exp(k^{-1}S_T(E_T))} \quad (19)$$

and defining U to be the average temperature of the system such that by the first law $S_R(U - E_j) = \frac{U - E_j}{T}$ we arrive at

$$\mathcal{P}_j = \exp\left(\frac{1}{kT}(U - TS(U) - E_j)\right). \quad (20)$$

³Above, the energy spectrum is assumed to be discrete. If it were continuous we would of course have

$$\mathcal{Z} = \frac{1}{h^3} \int e^{-\beta H} d^3q d^3p$$

where h is Planck's constant and H is the Hamiltonian, for the canonical formalism. It is worth noting that the h factors are included to ensure that \mathcal{Z} is dimensionless

Defining

$$\beta := \frac{1}{kT} \qquad F := U - TS \qquad (21)$$

the inverse temperature and Helmholtz free energy, a Legendre transformation of the energy creating a function dependent on T as opposed to S we then have

$$\mathcal{P}_j = e^{\beta(F-E_j)}. \qquad (22)$$

The sum of probabilities is equal to one

$$e^{\beta F} \sum_j e^{-\beta E_j} = 1 \qquad (23)$$

allowing us to define

$$\mathcal{Z} := e^{-\beta F} = \sum_j e^{-\beta E_j} \qquad (24)$$

the partition function. Notice that

$$\sum_j \mathcal{P}_j = \frac{1}{\mathcal{Z}} \sum_j e^{-\beta E_j} = 1 \qquad (25)$$

helping us understand that the partition function gets its name from telling us how the energy contributions are partitioned throughout the ensemble.

It should be highlighted that the canonical and grand canonical ensembles have different uses. In the case of a canonical ensemble, the system is only able to exchange heat with the reservoir whilst in the case of the grand canonical ensemble, the system is able to exchange heat and particles - hence the addition of the chemical potential which should model such an exchange. Additionally, it is worth pointing out that in eq. 18 one is essentially *tracing out* the reservoir an idea we should keep in mind for pages to follow.

An Example - The Ideal Gas Consider a gas of N particles without external potential and mutual interactions [20] in a volume V in contact at equilibrium with a heat and particle reservoir at temperature T and chemical potential μ . The Hamiltonian for the ideal gas is purely kinetic

$$H(p) = \sum_{i=1}^N \frac{\vec{p}_i^2}{2m}. \qquad (26)$$

The grand canonical partition function has within it the canonical partition function

$$\mathcal{Z}_G = \sum_i^N e^{-\beta(E_i - \mu N_i)} = \sum_i e^{-\beta E_i} e^{\beta \mu N_i} = \sum_i \mathcal{Z}_C e^{\beta \mu N_i} = \sum_i \mathcal{Z}_C z_i^N \quad (27)$$

where z is the fugacity. So let's start with the canonical partition function. To begin with, the Hamiltonian is a continuous operator in the position basis and we have a factorisable partition function due to the particles being identical giving

$$\mathcal{Z}_C = \frac{V^N}{N! h^{3N}} \prod_{i=1}^N \int_{-\infty}^{\infty} d^3 p_i \exp\left(\frac{-\vec{p}_i^2}{2mk_B T}\right) = \frac{V^N}{N! h^{3N}} \left(\int_{-\infty}^{\infty} d^3 p_i \exp\left(\frac{-\vec{p}_i^2}{2mk_B T}\right) \right)^N. \quad (28)$$

This is a friendly Gaussian integral $\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$ in $3N$ dimensions giving

$$\mathcal{Z}_C = \frac{V^N (2\pi mk_B T)^{3N/2}}{N! h^{3N}} \quad (29)$$

As a preliminary result, identifying that without the dimensional corrections we have a quantity which is the momentum cubed we can define the characteristic thermal momentum

$$p_T = \sqrt{2\pi mk_B T} \quad (30)$$

which gives the *thermal de Broglie wavelength*

$$\lambda_T = \frac{h}{p_T} = \frac{h}{\sqrt{2\pi mk_B T}} \quad (31)$$

that characterises the regime under which quantum effects become prevalent for an ideal gas if

$$\frac{V}{N\lambda_T^3} \leq 1.$$

Moving on, the grand canonical partition function

$$\mathcal{Z}_G = \sum_{N=0}^{\infty} \frac{1}{N!} \left(\frac{Vz}{\lambda_T^3} \right)^N \quad (32)$$

and recalling $\sum_{n=0}^{\infty} \frac{x^n}{n!} = e^x$ we have

$$\mathcal{Z}_G = \exp\left(\frac{Vz}{\lambda_T^3}\right) \implies \Phi = -k_B T \left(\frac{Vz}{\lambda_T^3}\right). \quad (33)$$

The grand canonical potential allows us to analyse various facets of the system through the relation

$$d\Phi = -PdV - SdT - Nd\mu \quad (34)$$

so

$$N = - \left(\frac{\partial \Phi}{\partial \mu} \right)_{T,V} = \frac{Vz}{\lambda_T^3} \quad P = - \left(\frac{\partial \Phi}{\partial V} \right) = -k_B T \left(\frac{z}{\lambda_T^3} \right) \quad (35)$$

combining the above

$$PV = Nk_B T \quad (36)$$

the equation of state for ideal gases.

1.2.3 Statistical Mechanics for Quantum Equilibrium Thermodynamics

The *Quantum* Ergodic Hypothesis

A given statistical quantum state $|\psi\rangle = \sum_n c_n |\psi_n\rangle$ satisfies [20]

◇ **Equiprobability** Over long enough time, all states contribute equally to the system

$$\overline{c_n^* c_{n'}} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt c_n^*(0) c_n(0) = \begin{cases} r, & E \leq E_n \leq E + \delta E \\ 0. & \end{cases} \quad (37)$$

◇ **Random Phase** If $n \neq n'$ then

$$\overline{c_n^* c_{n'}} = 0 \quad (38)$$

the phase of the wavefunction is a random variable. This presupposes weak coupling to the environment which randomises the phase.

Consider once more eq. (25)

$$\sum_j \mathcal{P}_j = \frac{1}{\mathcal{Z}} \sum_j e^{-\beta E_j} = 1. \quad (39)$$

If we had a quantum mechanical system formed of *weakly interacting* identical sub-systems at equilibrium, with a Hamiltonian that has a discrete spectrum this equation would only need to be modified slightly

$$\text{Tr} \hat{\rho} = \sum_j \mathcal{P}_j = \sum_j \langle j | \hat{\rho} | j \rangle = \frac{1}{\mathcal{Z}} \sum_j e^{-\beta E_j} = 1. \quad (40)$$

where the probability distribution has now been upgraded to a density matrix and the phase space furnished with a Hilbert space. And so, we are able to associate this canonical ensemble⁴ with the

⁴A similar process can be carried out for grand canonical ensembles which are used to describe quantum gases. These aren't too useful for us.

density matrix

$$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{\mathcal{Z}} = \frac{1}{\mathcal{Z}} \sum_j e^{-\beta E_j} |j\rangle\langle j| \quad (41)$$

where E_j are the eigenvalues and $|j\rangle$ are the corresponding eigenkets of the Hamiltonian of this system, that also provide a *complete* basis for this Hilbert space. A density matrix of this form is known as a **Gibbs state** [21, 22]. In this context, the partition function can be found as

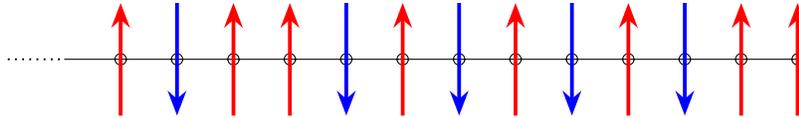
$$\mathcal{Z} = e^{-\beta F} = \text{Tr} \left\{ e^{-\beta\hat{H}} \right\} \quad (42)$$

and is what normalises the density matrix. Quantum canonical ensembles or Gibbs states stem from *weakly interacting* sub-systems as described earlier. The Hamiltonians of such systems are said to be *local* and take the form

$$\hat{H} = \sum_i h_i \otimes \mathcal{I} \quad (43)$$

that has bounded strength and acts non-trivially on at most $k < N$ particles.

An Example - Ideal Quantum Paramagnet Consider N quantum spin- $\frac{1}{2}$ particles in a magnetic field, \vec{B} .



We can describe this system through the Hamiltonian

$$\hat{H} = - \sum_{i=1}^3 \mu_B \vec{h} \cdot \vec{\sigma}_i \quad (44)$$

where σ_i are the Pauli matrices, μ_B is the Bohr magneton and \vec{h} is the magnetic field strength vector which I will take to be h in each direction. The partition function for a singular spin can be found

$$\mathcal{Z} = \text{tr} \left\{ e^{\beta\hat{H}} \right\} = \text{tr} \left\{ e^{\beta \sum_i \mu_B h \sigma_i} \right\} \quad (45)$$

$$= \text{tr} \left(\begin{array}{cc} 3 \cosh(\beta\mu_B h) + \sinh(\beta\mu_B h) & (1 - i) \sinh(\beta\mu_B h) \\ (1 + i) \sinh(\beta\mu_B h) & 3 \cosh(\beta\mu_B h) - \sinh(\beta\mu_B h) \end{array} \right) \quad (46)$$

$$\mathcal{Z} = 6 \cosh(\beta\mu_B h) \quad (47)$$

and so the partition function for all N spins is

$$\mathcal{Z} = (6 \cosh(\beta\mu_B h))^N. \quad (48)$$

From here, we may use the Helmholtz free energy to investigate the entropy and investigating the magnetic susceptibility we derive the Curie law. (Finish off this exercise.)

Reflecting on the thinking behind the exercise we just carried out we can see the ideas of statistical mechanics and their power. We have a system of *weakly interacting* spin- $\frac{1}{2}$ particles that are on the average at the same temperature. That is, they are at equilibrium with each other. We focus on a single spin and take all the rest to be our reservoir giving us a canonical ensemble through which we can find the partition function for this single spin. Since the system is made of only spins, this allows us to build a partition function for the whole system making use of the partition function for a single spin. This also gives insight into why Gibbs states are reduced density matrices. The reduction occurs when you trace out your chosen reservoir, which in this case would be the rest of the spins.

Connecting Gibbs and von Neumann Entropy

For quantum states the von Neumann entropy quantifies the informational entropy. If a system is weakly coupled to a bath at equilibrium we may associate a canonical ensemble and Gibbs entropy to it. In this circumstance, the von Neumann entropy is equal to the Gibbs entropy giving an explicit connection between information and thermodynamics.

Consider the Gibbs entropy may be expressed in terms of the Gibbs Free Energy as

$$F = U - TS \implies S = -\beta(U - F) \quad (49)$$

$$S_G = -\beta(\langle \hat{H} \rangle - t \ln \mathcal{Z}) = -\beta \text{Tr} \{ \hat{\rho} \hat{H} \} + \ln \mathcal{Z} \quad (50)$$

and since this is the entropy of a Gibbs state we have

$$= -\beta \sum_{i=0}^N \frac{e^{-\beta E_i}}{\mathcal{Z}} E_i + \ln \mathcal{Z}. \quad (51)$$

For malleability, we may multiply the logarithm of the partition function by the trace of the density matrix, which is 1 giving

$$= -\beta \sum_{i=0}^N \frac{e^{-\beta E_i}}{\mathcal{Z}} E_i + \ln \mathcal{Z} \text{Tr} \{ \hat{\rho} \} \quad (52)$$

$$= -\beta \sum_{i=0}^N \frac{e^{-\beta E_i}}{\mathcal{Z}} E_i + \ln \mathcal{Z} \sum_{i=0}^N \frac{e^{-\beta E_i}}{\mathcal{Z}} = \sum_{i=0}^N \frac{e^{-\beta E_i}}{\mathcal{Z}} (-\beta E_i + \ln \mathcal{Z}) \quad (53)$$

$$= -\sum_{i=0}^N \frac{e^{-\beta E_i}}{\mathcal{Z}} \left(\ln \left(\frac{e^{-\beta E_i}}{\mathcal{Z}} \right) \right) \quad (54)$$

$$= -\sum_{i=0}^N \lambda_i \ln \lambda_i = -\text{Tr} \{ \hat{\rho} \ln \hat{\rho} \} = S_{vN}. \quad (55)$$

1.3 Nonequilibrium Thermodynamics

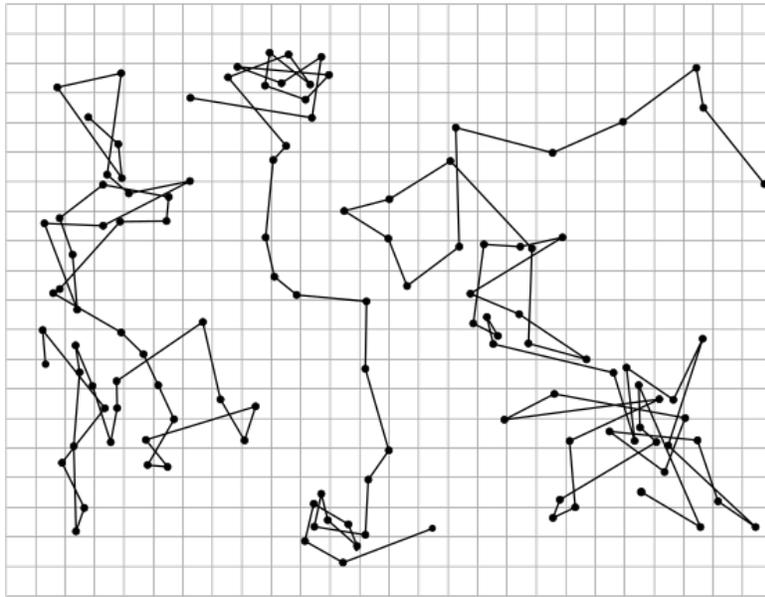


Figure 3: Reproduced from [23], three tracings of the motion of colloidal particles of radius $0.53 \mu\text{m}$, as seen under the microscope, are displayed. Successive positions every 30 s are joined by straight line segments (the mesh size is $3.2 \mu\text{m}$). Adapted by *MiraiWarren*.

Real physical systems are messy. It is often not the case that the constituents of a system comprise a homogeneous and isotropic state. To contend with this in the 1930s, Norwegian physicist Lar Onsager [24] proposed to model thermodynamic systems that were out of equilibrium by assuming that their constituents are in *local equilibrium*. In this context, whilst there is local equilibrium, the properties of the system vary temporally and spatially.

In general, this formulation involves the expression of time-derivatives of extrinsic parameters which are called *thermodynamic fluxes*

$$J_k = \frac{dX_k}{dt} \quad (56)$$

allowing us to express the rate of entropy production as

$$\frac{dS}{dt} = \sum_k \frac{\partial S}{\partial X_k} \frac{dX_k}{dt} = \sum_k F_k J_k \quad (57)$$

where F_k are *thermodynamic forces or affinities*. For systems in local equilibrium with small affinities, J_k can be written as a function of F_k

$$J_k = \sum_j L_{j,k} F_j \quad (58)$$

and $L_{j,k}$ are the kinetic coefficients up to first-order defined as

$$L_{j,k} = \left. \frac{\partial J_k}{\partial F_j} \right|_{F_j=0}. \quad (59)$$

The Fourth Law (Onsager's Theorem)

The matrix of kinetic coefficients is symmetric

$$L_{j,k} = L_{k,j}. \quad (60)$$

In essence, this shows that if a system is said to be time-reversible despite being in a non-equilibrium state, then the flow of macroscopic extrinsic parameters must exhibit symmetry expressed by the Onsager reciprocity relations. For a more detailed discussion consider [15, 24, 25].

1.3.1 The Thermodynamics of *microscopic* Stochastic Systems

Beyond the work of Onsager, random systems that are much farther away from equilibrium were studied by Langevin, Einstein and others throughout the 20th century mainly to deal with the idea of Brownian motion. Dealing with *stochastic forces* in these systems led to the emergence of concepts like fluctuation and dissipation which are an important part of modern nonequilibrium thermodynamics. Most notable is the development of the Langevin equation

$$m\ddot{x} + m\gamma\dot{x} + V'(x) = \zeta(t) \quad (61)$$

where m is the mass of the particle, γ is a damping coefficient, $V'(x)$ is a conservative force and $\zeta(t)$ is a stochastic force. This force is seen to describe the randomness in an open system due to thermal fluctuations. Let's now examine how these concepts evolved to contribute to modern nonequilibrium thermodynamics.

1.3.2 Fluctuation Theorems

When introducing entropy via Clausius' inequality (14) we saw that the change in entropy was defined for an irreversible process and so the 2nd Law (15) may be interpreted as the fact that on long time scales, processes are irreversible leading to the related concept of the *arrow of time*. This is contentious because clearly we see unitary time dynamics everywhere, especially in quantum systems. This is known as Loschmidt's paradox or the reversibility paradox [26]. We must therefore, find a way to recover the second law which is apparent at large scales, from the regime of small interactions where reversibility dominates. This is the role of the Fluctuation Theorems [27, 28, 29, 30, 31] that reconcile this difference between the regimes.

A *macroscopic* reversible system is one whose phase space contains an anti-(time reversed) trajectory corresponding to every trajectory in the space and where both of these classes of trajectories is equally likely. On the other hand, if the probability of observing anti-trajectories is small than a

macroscopic system is said to be irreversible [31]. In this setting the mechanism to relate *microscopic* reversibility to *macroscopic* irreversibility must then be probability. This is the route that Evans and Searle [27, 28] pursued when having to face this paradox in the context of describing the statistical mechanics of sheared liquids which involved thermodynamic fluctuations. They show that for a system that evolves from an initial state of equilibrium to a nonequilibrium state we have [13]

$$\frac{\mathcal{P}_\tau(+\Delta S)}{\mathcal{P}_\tau(-\Delta S)} = e^{\Delta S/k_B} \quad (62)$$

the ratio of probabilities (\mathcal{P}) of observing positive and negative entropy production up to time $\tau > 0$ may be expressed as an exponential function of the change in entropy. In such a picture, irreversible processes that occur forwards in time produce entropy whilst reversible processes which can occur backwards in time produce negative entropy. This is a sensible heuristic because what it expresses is that negative entropy production is exponentially unlikely at whilst for small systems becomes more likely. Similarly, this argument can be given in terms of time, that is negative entropy production is more likely to occur on very small time scales and vanishingly probable to occur on larger time scales. From (54) one attains the integrated fluctuation theorem

$$\langle e^{-\Delta S/k_B} \rangle = 1 \quad (63)$$

which implies

$$\langle \Delta s \rangle \geq 0 \quad (64)$$

where $\langle \cdot \rangle$ is denoting an average. That is, on average even in a nonequilibrium system, we expect a generalisation of the Clausius inequality and the second law to hold. The relations presented above are largely of a heuristic nature and form a phenomenological foundation for more formal nonequilibrium thermodynamics.

In the case of equilibrium thermodynamics, the Carnot cycle told us how to extract the most work out of a system. Make it cyclic so that there is no change in entropy and you get maximum work. But in the case of nonequilibrium thermodynamics where the situation is less clear we need some new tools. The formalisation of the ideas discussed in 1.3.2, by Crooks [30] and Jarzynski [29] amongst others give us what we need.

1.3.3 Jarzynski's Equality

Jarzynski's Equality as a Generalised 2nd Law

This equality gives us a way to calculate the work done in nonequilibrium processes by bringing to light a fundamental relationship between nonequilibrium work and equilibrium free energy.

$$-k_B T \ln \langle e^{-\beta W} \rangle = \Delta F \quad (65)$$

The change in free energy between equilibrium states can be determined by the average work done by large ensembles out-of-equilibrium states.

Making use of (65) and Jensen's inequality $\langle e^x \rangle \geq e^{\langle x \rangle}$ we obtain the inequality

$$\langle W \rangle \geq \Delta F. \quad (66)$$

This expresses that even in nonequilibrium thermodynamics one can at best on the average not create entropy but in most cases all your work is not going to be passed on to the system, you'll create some entropy on the way. As such, this can be seen as a generalisation of the 2nd law of thermodynamics to a nonequilibrium.

A statement related to (56) is also obtained from (64) where the probability of observing some work W below $\Delta F - \zeta$: $\zeta > 0$ is found [13]

$$P[W < \Delta F - \zeta] = e^{-\beta \zeta}. \quad (67)$$

where the probability of observing a process where the work is close to the the macroscopically forbidden $W < \Delta F$ regime is exponentially low.

Consider a system [13, 9], that is weakly coupled to some environment at inverse temperature β and under-damped with a work stochastic parameter⁵ λ . Denoting a microstate in the phase space of this system as $\Gamma = (q_i, p_i)$ with Hamiltonian $H = H(\Gamma; \lambda)$ we may describe the evolution of probability distributions over this phase space through the Liouville equation

$$\frac{\partial \mathcal{P}(\Gamma; \lambda)}{\partial t} = - \{ \mathcal{P}(\Gamma; \lambda), H(\Gamma; \lambda) \} \quad (68)$$

where $\{ \cdot, \cdot \}$ is the Poisson bracket. Since the system is weakly coupled we can assume that is at equilibrium with the environment initially and described by a canonical ensemble

$$\mathcal{P}_0(\Gamma; \lambda) = \frac{e^{-\beta H(\Gamma; \lambda)}}{\mathcal{Z}(\Gamma; \lambda)} \quad (69)$$

⁵One can think of this quantity as the force being applied to the system at a given time. Note also that the nonequilibrium physics is originating from this parameter.

which is then evolved out of equilibrium by (57). The intrinsic work [32] may be described as the difference in the Hamiltonian over a time τ on a path in phase space from an initial point Γ_0 to Γ_τ

$$W = H(\Gamma_\tau; \lambda_\tau) - H(\Gamma_0; \lambda_0). \quad (70)$$

Note that $\Gamma_\tau; \lambda_\tau$ and $\Gamma_0; \lambda_0$ are both equilibrium states but the states connecting them **need not be**. To derive Jarzynski's equality, we now consider the average work distribution over the initial state and conditions

$$\langle e^{-\beta W} \rangle = \int d\Gamma_0 \mathcal{P}_0(\Gamma_0; \lambda_0) e^{-\beta W} = \int d\Gamma_0 \frac{e^{-\beta H(\Gamma_0; \lambda_0)}}{\mathcal{Z}(\Gamma_0; \lambda_0)} e^{-\beta W} \quad (71)$$

$$= \int d\Gamma_0 \frac{e^{\beta H(\Gamma_\tau; \lambda_\tau)}}{\mathcal{Z}(\Gamma_0; \lambda_0)} \quad (72)$$

where we made use of (59) allowing us to express the average work distribution in terms of the final state probability. Next we change the variables of integration

$$= \frac{1}{\mathcal{Z}(\Gamma_0; \lambda_0)} \int d\Gamma_\tau \left| \frac{\partial \Gamma_\tau}{\partial \Gamma_0} \right|^{-1} e^{\beta H(\Gamma_\tau; \lambda_\tau)} = \frac{1}{\mathcal{Z}(\Gamma_0; \lambda_0)} \int d\Gamma_\tau e^{\beta H(\Gamma_\tau; \lambda_\tau)} = \frac{\mathcal{Z}(\Gamma_\tau; \lambda_\tau)}{\mathcal{Z}(\Gamma_0; \lambda_0)} \quad (73)$$

where that the Jacobian is equal to 1 by Liouville's Theorem and we have made use of the definition of the partition function. Recalling the definition of the free energy in terms of the partition function $F = -k_b T \ln \mathcal{Z}$ we have

$$\langle e^{-\beta W} \rangle = e^{-\beta(F(\Gamma_\tau; \lambda_\tau) - F(\Gamma_0; \lambda_0))} = e^{-\beta \Delta F}. \quad (74)$$

1.3.4 Crooks' Fluctuation Theorem

Where Jarzynski's equality developed a relationship between an average of nonequilibrium work distributions and the free energy distributions of equilibrium states, Crooks' Fluctuation Theorem [30] develops a more pointed relationship between the probability of observing forward and reverse processes through work distributions. In effect, formalising the heuristic argument of Evans and Searle [28] presented as (56).

To derive this result, as described in [33, 9, 13], we again consider the evolution of a thermodynamic system as described in 1.3.3 during $t \in [0, \tau]$ under the stochastic work parameter λ_t . A thermodynamic process or trajectory may be expressed as an ordered set of microstates $\{\Gamma_0, \Gamma_1, \dots, \Gamma_N\}$ where the microstate Γ_n corresponds to the microstate occupied at time $t_n = \frac{n\tau}{N}$. Next we make two assumptions;

- This process is Markovian: a microstate Γ_{n+1} is sampled randomly from a transition probability \mathcal{P} that depends on Γ_n only.

- The system satisfies the principle of detailed balance locally, it is microscopically reversible

$$\frac{\mathcal{P}(\Gamma_0 \rightarrow \Gamma'; \lambda)}{\mathcal{P}(\Gamma_0 \leftarrow \Gamma'; \lambda)} = \frac{e^{-\beta H(\Gamma'; \lambda)}}{e^{-\beta H(\Gamma_0; \lambda)}}. \quad (75)$$

This means that the transition from one microstate to the next due to the work parameter is reversible and that local transitions occur between states at equilibrium with their environment. This captures the idea of local equilibrium and global nonequilibrium in the process.

For a forward process, we have that first the work parameter is updated, then a new microstate is sampled at random. In a reverse process these two steps would be reversed. In either case, it is clear that a process from $t = 0$ to $t = \tau$ can be constructed as the product of smaller processes. In this context we have the change in energy

$$\Delta E = H(\Gamma_N, \lambda_N) - H(\Gamma_0, \lambda_0) \quad (76)$$

as the differences in the Hamiltonian of the final and initial state. By the first law this can be expressed in terms of work and *heat* energy. The work will correspond to a change in the work parameter

$$W = \sum_{i=0}^{N-1} H(\Gamma_i, \lambda_{i+1}) - H(\Gamma_i, \lambda_i) \quad (77)$$

whilst change in *heat* energy will correspond to changes in the microstate due to the environment.

$$Q = \sum_{i=0}^{N-1} H(\Gamma_{i+1}, \lambda_{i+1}) - H(\Gamma_i, \lambda_{i+1}). \quad (78)$$

For the result, we describe the calculation from [33]. Consider now a trajectory $\varphi = \{\Gamma_0, \Gamma_1, \dots, \Gamma_N\}$. The probability that such a trajectory occurs can be expressed as the probability of all the subprocesses occurring as a result of Markovianity

$$\mathcal{P}(\varphi) = \mathcal{P}(\Gamma_0 \rightarrow \Gamma_1; \lambda_1) \mathcal{P}(\Gamma_1 \rightarrow \Gamma_2; \lambda_2) \dots \mathcal{P}(\Gamma_{N-1} \rightarrow \Gamma_N; \lambda_N). \quad (79)$$

Let φ_R denote the time-reversed trajectory and then consider the ratio of the likelihood that the forward trajectory occurs and the likelihood that reverse trajectory occurs

$$\frac{\mathcal{P}(\varphi)}{\mathcal{P}(\varphi_R)} = \frac{\mathcal{P}(\Gamma_0 \rightarrow \Gamma_1; \lambda_1) \mathcal{P}(\Gamma_1 \rightarrow \Gamma_2; \lambda_2) \dots \mathcal{P}(\Gamma_{N-1} \rightarrow \Gamma_N; \lambda_N)}{\mathcal{P}(\Gamma_0 \leftarrow \Gamma_1; \lambda_1) \mathcal{P}(\Gamma_1 \leftarrow \Gamma_2; \lambda_2) \dots \mathcal{P}(\Gamma_{N-1} \leftarrow \Gamma_N; \lambda_N)}. \quad (80)$$

But by the 2nd assumption, each step is microscopically reversible and so the detailed balance condition is obeyed by every contributor to (74) giving

$$\frac{\mathcal{P}(\varphi)}{\mathcal{P}(\varphi_R)} = \frac{e^{-\beta H(\Gamma_1; \lambda_1)} e^{-\beta H(\Gamma_2; \lambda_2)} \dots e^{-\beta H(\Gamma_N; \lambda_N)}}{e^{-\beta H(\Gamma_0; \lambda_1)} e^{-\beta H(\Gamma_1; \lambda_2)} \dots e^{-\beta H(\Gamma_{N-1}; \lambda_N)}} \quad (81)$$

which comparing with (72) gives

$$\frac{\mathcal{P}(\varphi)}{\mathcal{P}(\varphi_R)} = e^{-\beta Q} \quad (82)$$

where Q is the energy exchanged with the environment and $-\beta Q$ is the entropy change in the bath. If one assumes that the trajectories start and end at equilibrium states have

$$\frac{\mathcal{P}(\varphi)}{\mathcal{P}(\varphi_R)} = \frac{e^{\beta F(\lambda_0) - \beta H(\Gamma_0, \lambda_0)} \prod_{i=1}^N \mathcal{P}(\Gamma_i \rightarrow \Gamma_{i+1}; \lambda_{i+1})}{e^{\beta F(\lambda_N) - \beta H(\Gamma_N, \lambda_N)} \prod_{i=1}^N \mathcal{P}(\Gamma_i \leftarrow \Gamma_{i+1}; \lambda_{i+1})} = e^{-\beta(Q + \Delta F - \Delta E)} \quad (83)$$

$$\frac{\mathcal{P}(\varphi)}{\mathcal{P}(\varphi_R)} = e^{-\beta(-W^F(\varphi) + \Delta F)} \quad (84)$$

by the first law, where W^F denotes the work of the forward process such that $W^F(\varphi) = -W^R(\varphi_R)$. Finally this can be written in terms of work distributions as opposed to trajectories by finding the average work over all possible trajectories [9]

$$\mathcal{P}(+W) = \int d\varphi \mathcal{P}(\varphi) \delta(W - W^F(\varphi)) \quad \mathcal{P}(-W) = \int d\varphi_R \mathcal{P}(\varphi_R) \delta(W + W^R(\varphi)) \quad (85)$$

which by applying to (78) one attains Crook's Theorem

$$\frac{\mathcal{P}(+W)}{\mathcal{P}(-W)} = e^{-\beta(W - \Delta F)}. \quad (86)$$

Interestingly, if one integrates the result over the forward work distribution, one attains Jarzynski's equality. Whilst Crooks' theorem is a broader statement than the Jarzynski equality, one notes that Crooks' theorem stands only for Markov processes whilst Jarzynski's equality does not share this limitation. To model a situation where correlations can form between the bath and a system one would be able to employ the Jarzynski equality and not the Crooks fluctuation theorem. This theorem has been experimentally verified in the interesting setting of RNA folding [34].

With the Jarzynski equality and Crooks theorem in hand, the fluctuation theorems have given us a tool set with which to relate nonequilibrium work to equilibrium state changes.

2 Quantum Thermodynamics & Information

In this section I will review what in my perspective are the most crucial and foundational elements of the field which is beginning to be established around quantum thermodynamics. Namely, I will introduce recent grounding results around the generalisation of Carnot cycles [35, 9], the quantum fluctuation theorems [36, 32] and entropy production in a quantum thermodynamic context [37]. This is a bare bones presentation and leaves out treatments of quantum thermometry [38], quantum engines [39] and much more. For a more thorough and complete review consider [40].

Before we jump in it's good to have a word about dynamics generally in this context. The evolution of an open quantum system is given by a generalised form of the Heisenberg/von Neumann/quantum Liouville equation known as the GKSL or *Lindblad* master equation [6, 41, 42].

$$\dot{\hat{\rho}}(t) = \hat{\mathcal{L}}(\hat{\rho}) = -i [\hat{H}, \hat{\rho}] + \sum_{a>0} \Gamma_a \left(\hat{L}_a \hat{\rho} \hat{L}_a^\dagger - \frac{1}{2} \{ \hat{L}_a^\dagger \hat{L}_a, \hat{\rho} \} \right) \quad (87)$$

Here the first term describes unitary time evolution, Γ describes the decay rate of the coupling between the bath and the system and \hat{L}_a are the Lindblad operators which describe the interaction between the system and environment. This equation is Markovian, meaning it is local in time and the system has no memory or back propagation effects. As such, no correlations can be established between the system and the bath regardless of coupling strength. A system is said to be weakly coupled when the interaction term can be neglected that is $\Gamma_a \ll 1$. For a better presentation consider Chapter 3 from Preskill's notes [6] and for a comprehensive treatment [41].

This being said, it is of course of deep interest to allow a bath to establish correlations with a system. Especially when one is trying to examine the quantum thermodynamics associated to a quantum information protocol⁶ or the entropy production of a system coupled to a bath in a quantum setting. Several approaches exist here such as the derivation of completely new non-Markovian master equations [41], Collisional models [43, 44], modifying the master equation ex: tweaking its coupling parameters and making them negative or using interesting models that allow one to capture the non-Markovian dynamics within some reduced state [45, 46].

2.1 The 1st & 2nd laws for equilibrium thermodynamics in a quantum context

Whilst we briefly met quantum equilibrium thermodynamics when playing with the tools of statistical mechanics in a quantum context we did not properly treat this physics in the dept it requires. Even when weakly-coupled, quantum systems often get entangled with their environment meaning that there is some thermodynamic cost for the maintenance of these correlations, something which classical systems needn't be concerned with. This means that the way we think of *heat* and *work* is going to change in a quantum context for different equilibrium states. Following the approach of [35, 9] we consider two equilibrium cases.

⁶This alludes to my own work, where I treat the logical qubit in the register of the DQC1 complexity class [10] as a system and the mixed state ancillas as the bath. Here, correlations established between the bath and system are not only present but essential for the computation.

Gibbs States have minimal free energy and maximal entropy

If we define the free energy for an arbitrary quantum state modeling an open quantum system taking $S(\hat{\rho})$ to be the von Neumann entropy $S(\hat{\rho}) = -\text{tr}\{\hat{\rho} \ln \hat{\rho}\}$ we have

$$F(\hat{\rho}) = \langle \hat{H} \rangle - tS(\hat{\rho}). \quad (88)$$

For a Gibbs state, this will coincide with the Gibbs free energy

$$F(\hat{\rho}_\beta) = -\beta^{-1} \ln \mathcal{Z} = -\beta^{-1} \ln \left(\text{tr}\{e^{-\beta \hat{H}}\} \right). \quad (89)$$

In general we have

$$F(\hat{\rho}) = \text{tr}\{\hat{\rho} \hat{H}\} + \beta^{-1} \text{tr}\{\hat{\rho} \ln \hat{\rho}\} = \beta^{-1} \text{tr}\{\hat{\rho} (\ln \hat{\rho} + \beta \hat{H})\} \quad (90)$$

by linearity of the trace. Considering the relative entropy of this arbitrary state $\hat{\rho}$ and the Gibbs state $\hat{\rho}_\beta$ we have

$$D(\hat{\rho} || \hat{\rho}_\beta) = \text{tr}\{\hat{\rho} \ln \hat{\rho}\} - \text{tr}\{\hat{\rho} \ln \hat{\rho}_\beta\} \quad (91)$$

which can be expressed in terms of the free energy as

$$D(\hat{\rho} || \hat{\rho}_\beta) = \beta (F(\hat{\rho}) - F(\hat{\rho}_\beta)). \quad (92)$$

But, the relative entropy is known to be non-negative by Klein's inequality [47].

$$D(\cdot || \cdot) \geq 0. \quad (93)$$

As a result the Gibbs free energy is the lowest possible free energy or the free energy of the Gibbs state is minimal. The first law of thermodynamics can be stated in this context as

$$dE = tdS + dF \quad (94)$$

so if Gibbs states minimise the free energy, they maximise the von Neumann entropy, which happens to be the Gibbs Entropy. With this in mind, we may also say that for fully-degenerate Hamiltonians, where all microstates have equal energy, the Gibbs state coincides with the maximally mixed state

$$\rho_{\mathcal{M}} = \frac{1}{d} \sum_{i=0}^d |i\rangle\langle i| \quad (95)$$

where d is the dimension of the system.

2.1.1 Gibbs States

As introduced in 1.2.3, Gibbs states are quantum states that represent open quantum systems that can be modeled by a canonical ensemble and as such take the form

$$\hat{\rho}_\beta = \frac{e^{-\beta\hat{H}}}{\mathcal{Z}} \quad (96)$$

where \mathcal{Z} is the partition function and \hat{H} is a local Hamiltonian.

This means that the system is weakly coupled with some bath at equilibrium with temperature β^{-1} . It is worth emphasising that Gibbs states represent situations where no correlations can be formed between the environment and the system in question. The entropy of the Gibbs state is the Gibbs entropy which can be expressed in terms of the Gibbs free energy as

$$S_\beta = \beta(E - F) = \beta(\text{tr}\{\hat{\rho}\hat{H}\} - F_\beta) \quad (97)$$

so for quasistatic, isothermal processes we have

$$dS_\beta = \beta(dE - dF) = \beta(\text{tr}\{d\hat{\rho}\hat{H}\} + \text{tr}\{\hat{\rho}d\hat{H}\} - dF_\beta) \quad (98)$$

but $\text{tr}\{\hat{\rho}d\hat{H}\}$ is an expression of work and so an expression of the change in free energy giving

$$dS_\beta = \beta\text{tr}\{d\hat{\rho}\hat{H}\} = \beta\delta Q. \quad (99)$$

As such, our first law of thermodynamics changes in this context to

$$dE = \delta Q + \delta W = \text{tr}\{\delta\hat{\rho}\hat{H}\} + \text{tr}\{\hat{\rho}\delta\hat{H}\} \quad (100)$$

where work is identified with a change in the Hamiltonian and heat is identified with a change in the state. This recovers the familiar

$$dE = tdS + dF \quad (101)$$

where tdS is the entropic cost associated to the work done for change in energy.

2.1.2 Quantum Thermal Area Law for Gibbs States

When considering a system whose dynamics are described by a local Hamiltonian we may upper bound an expression of the correlations formed between two subsystems, known as the *mutual information*, through a free energy argument – provided these subsystems form Gibbs states.

Mutual Information

If a quantum system may be partitioned into two subsets A and B then the correlations formed between these two subsets may be quantified by the mutual information defined as

$$\mathcal{I}(A : B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}) = D(\rho_{AB} || \rho_A \otimes \rho_B) \quad (102)$$

where ρ_i is the reduced density matrix with j having been traced out. This is effectively the relative entropy between the system and a separable version of the system where correlations have been traced out where this difference then quantifies the correlations in the system.

Making this more tangible, consider a 1D Ising Chain governed by a transverse Ising Hamiltonian. Then if we may partition the system into two thermal states, the correlations formed across these two subsystems will be upper bounded by the interaction term of the boundary of these two subsystems. That is the interaction of their edge spins. To prove this consider [21, 48] that as shown before the Gibbs free energy is the minimal free energy

$$F(\hat{\rho}_\beta^{AB}) \leq F(\hat{\rho}_\beta^A \otimes \hat{\rho}_\beta^B). \quad (103)$$

This being said, both free energies maybe associated to a Gibbs entropy since they are associated to thermal states via $F(\hat{\rho}) = \langle \hat{H} \rangle - tS(\hat{\rho})$ giving

$$\mathcal{I}(A : B) = S(\hat{\rho}_\beta^{AB}) - S(\hat{\rho}_\beta^A \otimes \hat{\rho}_\beta^B) \leq \beta \left(\text{tr}\{\hat{H}\hat{\rho}_\beta^A \otimes \hat{\rho}_\beta^B\} - \text{tr}\{\hat{H}\}\hat{\rho}_\beta^{AB} \right). \quad (104)$$

where the LHS is equal to the mutual information by additivity of the entropy. Since for Gibbs states we have local Hamiltonians we have

$$\hat{H} = \hat{H}_A + \hat{H}_B + \hat{H}_I \quad (105)$$

where \hat{H}_I is the interacting term. By definition the expectation values of $\hat{H}_A + \hat{H}_B$ agree for the separable and joint state since they include no interaction

$$\text{tr}\{(\hat{H}_A + \hat{H}_B)\hat{\rho}_\beta^A \otimes \hat{\rho}_\beta^B\} = \text{tr}\{(\hat{H}_A + \hat{H}_B)\hat{\rho}_\beta^{AB}\} \quad (106)$$

This gives

$$\mathcal{I}(A : B)_{\rho_\beta^{AB}} \leq \beta \left(\text{tr}\{\hat{H}\}I\hat{\rho}_\beta^A \otimes \hat{\rho}_\beta^B\} - \text{tr}\{\hat{H}_I\}\hat{\rho}_\beta^{AB} \right) \quad (107)$$

which can be manipulated through the usual operator norm inequalities

$$\leq \|\hat{H}_I\| \left(\|\hat{\rho}_\beta^A \otimes \hat{\rho}_\beta^B - \hat{\rho}_\beta^{AB}\| \right) \leq \|\hat{H}_I\| \times \|\hat{\rho}_\beta^A \otimes \hat{\rho}_\beta^B - \hat{\rho}_\beta^{AB}\| \quad (108)$$

$$\leq \|\hat{H}_I\| \times \left(\|\hat{\rho}_\beta^A \otimes \hat{\rho}_\beta^B\| + \|\hat{\rho}_\beta^{AB}\| \right) = 2\|\hat{H}_I\|. \quad (109)$$

Finally we have

$$\mathcal{I}(A : B)_{\rho_\beta^{AB}} \leq 2\beta\|\hat{H}_I\|. \quad (110)$$

2.1.3 Non-Gibbsian Equilibrium States

Such a state is still weakly coupled to its bath such that it does not continuously receive energy from the bath, but it differs from a Gibbs state in that correlations may be established with the bath. Thus, the dynamics of such a system are implicitly non-Markovian. In this context, heat may not exclusively be associated with changes in the state as some heat may contribute to the maintenance of these established correlations.

In such a context, one assumes that some reduced part of the ensemble can be thought of as a stationary Gibbs state

$$\hat{\sigma} = \frac{e^{-\beta(\hat{H}_\Delta + \Delta)}}{\mathcal{Z}_\Delta} \quad (111)$$

where \hat{H}_Δ is the reduced Hamiltonian, \mathcal{Z}_Δ is the modified partition function and Δ includes the interaction between the system and bath as well as contributions due to quantum correlations. Now we can quantify the entropy of the non-Gibbsian state using the von Neumann entropy which is well defined for all quantum states and use this to modify the quantum first law for Gibbs states (99) to a non-Gibbsian context by considering the difference in entropy between this non-Gibbsian state and the reduced stationary state (101). Consider the modification to (97)

$$dS = \beta(\mathcal{E} - \mathcal{F}) = \beta(\text{tr}\{\hat{\sigma}\hat{H}\} - (F + tD(\hat{\sigma}||\hat{\rho}))) \quad (112)$$

where \mathcal{E} is the internal energy given by the free energy of the reduced Gibbs state and we use difference in entropy (relative entropy) between the entropy of the stationary state and the non-Gibbsian state to define the *information free energy*⁷ [49]. For an isothermal, quasistatic process we have

$$dS = \beta(\text{tr}\{d\hat{\sigma}\hat{H}\} + (\text{tr}\{\hat{\sigma}d\hat{H}\} - dF)) \quad (113)$$

allowing us to identify

$$dS = \beta(\delta Q_{tot} - \delta Q_c) = \beta\delta Q_{ex} \quad (114)$$

and

$$d\mathcal{E} = \delta W_{ex} + \delta Q_{ex} \implies dE = tdS + dF. \quad (115)$$

Most notable here is the definition of $\delta Q_c = dF - \text{tr}\{\hat{\sigma}d\hat{H}\}$ the energetic cost of maintaining coherence and quantum correlations established with the bath. It is good to acknowledge that the robustness of the first law is due to the phenomenological nature of equilibrium thermodynamics and so it stands to reason that the first law should hold under minor alterations.

With these definitions in hand we can now present the result of Gardas and Deffner [35] which shows that the efficiency of the Carnot engine rings through also for equilibrium thermodynamics in a quantum context.

⁷This is a non-equilibrium state function [49]

2.1.4 Quantum Carnot Cycles & the 2nd Law

Let's think of a quantum system that is weakly coupled to two equilibrium heat baths such that one bath is hotter than the other, say $T_1 > T_2$. Correlations may be established between the baths and the system and as such for generality we use the structure of non-Gibbsian equilibrium states established above, to describe the thermodynamics of the quantum system. Given the setup we can anticipate a Carnot cycle taking place with four strokes, alternating between isothermal and isentropic processes (during which and extensive control parameter ω is varied).

1 \rightarrow 2 **1st Isothermal stroke** - Heat $Q_{ex,1}$ is absorbed from the T_1 reservoir by the system allowing it to carry out work $W_{ex,1}$ on the environment at constant temperature.

$$W_{ex,1} = \mathcal{F}(w_2, T_1) - \mathcal{F}(w_1, T_1) \quad Q_{ex,1} = T_1(\mathcal{S}(\omega_2, T_1) - \mathcal{S}(\omega_1, T_1)) \quad (116)$$

Notice that the work carried out is denoted by the variation of the work parameter and is expressed in terms of the change in free energy. On the other hand, the change in heat is expressed in terms of change in entropy.

2 \rightarrow 3 **1st Isentropic stroke** - The temperature gradient has been equalised but the system continues to do work, cooling it to T_2 . Since there is no exchange, there is no entropic cost, $\Delta\mathcal{S} = 0$. As such, the work is equal to the change in energy

$$W_{ex,2} = \Delta\mathcal{E} = \mathcal{E}(\omega_3, T_2) - \mathcal{E}(\omega_2, T_1) = \Delta\mathcal{F} - (T_1 - T_2)\mathcal{S}(\omega_3, T_2) \quad (117)$$

which we've expressed in terms of the free energy.

3 \rightarrow 4 **2nd Isothermal stroke** - The work $W_{ex,3}$ is performed on the system such that the system exchanges heat $Q_{ex,3}$ with the reservoir at T_2 to remain at equilibrium with T_2 .

$$W_{ex,3} = \Delta = \Delta\mathcal{F}(\omega_4, T_2) - \Delta\mathcal{F}(\omega_3, T_2) \quad Q_{ex,3} = T_2(\mathcal{S}(\omega_4, T_2) - \mathcal{S}(\omega_3, T_2)). \quad (118)$$

4 \rightarrow 1 **2nd Isentropic stroke** - Further work is carried out on the system but it is not allowed to exchange heat with the bath at T_2 , as such it again reaches the temperature T_1 , completing the cycle

$$W_{ex,4} = \Delta\mathcal{E} = \Delta\mathcal{F} - (T_1 - T_2)\mathcal{S}(\omega_1, T_1) \quad (119)$$

reflecting the isentropic condition $\mathcal{S}(\omega_1, T_1) = \mathcal{S}(\omega_4, T_2)$ as in 2 \rightarrow 3.

From the above we find that the efficiency of this cycle is given by

$$\eta = \frac{\sum_i W_{ex,i}}{Q_{ex,1}} = 1 - \frac{T_2}{T_1} \quad (120)$$

which is in agreement with the classical Carnot efficiency. Note that in the *output* portion of the efficiency ratio we are including the thermodynamic cost to maintain the non-Gibbsian correlations.

As a result, we have that the Carnot statement of the 2nd Law of thermodynamics is observed even in a quantum context. That is *no engine operating between two heat reservoirs can be more efficient than a Carnot engine operating between those same reservoirs*.

Having discussed the physics of equilibrium thermodynamics in the quantum regime we now turn our attention to non-equilibrium thermodynamics in this context. A situation which within short time dynamics is much more prevalent than its counterpart.

2.2 Quantum Fluctuation Theorems

The celebrated results of Jarzynski [29] and Crooks [30] that allowed people to begin to quantify nonequilibrium work in terms of free energy differences was soon applied to quantum systems by Tasaki [50], giving the Tasaki-Crooks quantum fluctuation theorem. This work was redeveloped in the language of characteristic functions as opposed to distribution functions and expanded to more general quantum systems some time later by Campisi, Talkner and Hänggi [51]. Two excellent and comprehensive reviews of this area are [32, 36]. Very recently, the Tasaki-Crooks quantum fluctuation theorem was experimentally validated using IBM quantum computers by Campisi and others [52].

2.2.1 Work is not an Observable

What makes it difficult to recast the fluctuation theorems in a quantum setting is mainly dealing with the notion of Work. Work is not an observable [53] and so cannot have an associated operator in any sense. Several attempts were made to develop such a formalism but in [53] it was shown that this can conclusively bear no fruit. This should not be too surprising if one keeps in mind the 1st law of thermodynamics as described in the first section. Work is not an exact differential, that is it has to be described through a process and as such in a quantum context cannot be described by some Hermitian operator whose eigenvalues can be obtained by a single projective measurement. We must therefore make two measurements at separate times to ascertain the energy of the system at different points and through this the work.

This formalism for work known as the two-time or two-point energy measurement approach is still contentious. The act of measurement has an associated thermodynamic cost to it which spoils the completeness of this framework. This puts a thermodynamic burden on a measuring device or observer which impedes the thermodynamics of such a non-equilibrium system from being self-contained. This was pointed out and remedied in [54] fairly recently where a technique involving differences in the energy eigenvalues is used to define the average work. A version of Jarzynski's equality was shown to hold in such a scheme. For our purposes we will stick to the two-point approach.

2.2.2 Tasaki-Crooks Fluctuation Theorem and the quantum Jarzynski equality

Need to write out this derivation.

2.3 Quantum Landauer Bounds

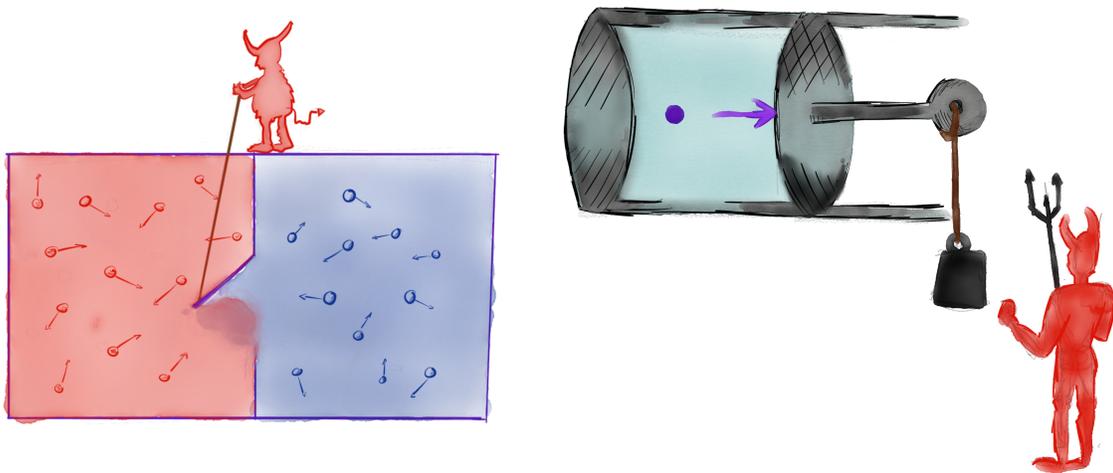
The 2nd law of thermodynamics gives us information about the nature of entropy in a system. We expect it to always be monotonically increasing. Landauer bounds also give us information about entropy but do this in relation to heat dissipation to the bath such that

$$\beta\Delta Q \geq \Delta S. \quad (121)$$

More recently, this bound has been expanded upon in equilibrium and non-equilibrium quantum thermodynamic settings [55, 1, 2, 44] offering a rich tool set to examine the relationships between heat and information exchanges. In this section we will introduce the major results related to these new quantum Landauer bounds and briefly introduce the original context which led to (121) in the first place.

2.3.1 Landauer's Erasure Principle, Szilard's Engine & Maxwell's Demon

In the late 19th century, Maxwell [56] came up with a thought experiment that seemingly violated the 2nd law of thermodynamics. He envisaged a gas in a box with a trap door that may be opened and closed in the middle to create a partition, and a demon in control of this trap door. With perfect knowledge of the velocities and random motions of the constituents of this gas, the demon can open and close the trap door systematically separating faster particles one side and slower ones on the other. Decreasing the entropy of the system and violating the 2nd law of thermodynamics. Half a century later, Szilard [57] refined this thought experiment making it more tractable by imagining a single particle gas in a container. This container may be split into two partitions, put into contact with a bath and a piston added to it. If the demon is aware of the position of the particle then it may constrain the particle to half the vessel such that when a piston is connected to it isothermal expansion occurs resulting in work. This results in [58]



$$W_{\text{extracted}} = \Delta Q = t\Delta S = k_B t \ln 2 \quad (122)$$

where the 2 appears as a result of the two microstates related to the two partitions of the vessel and we have a full conversion of heat into work, a process which violates the 2nd law of thermodynamics. Landauer's erasure principle is what rectifies this violation. A naïve argument would be that for the demon to acquire knowledge of the particle he is affecting the entropy of the system in such a way as to balance this work being done, but classically measurement entails no work. The most complete argument was given by Bennett [59] and involves the notion of memory. Here, the argument is made that for work extraction to occur cyclically the demon must erase his memory of the position of the particle at each new cycle. Giving

$$W_{\text{erasure}} = t\mathcal{H} = -k_B t \ln 2 \quad (123)$$

where \mathcal{H} is the information content or Shannon entropy of the erased information. This is Landauer's erasure principle in action, where a bit of information being deleted results in heat dissipation. Clearly, the sum of the work contributions is 0, reconciling our paradox and violation of the 2nd law.

Shannon Entropy

In his seminal work [60], Claude Shannon wanted to come up with a quantity to articulate the amount of information carried by a string or message. Particularly, in the context of encoding where information may be lost on the way. To do so, he felt it was a good idea to quantify how *surprising* some outcome would be i.e. unlikely. So we have some quantity

$$\mathcal{H}(x_i) \propto \frac{1}{\mathcal{P}(x_i)} \quad (124)$$

but when the event is going to occur with certainty this would give a surprise of 1 also, so a way of dealing with this is to use a logarithmic function

$$\mathcal{H}(x_i) = \ln \frac{1}{\mathcal{P}(x_i)} \quad (125)$$

so for a whole probability distribution we have

$$\mathcal{H}(x_i) = \sum_i \mathcal{P}(x_i) \ln \frac{1}{\mathcal{P}(x_i)} = - \sum_i \mathcal{P}(x_i) \ln \mathcal{P}(x_i) \quad (126)$$

which we know to be the Shannon entropy. Evidently, this is nothing more than the von Neumann entropy for classical probability distributions.

2.3.2 Reeb & Wolf's Landauer Bound

To obtain the more general result (121) in a quantum context for an initial state weakly coupled to a bath at equilibrium with inverse temperature β

$$\hat{\rho}_{SB}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_B^\beta \quad (127)$$

with dynamics governed by

$$\hat{H}_{tot}(t) = \hat{H}_S(t) + \hat{H}(t)_B + \hat{H}_I(t) \quad (128)$$

where the system will be driven out of equilibrium. The final state is by the unitary time-evolution operator

$$\hat{U}_{SB} = \hat{T} \exp \left(-\frac{i}{\hbar} \int_0^\tau dt \hat{H}_{tot}(t) \right) \implies \hat{\rho}_{SB}(\tau) = \hat{U}_{SB} \hat{\rho}_{SB} \hat{U}_{SB}^\dagger \quad (129)$$

where \hat{T} is the time ordering operator. Consider the definition for the entropy production [36]

$$\Sigma = \Delta S - \beta \Delta Q \quad (130)$$

where ΔS is the change in von Neumann entropy between the initial and final state and δQ is the heat exchanged with the bath.

$$\Delta S = S(\hat{\rho}_S(\tau)) - S(\hat{\rho}_S(0)) \quad \Delta Q = \text{tr} \left\{ \hat{H}_B \hat{\rho}_B^\beta \right\} - \text{tr} \left\{ \hat{H}_B \hat{\rho}_B(\tau) \right\} \quad (131)$$

$$\Sigma = -\text{tr} \left\{ \hat{\rho}_S(\tau) \ln \hat{\rho}_S(\tau) \right\} + \text{tr} \left\{ \hat{\rho}_S(0) \ln \hat{\rho}_S(0) \right\} - \beta \left(\text{tr} \left\{ \hat{H}_B \hat{\rho}_B^\beta \right\} - \text{tr} \left\{ \hat{H}_B \hat{\rho}_B(\tau) \right\} \right) \quad (132)$$

$$= -\text{tr} \left\{ \hat{\rho}_S(\tau) \ln \hat{\rho}_S(\tau) \right\} + \beta \text{tr} \left\{ \hat{H}_B \hat{\rho}_B(\tau) \right\} + \text{tr} \left\{ \hat{\rho}_S(0) \ln \hat{\rho}_S(0) \right\} - \beta \text{tr} \left\{ \hat{H}_B \hat{\rho}_B^\beta \right\} \quad (133)$$

by linearity of trace

$$= \text{tr} \left\{ \hat{\rho}_{SB}(\tau) \left(-\ln \hat{\rho}_S(\tau) + \beta \hat{H}_B \right) \right\} + \text{tr} \left\{ \hat{\rho}_{SB}(0) \left(-\ln \hat{\rho}_S(0) + \beta \hat{H}_B \right) \right\} \quad (134)$$

$$= \mathcal{F}(\hat{\rho}_{SB}(\tau)) - \mathcal{F}(\hat{\rho}_{SB}(0)) \quad (135)$$

$$= \beta^{-1} [D(\hat{\rho}_{SB}(\tau) || \hat{\rho}_{SB}(0))] \quad (136)$$

and the relative entropy is known to be non-negative giving

$$\Sigma = \Delta S - \beta \Delta Q \geq 0 \quad (137)$$

$$\therefore \beta \Delta Q \geq \Delta S, \quad (138)$$

the generalised Landauer bound (121). This bound relates the heat exchanged with the bath to the entropy change in the system, in some sense saying that the heat exchanged with the bath is going to bound the correlations formed with the bath. Explicitly [36] imagine a situation where

$$\frac{1}{2} (|0\rangle\langle 0| + |1\rangle\langle 1|) \rightarrow |0\rangle\langle 0|, \quad (139)$$

here the von Neumann entropy has changed from 2 to 0, meaning that we have at least $|Q| = \beta^{-1} \ln 2$ dissipated to the bath as a result of erasure, recovering the original statement of Landauer's principle. A version of this argument is given in [37] but some years later, this line of attack was improved drastically by Reeb & Wolf [55] where they were able to turn this inequality into a more general equality using the mutual information and relative entropy as well as giving a sharper and more explicit version of the inequality for finite reservoirs. We will now review the main results of [55]. Before this we restate the notation of [55], in particular Δ is the entropy change in the reservoir

$$\Delta = S(\hat{\rho}'_R) - S(\hat{\rho}_R), \quad (140)$$

$S(A|B)$ is the conditional entropy of a bipartite state where A is conditioned on B

$$S(A|B) = S(\hat{\rho}_{AB}) - S(\hat{\rho}_B) \quad (141)$$

and the decrease in the entropy of the system is denoted

$$\Delta S = S(\hat{\rho}_S) - S(\hat{\rho}'_S). \quad (142)$$

The 2nd Law Lemma *Let $\hat{\rho}_{SR} = \hat{\rho}_S \otimes \hat{\rho}_R$ be the initial state of a system where a finite reservoir is in a Gibbs state $\hat{\rho}_R = \frac{e^{-\beta \hat{H}}}{\mathcal{Z}}$ with final state $\hat{\rho}'_{SR} = \hat{U}(\hat{\rho}_S \otimes \hat{\rho}_R)\hat{U}^\dagger$. Then*

$$\Delta = \Delta S + I(S' : R') \geq \Delta S, \quad (143)$$

the reservoir's entropy increase Δ is larger than the system's entropy decrease ΔS . Consider $\Delta - \Delta S$ we have

$$\Delta - \Delta S = S(\hat{\rho}'_R) - S(\hat{\rho}_R) + S(\hat{\rho}'_S) - S(\hat{\rho}_S) \quad (144)$$

so by additivity of the von Neumann entropy we have

$$= S(\hat{\rho}'_R) + S(\hat{\rho}'_S) - S(\hat{\rho}_{SB}) = S(\hat{\rho}'_R) + S(\hat{\rho}'_S) - S(\hat{\rho}'_{SB}) \quad (145)$$

by the invariance of global entropy under unitary evolution. But the equation on the right is nothing more than the mutual information across the system and the bath after evolution

$$= \mathcal{I}(S' : R')_{\rho'_{SR}} \geq 0 \quad (146)$$

since the mutual information is non-negative by Jensen's inequality. Finally giving,

$$\Delta = \Delta S + \mathcal{I}(S' : R') \geq \Delta S. \quad (147)$$

Notably, the change of entropy in the bath is equal to the change of entropy in the system when the mutual information is 0. This shows that $\Delta = \Delta S$ occurs if no correlations are formed between the bath and the system. One can also interpret this as a generalisation of Landauer's principle showing that the change in entropy of the bath, and so heat exchanged with the bath by the first law, is greater than the change in entropy of the system.

Before moving on, note that the relative entropy has the property

$$D(\sigma||\rho) = \infty \iff \text{supp}[\sigma] \not\subseteq \text{supp}[\rho] \quad (148)$$

where $\text{supp}[\hat{\rho}]$ is $x \in \mathbb{C} : \hat{\rho}(x) \neq 0$.

Equality form of Landauer's Principle

Let $\hat{\rho}_{SR} = \hat{\rho}_S \otimes \hat{\rho}_R$ be the initial state of a system where a finite reservoir is in a Gibbs state $\hat{\rho}_R = \frac{e^{-\beta\hat{H}}}{\mathcal{Z}}$: $\beta \in [-\infty, +\infty]$ with final state $\hat{\rho}'_{SR} = \hat{U}(\hat{\rho}_S \otimes \hat{\rho}_R)\hat{U}^\dagger$. Then

$$\beta\Delta Q = \Delta S + \mathcal{I}(S : R) + D(\hat{\rho}'_R||\hat{\rho}_R). \quad (149)$$

To begin with consider $\beta \in (-\infty, \infty)$ by the 2nd Law Lemma we have

$$\Delta S + \mathcal{I}(S' : R') = \Delta = S(\hat{\rho}'_R) - S(\hat{\rho}_R) \quad (150)$$

$$= -\text{tr}\{\hat{\rho}'_R \ln \hat{\rho}'_R\} + \text{tr}\left\{\hat{\rho}_R \ln \frac{e^{-\beta\hat{H}}}{\mathcal{Z}}\right\} \quad (151)$$

$$= -\text{tr}\{\hat{\rho}'_R \ln \hat{\rho}'_R\} + \text{tr}\{\hat{\rho}_R(-\beta\hat{H} - \hat{1} \ln \mathcal{Z})\} \quad (152)$$

now adding a zero term for pliability and making use of the linearity of trace gives

$$= -\text{tr}\{\hat{\rho}'_R \ln \hat{\rho}'_R\} - \beta \text{tr}\{\hat{\rho}_R \hat{H}\} - \ln \mathcal{Z} \text{tr}\{\hat{\rho}_R\} + \beta \text{tr}\{\hat{\rho}'_R \hat{H}\} - \beta \text{tr}\{\hat{\rho}'_R \hat{H}\} \quad (153)$$

$$= -\text{tr}\{\hat{\rho}'_R \ln \hat{\rho}'_R\} + \beta \text{tr}\{\hat{H}(\hat{\rho}'_R - \hat{\rho}_R)\} - \ln \mathcal{Z} - \beta \text{tr}\{\hat{\rho}'_R \hat{H}\} \quad (154)$$

$$= -\text{tr}\{\hat{\rho}'_R \ln \hat{\rho}'_R\} + \beta\Delta Q - \ln \mathcal{Z} \text{tr}\{\hat{\rho}'_R\} + \text{tr}\{\hat{\rho}'_R \ln e^{-\beta\hat{H}}\} \quad (155)$$

$$= -\text{tr}\{\hat{\rho}'_R \ln \hat{\rho}'_R\} + \beta\Delta Q + \text{tr}\left\{\hat{\rho}'_R \left(\ln e^{-\beta\hat{H}} - \ln \mathcal{Z}\right)\right\} \quad (156)$$

$$= \beta\Delta Q - \text{tr}\{\hat{\rho}'_R \ln \hat{\rho}'_R\} + \text{tr}\{\hat{\rho}'_R \ln \hat{\rho}_R\} \quad (157)$$

$$= \beta\Delta Q - D(\hat{\rho}'_R||\hat{\rho}_R) \quad (158)$$

and finally

$$\beta\Delta Q = \Delta S + \mathcal{I}(S : R) + D(\hat{\rho}'_R||\hat{\rho}_R). \quad (159)$$

For the cases that $\beta = \pm\infty$ consider that $\hat{\rho}_R = \frac{\hat{P}_g}{\text{dim } \hat{P}_g}$, the normalised projection operator onto the ground state of \hat{H} . Meaning $\text{tr}\{\hat{H}\hat{\rho}'_R\} \geq \text{tr}\{\hat{H}\hat{\rho}_R\} \implies \Delta Q \geq 0$. If $\Delta Q = 0$, then $\hat{\rho}'_R$ is supported in the ground state so (150) gives the following in this case

$$S(\hat{\rho}'_R) - S(\hat{\rho}_R) = -\text{tr}\{\hat{\rho}'_R \ln \hat{\rho}'_R\} - \ln \text{dim } \hat{P}_g = -D(\hat{\rho}'_R||\hat{\rho}_R) \quad (160)$$

so both sides of (149) are 0. In the case that $\beta = \pm\infty$ and $\Delta Q > 0$, then $D(\hat{\rho}'_R||\hat{\rho}_R) = \infty$ since $\hat{\rho}'_R$ has support outside the ground state and so outside the support of $\hat{\rho}_R$ so both sides are equal to $\pm\infty$.

2.3.3 Nonequilibrium Landauer Bounds

Need to summarise [1, 2]

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