
Quantifying Dissipation via Thermodynamic Length

Matteo Scandi



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Matteo Scandi

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Theoretical and Mathematical Physics
Ludwig-Maximilians-Universität and
Technische Universität
München

Supervisor: Juan Ignacio Cirac Sasturain

Second Referee: Martí Perarnau-Llobet

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Bring' vor, was wahr ist;
Schreib' so, dass es klar ist
Und verficht's, bis es mit dir gar ist!

Ludwig Boltzmann, *Vorlesungen über
die Principe der Mechanik*

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Introduction

This thesis is a whole divided into three parts: in the first chapter, the framework of quantum thermodynamics is presented, and it is shown how one can define thermodynamic functionals and transformations in complete analogy to the classical case, obtaining a formalism in which the second law can be rigorously demonstrated; the second chapter, on the other hand, is focused on how the quantum mechanical unitary evolution can be generalised to the case in which part of the system is not accessible and how, under some approximations, one can derive an expression of the dissipative dynamics; moreover, it is shown how a quasi-adiabatic thermodynamic protocol can be implemented in this formalism; finally, in the third chapter, the concept of thermodynamic length is introduced and explored. This corresponds to the possibility of defining a metric on the manifold of equilibrium thermal states, whose geodesics will describe optimal finite-time processes. The results studied have been already treated in the literature for the classical case, famously in a paper by Crooks [7]. The derivation given was obtained independently and can be thought as the generalisation of the classical formalism to the case in which the observables do not necessarily commute. Moreover, the formalism is extended to account for imperfect thermalisation. Some applications of this framework have been given in appendix D and E: in the first, it is shown how to minimise the dissipation during a discrete Landauer erasure protocol; in the latter, the optimisation of a Carnot-like quantum thermal machine is used to illustrate how the formalism can be generalised to the strong coupling regime.

The notations used throughout the work have been listed in appendix A, and will be sometimes used without further introduction, in order to keep the exposition clean. The reader is referred to this appendix in case of confusion.

Chapter 1

Elements of quantum information and quantum thermodynamics

The law that entropy always increases holds, I think, the supreme position among the laws of Nature. If someone points out to you that your pet theory of the universe is in disagreement with Maxwell's equations – then so much the worse for Maxwell's equations. If it is found to be contradicted by observation – well, these experimentalists do bungle things sometimes. But if your theory is found to be against the second law of thermodynamics I can give you no hope; there is nothing for it but to collapse in deepest humiliation.

Sir Arthur Stanley Eddington, *The Nature of the Physical World*

In this chapter some elements of quantum information and quantum thermodynamics are listed. In the first two sections the fundamental functionals of quantum information and quantum thermodynamics will be defined and motivated. Moreover, it will be shown how to connect the free energy of a close to equilibrium state to its distinguishability from a thermal state. Then, thermodynamic transformations will be generalised to the quantum regime. Finally, the second law of thermodynamics will be proven in this formalism.

1.1 Fundamental functionals in quantum information

In this section, in order to clarify the motivations behind the introduction of quantum information functionals, their classical counterparts will be first discussed.

In classical information theory the entropy associated to a probability distribution over a discrete space Ω is defined as:

$$S(p) = - \sum_{x \in \Omega} p(x) \log [p(x)].$$

If one interprets Ω as the set of possible outcomes of an experiment and p as the experimental distribution of data, then $S(p)$ can be interpreted as a measure of the ignorance

of the observer about the state x ; this can be understood examining the behaviour of this quantity in limiting cases: if the output of the experiment is deterministic, that is if for some x_0 , $p(x_0) = 1$, then $S(p) = 0$; on the other hand, if all the x are equiprobable, then S attains its maximum.

In analogy with the classical case, one can define the von Neumann entropy of a density matrix ρ as:

$$S(\rho) = -\text{Tr} [\rho (\log [\rho])];$$

this quantity is a suitable candidate for being interpreted as thermodynamic entropy, as it is non negative (with $S(\rho) = 0$ only for pure states), extensive¹ and non decreasing under the action of completely positive trace preserving maps.

A clearer interpretation comes from statistical inference theory, the study of how to deduce a model which best fits a set of experimental data. Assume an experiment to be well described by the distribution p_1 ; then, the probability of observing the sequence of outcomes $\{x_1, \dots, x_n\}$ upon repeating the experiment independently n times is given by:

$$P(\{x_1, \dots, x_n\} | p_1) = \prod_{i=1}^n P(x_i | p_1) = \exp \left(\sum_{i=1}^n \log [P(x_i | p_1)] \right).$$

Thanks to the independence of the different realisations of the experiment, the law of large numbers applies, so that:

$$\sum_{i=1}^n \log [P(x_i | p_1)] \stackrel{n \gg 1}{\approx} -nS(p_1).$$

Since, asymptotically, the dependence on the particular sequence of outcomes becomes progressively irrelevant, one can give the following informal estimate²:

$$P(\{x_1, \dots, x_n\} | p_1) \stackrel{n \gg 1}{\approx} \frac{1}{\exp(nS(p_1))}$$

$$\Rightarrow S(p_1) = \lim_{n \rightarrow \infty} \frac{1}{n} \log [\# \text{ typical sequences}].$$

This result can be understood looking at the two limit cases of perfect knowledge and complete ignorance: in the first case, there will be only one sequence generated by the

¹In this context, one refers to extensivity to be the property that on a product state the entropy decomposes as: $S(\rho \otimes \sigma) = S(\rho) + S(\sigma)$. It should be noted that this equality is not true for arbitrary states: a weaker condition can be proved, namely subadditivity, corresponding to the inequality $S(\rho^{AB}) \leq S(\rho^A) + S(\rho^B)$; this relation can be easily interpreted, accounting for the possible increase in the entropy as a consequence of the the loss of information resulting from neglecting the correlations between the two systems.

²This argument can be made rigorous, see for example [13, 32]. The concept of typicality informally used here refers to the fact that, if one interprets the sequence of experiment's outputs as an element of the sample space of a Bernoulli scheme, the argument just given holds on a full measure set.

probability distribution, so that $S(p_1) = \lim_{n \rightarrow \infty} (1/n) \log [1] = 0$; in the other case, all the possible sequences will be expected, so that the entropy will attain its maximum, namely: $S(p_1) = \lim_{n \rightarrow \infty} (1/n) \log [|\Omega|^n] = \log [|\Omega|]$. As it can be seen, the entropy is connected to the possibility of reducing the number of strings of expected outcomes to a subset of the full phase space; therefore, the bigger the entropy, the less predictive power the distribution p_1 will have or, equivalently, the bigger the ignorance about the state of the system.

Another relevant problem in inference is the one of distinguishing two probability distributions based on the experimental data they produce³. For this reason, it is useful to consider the relative probability of observing a sequence of outcomes $\{x_1, \dots, x_n\}$ given that the state is described by the distribution p_1 or by p_2 ; in formulae:

$$\frac{P(\{x_1, \dots, x_n\} | p_1)}{P(\{x_1, \dots, x_n\} | p_2)} = \exp \left(\sum_{i=1}^n (\log [P(x_i | p_1)] - \log [P(x_i | p_2)]) \right).$$

Assuming the system to be truly described by p_1 , the asymptotic value of the exponent (divided by n) is:

$$S(p_1 || p_2) = \sum_{x \in \Omega} p_1(x) (\log [p_1(x)] - \log [p_2(x)]).$$

This quantity, called relative entropy, translates naturally to the quantum case as:

$$S(\rho_1 || \rho_2) = \text{Tr} [\rho_1 (\log [\rho_1] - \log [\rho_2])],$$

and it is used as one of the canonical measure of distinguishability in quantum information. An important result, known as Klein's inequality, gives the following relationship:

$$S(\rho || \sigma) \geq 0, \quad \text{with equality iff } \rho \equiv \sigma,$$

which can be equivalently restated saying that the relative entropy is a premetric on the space of density matrices; unfortunately though, it cannot be promoted to a metric, since it is not symmetric nor the triangle inequality holds in general.

Finally, in the context of bipartite systems, it is useful to define the mutual information as:

$$I(A|B) := S(\rho^A) + S(\rho^B) - S(\rho^{AB}).$$

This functional has the intuitive interpretation of quantifying the amount of correlation between the two subsystems. It is easy to see that it can be connected to the relative entropy through the identity:

$$I(A|B) = S(\rho^A) + S(\rho^B) - S(\rho^{AB}) = S(\rho^{AB} || \rho^A \otimes \rho^B);$$

then, it trivially follows from Klein's inequality that the mutual information is non negative and equal to zero if and only if the full system is in a product state.

³It is crucial to understand that problems in inference theory are far from being simple issues for experimentalists alone; the intrinsic probabilistic nature of quantum mechanics rises these problems from experimental nuances to fundamental limitations on the possibility of distinguishing two quantum states.

1.2 Thermodynamic functionals and their expansions

In quantum thermodynamics the Gibbs state associated to a Hamiltonian H_0 is defined as:

$$\omega_\beta(H_0) \equiv \omega_0 := \frac{e^{-\beta H_0}}{\text{Tr}[e^{-\beta H_0}]} \equiv \frac{e^{-\beta H_0}}{Z_0}.$$

In strict analogy with the procedure to deduce the canonical ensemble in classical statistical mechanics, this functional form can be derived fixing an average energy $\langle H_0 \rangle_\rho = \text{Tr}[\rho H_0]$ and requiring ρ to maximise the entropy; in this context, β can be identified with the Lagrange multiplier used to enforce the constraint⁴. Another possible characterisation of the Gibbs state is demanding ω to be *completely passive*, meaning that one cannot extract any work from an arbitrary number of copies of ω via unitary transformations alone [26]. In this regard, it is useful to define, in analogy to the classical case, the free energy of a state as:

$$F[(\rho; H)_\beta] = \langle H \rangle_\rho - \theta S(\rho),$$

where θ is the temperature and k_B is set to 1. It is worth noticing that Gibbs states minimise the free energy for fixed $\langle H \rangle$, so that the two definition above clearly appear to be equivalent.

Thermodynamical functionals evaluated on a Gibbs state take a particularly simple form, resembling their classical counterparts; the entropy of a Gibbs state, for example, is given by:

$$S(\omega_\beta(H)) = \beta \langle H \rangle_\omega + \log[Z_H],$$

so that the free energy takes the form:

$$F[\omega_\beta(H)] = -\theta \log[Z_H].$$

A useful identity is given by the following:

Lemma 1. *Let $\omega_\beta(H)$ be a thermal state and ρ an arbitrary density matrix; then the following identity holds:*

$$\beta \Delta F \Big|_{\omega_\beta(H)}^\rho := \beta(F[(\rho; H)_\beta] - F[\omega_\beta(H)]) = S(\rho || \omega_\beta(H)). \quad (1.1)$$

Proof. By direct calculation:

$$\begin{aligned} \beta \Delta F \Big|_{\omega_\beta(H)}^\rho &= \beta(F[(\rho; H)_\beta] - F[\omega_\beta(H)]) = \beta \text{Tr}[H\rho] + \text{Tr}[\rho \log[\rho]] + \log[Z_H] = \\ &= \text{Tr}[\rho \log[\rho]] - \text{Tr}\left[\rho \log\left[\frac{e^{-\beta H}}{Z_H}\right]\right] = S(\rho || \omega_\beta(H)). \end{aligned}$$

□

⁴This method is common in information theory, and goes under the name of principle of maximum entropy; for this reason this type of derivation is often referred to as information theoretical. The simple idea underlying this procedure is to choose the most unconstrained distribution which reflects the information one has about the system; for example, in this case, in which one assumes to have experimental access only to the average energy, the distribution is chosen to be the one for which the maximum ignorance about the system is encoded given this constraint.

It is worth noticing that in this way a purely mathematical object, the relative entropy, which describes the distinguishability of two probability distributions, is connected with a physically quantity, namely the difference between the non equilibrium free energy and the equilibrium one. Thanks to the classical connection between free energy and work, this quantity can be interpreted as the work one can do using a system out of equilibrium as a resource and, for this reason, this quantity is sometimes referred to in the literature as availability.

To clearly understand the importance of identity (1.1), it is interesting to examine the mixing paradox, a variation of the Gibbs paradox: take two different ideal gases in two separate compartments of a box, divided by a sliding door; opening the door will increase the entropy of the system, since the volume available to each of the two substances increases. The paradox then arises from the following observation: if the degree of distinguishability between the two gases is finite, then the entropy will always increase by a fixed amount, while if the distinguishability is zero, since the macrostate will not be affected by the opening of the door, the entropy will stay constant. This apparent discontinuity has been used to argue that there is some subjectivity in the description of a thermodynamics state: in fact, it is not that insensible to think that an experimentalist which has more control over a system, which can come from the ability of better probing the nature of the substances contained, will loose the extra work which could come from exploiting this information, while someone who didn't have perfect experimental control from the beginning won't be affected by the mixing [17]. This kind of argument can be formulated in the quantum framework as well, and it can be seen as a possible justification of the interpretation of thermodynamics as a resource theory. What is different in the quantum realm is the possibility of objectively defining what it actually means for two systems to be intrinsically difficult to be distinguished, quantity which, as it was shown in the previous section, is measured by the relative entropy: for this reason, the relative entropy itself can be interpreted as the entropy produced during a thermalisation process. Then, lemma 1 can be seen as the formalisation of this intuition. Moreover, it can be seen how the discontinuity cease to exists in the quantum regime, since $S(\rho||\omega_\beta(H))$ approaches continuously 0 as $\rho \rightarrow \omega_\beta(H)$.

Some expansion will be now given, which will be of use in the investigation of system close to equilibrium and in order to better understand quasi-isothermal processes.

Before starting, it is convenient to define the operator associated to a full rank density matrix ρ , \mathcal{J}_ρ and its inverse:

$$\mathcal{J}_\rho[A] = \int_0^1 d\tau \rho^{1-\tau} A \rho^\tau \quad \mathcal{J}_\rho^{-1}[A] = \int_0^\infty dx (\rho + x)^{-1} A (\rho + x)^{-1}$$

The following results are consequences of lengthy but somehow straightforward calculations and, for this reason, their demonstration is deferred to the appendix B.

Let H_t be a smooth family of Hamiltonians, and let $\omega_\beta(H_t)$ be the corresponding family of Gibbs states; then one can give the expansion:

$$\omega_t =_{\mathcal{O}(t^2)} \omega_0 + t\omega'_0 = \omega_0 \left(\mathbb{1} - \beta t \left[\omega_0^{-1} \mathcal{J}_{\omega_0} [H'_0] - \langle H'_0 \rangle_{\omega_0} \right] \right).$$

This expansion is useful in order to derive the following expression for the change of free energy between two close thermal states:

$$\begin{aligned} \beta \Delta F \Big|_{\omega_\beta(H)}^{\omega_\beta(H+\varepsilon H')} &= S(\omega_\beta(H+\varepsilon H') || \omega_\beta(H)) =_{\mathcal{O}(\varepsilon^3)} \frac{\varepsilon^2}{2} \left(\text{Tr} [H' \mathcal{J}_\omega [H']] - \langle H' \rangle_\omega^2 \right) = \\ &= \frac{\varepsilon^2}{2} \left(\int_0^1 d\tau \text{Tr} [\omega^{1-\tau} H' \omega^\tau H'] - \langle H' \rangle_\omega^2 \right) =: \frac{\varepsilon^2}{2} \text{cov}_\omega(H', H'), \end{aligned}$$

where the generalised covariance commonly used in linear response theory [20] has been implicitly defined. This expansion is a consequence of a slightly more general result: given an arbitrary state ρ and a traceless perturbation ρ_1 , one has that:

$$S(\rho + \varepsilon \rho_1 || \rho) =_{\mathcal{O}(\varepsilon^3)} \frac{\varepsilon^2}{2} \text{Tr} [\rho_1 \mathcal{J}_\rho^{-1} [\rho_1]] = \frac{\varepsilon^2}{2} \int_0^\infty dx \text{Tr} [\rho_1 (\rho + x)^{-1} \rho_1 (\rho + x)^{-1}]; \quad (1.2)$$

plugging the expansion for the thermal state in equation 1.2, one gets the expression above.

1.3 Quantum thermodynamical transformations

A thermodynamic protocol is described as a continuous or discrete trajectory in the thermodynamic space, which is defined as the collection of points of the form $(\rho; H)_\beta$, where:

1. $\beta = (k_B \theta)^{-1}$ indicates the inverse temperature ($\beta \in \mathbb{R}^+$) of the external bath, which is assumed to be an infinite dimensional system in the Gibbs state $\omega_{beta}(H^B)$ to which the system is weakly coupled;
2. ρ is a full rank density matrix which indicates the state of the system, and
3. H is a traceless⁵ Hermitian operator on the state space, which denotes the system Hamiltonian.

The case in which $\rho = \omega_{beta}(H)$ will play a particular role in what follows, so the notation $(\omega; H)_\beta$ will be reserved to the case in which ω is the thermal state of the base point Hamiltonian. It can be seen that, since for any ρ one can give a H such that $H \rightarrow \rho = e^{-\beta H} / Z$, the space of ρ s and the space of H s are diffeomorphic. Thanks to the diffeomorphism between the space of Hermitian operators and \mathbb{R}^N (for some suitable N), the thermodynamic space is then diffeomorphic to \mathbb{R}^{2N+1} .

Given an arbitrary point $(\rho_0; H_0)_{\beta_0}$, it is not in general possible to reach all the manifold via thermodynamic transformations; in particular, the points accessible are given by the three classes of operations:

⁵This restriction is justified from the possibility of decomposing any operators as:

$$H = \text{Tr} [H] \mathbb{1} + \hat{H}$$

where \hat{H} is traceless and the first term only corresponds to a constant shift in the energy.

1. Quenches: corresponding to a change in the system Hamiltonian so fast that the state will be unaffected. Then, the point can be mapped as:

$$(\rho_0; H_0)_{\beta_0} \longrightarrow (\rho_0; H_x)_{\beta_0};$$

2. Isothermal transformations: corresponding to a change in some parameters of the Hamiltonian, while in contact with a bath, so that the system continuously tries to reach the equilibrium state. Indicating with $V_t^{(H)}$ the equilibration map with steady state $(\omega; H)_{\beta_0}$, the points reachable can be expressed by:

$$(\rho_0; H_0)_{\beta_0} \longrightarrow \left(V_t^{(H_x)} [\rho_0]; H_x \right)_{\beta_0} \quad t \geq 0;$$

3. Changes in β : corresponding to the possibility of connecting the system with baths at different temperatures:

$$(\rho_0; H_0)_{\beta_0} \longrightarrow (\rho_0; H_0)_{\beta_x}.$$

It is possible to associate to each point $(\rho; H)_\beta$ in the thermodynamic space the internal energy as:

$$U = \text{Tr} [\rho H].$$

Moreover, in analogy with the classical case, one can define the work done by the system on the environment during the transformation $(\rho_t; H_t)_{\beta_t}$, realised in time T , as:

$$W = - \int_0^T dt \text{Tr} [\rho_t \dot{H}_t]; \quad (1.3)$$

this definition can be thought as the generalisation of the one for the work done during a discrete transformation $(\rho_1; H_1)_{\beta_1} \rightarrow (\rho_2; H_2)_{\beta_2}$:

$$W = \text{Tr} [\rho_1 (H_1 - H_2)],$$

which can be simply interpreted as the average energy difference due to the change of Hamiltonian. From the formal expression of the first law of thermodynamics:

$$dU = -dW + dQ$$

one can give an expression of the heat absorbed by the system (dQ) as:

$$dQ = dU + dW = (\text{Tr} [\rho_t H_t]' - \text{Tr} [\rho_t \dot{H}_t]) dt = \text{Tr} [\dot{\rho}_t H_t] dt, \quad (1.4)$$

which, again, can be thought as the continuous version of the discrete case:

$$\Delta Q = \text{Tr} [H_2 (\rho_2 - \rho_1)].$$

Lastly, it will be useful to define two particular classes of ideal transformations, isothermals and adiabatics, which will be used to define the quantum Carnot cycle in appendix E. Then, the ideal isothermal transformation corresponding to a parametric family of Hamiltonians H_t at temperature $\theta = \beta^{-1}$ is simply given by the trajectory in the thermodynamical space $(\omega_t; H_t)_\beta$.

On the other hand, given the thermal state of a Hamiltonian H at temperature θ , the points reachable via an adiabatic transformation $\mathcal{A} \left[(\omega; H)_\beta \right]$ are given by the implicit expression:

$$(\rho_x; H_x)_{\beta_x} \in \mathcal{A} \left[(\omega; H)_\beta \right] \iff \rho_x = \frac{e^{-\beta_x H_x}}{\text{Tr} [e^{-\beta_x H_x}]} \quad \text{and} \quad \rho_x \equiv \omega_\beta(H). \quad (1.5)$$

The first condition means that under an adiabatic transformation the system always appears as it were in the thermal state of each Hamiltonian; on the other side, the second condition is the defining property of an adiabatic transformation, namely that the heat transfer is zero; this follows naturally from the definition (1.4) and the simple fact that ρ is unchanged during the transformation. This last property is important, because it implies that the work done in an adiabatic transformation $(\rho_1; H_1)_{\beta_1} \rightarrow (\rho_2; H_2)_{\beta_2}$ is a function of state, which means that it depends only on its endpoints, namely for any trajectory in the thermodynamic space one has:

$$W = -\Delta U = \text{Tr} [\rho_1 (H_1 - H_2)].$$

1.4 Second law of thermodynamics

Whenever one defines a mathematical object which is supposed to retain some physical meaning, there should be some concern about whether the definition is actually in agreement with experience; in doing so, much attention should be put in order not to be dragged astray by some superficial similarities or deceptive nomenclature. In order to understand this point, one should consider how the Shannon entropy got its name⁶ and why it is in fact problematic to identify this entropy with the thermodynamic one. For sure, the analogies shown in the previous sections between the classical formalism of equilibrium thermodynamics, which is well understood and experimentally proven, and the novel quantum setting already give some reassurance that the definitions given could actually mirror reality; if, though, the second law of thermodynamics wouldn't be true in this formalism, some serious concerns about the actual significance of this theory should rise. Therefore, it is now shown how one can deduce the law which, to say it with Eddington words, *holds*

⁶Shannon himself explains it how [36]: "My greatest concern was what to call it. I thought of calling it "information", but the word was overly used, so I decided to call it "uncertainty". When I discussed it with John von Neumann, he had a better idea. Von Neumann told me: «You should call it entropy, for two reasons. In the first place your uncertainty function has been used in statistical mechanics under that name, so it already has a name. In the second place, and more important, no one really knows what entropy really is, so in a debate you will always have the advantage»".

the supreme position among the laws of Nature" in this formalism.

Firstly, it should be noticed that the entropy is constant under unitary evolution $\rho_t := U_t \rho_0 U_t^\dagger$, thanks to the cyclicity of the trace:

$$S(\rho_t) = -\text{Tr} \left[U_t \rho_0 U_t^\dagger \log \left[U_t \rho_0 U_t^\dagger \right] \right] = -\text{Tr} \left[U_t \rho_0 U_t^\dagger U_t \log [\rho_0] U_t^\dagger \right] = -\text{Tr} [\rho_0 [\log(\rho_0)]] = S(\rho_0).$$

This means that the classical property of the entropy of staying constant under reversible transformations is satisfied in the quantum formalism as well.

The change in the entropy for the system and for the environment are defined as:

$$\begin{cases} \Delta S := S(\text{Tr}_B [\rho_t^{AB}]) - S(\text{Tr}_B [\rho_0^{AB}]) \\ \Delta := S(\text{Tr}_A [\rho_t^{AB}]) - S(\text{Tr}_A [\rho_0^{AB}]), \end{cases}$$

The second law of thermodynamics can be now proven in the formulation given in [29]:

Theorem. *Given a system ρ^{AB} starting in a product state $\rho_0^{AB} = \rho^A \otimes \rho^B$ and evolving under the unitary evolution $\rho_0^{AB} = \rho^A \otimes \rho^B \rightarrow \rho_t^{AB} = U_t \rho^A \otimes \rho^B U_t^\dagger$, then the change in entropy of the full system $A + B$ is always positive:*

$$\Delta S + \Delta = [S(\rho_t^A) - S(\rho^A)] + [S(\rho_t^B) - S(\rho^B)] = I(A_t|B_t) \geq 0.$$

Moreover, the entropy will stay constant if and only if the evolution doesn't create correlations between the two partitions.

Proof. It follows easily from the chain of equalities:

$$\begin{aligned} \Delta S + \Delta &= [S(\rho_t^A) - S(\rho^A)] + [S(\rho_t^B) - S(\rho^B)] = S(\rho_t^A) + S(\rho_t^B) - S(\rho^A \otimes \rho^B) \stackrel{(1)}{=} \\ &\stackrel{(1)}{=} S(\rho_t^A) + S(\rho_t^B) - S(\rho_t^{AB}) = I(A_t|B_t) \geq 0, \end{aligned}$$

where in (1) the constancy of the entropy under unitary transformations has been used, and the last inequality has been proven above. Finally, rewriting the mutual information as:

$$I(A_t|B_t) = S(\rho_t^{AB} || \rho_t^A \otimes \rho_t^B),$$

it can be seen that this quantity is zero if and only if there is no correlation between A and B, that is if the system is in a product state. \square

Besides, if ρ^B is supposed to be in the thermal state $\rho^B = \omega_\beta(H^B)$, the result can be further extended to give the following expression for the change of entropy of the system A:

$$\begin{aligned} \Delta S &\geq \Delta S - I(A_t|B_t) - S(\rho_t^B || \rho^B) = \\ &= \cancel{S(\rho_t^A)} - \cancel{S(\rho^A)} - \cancel{S(\rho_t^A)} - \cancel{S(\rho_t^B)} + \cancel{S(\rho^A)} + S(\rho^B) + \cancel{S(\rho_t^B)} + \text{Tr} [\rho_t^B \log \rho^B] = \\ &= \beta(\langle H^B \rangle_{\rho^B} + \log Z_B - \langle H^B \rangle_{\rho_t^B} - \log Z_B) = \beta(\langle H^B \rangle_{\rho^B} - \langle H^B \rangle_{\rho_t^B}) = -\beta \Delta Q_B, \end{aligned}$$

where $-\Delta Q_B$ is the heat released by B . This quantity can be interpreted as the heat absorbed by the system A only if, at least at the endpoints of the transformation, the total energy can be considered extensive, meaning that the interaction does not significantly affect the energy balance: nonetheless, this assumption does not limit the range of applicability of the last theorem with respect to the one of classical equilibrium statistical mechanics, in which weak coupling with the environment is always assumed⁷. Then, this expression is identical to the classical statement of the second law; furthermore, the conditions under which the inequality is saturated are given by:

$$\begin{cases} I(A_t|B_t) = 0 \\ S(\rho_t^B || \rho^B) = 0, \end{cases}$$

where the first statement coincides with the condition one gets from the second law, while the second implies that $\rho_t^B \equiv \rho^B = \omega(H^B)$, i.e. the evolution leaves the thermal state unaffected; this is of course clear from thermodynamical reasoning, because whenever a Gibbs state is brought out of equilibrium, some entropy must be produced. For completeness, it should be said that this inequality is sometimes called Landauer's bound; in order to motivate this identification, it is useful to revert the inequality, defining the entropy decrease and the the heat released from the system to the bath as:

$$\begin{cases} \tilde{\Delta}S = -\Delta S \\ \tilde{\Delta}Q = \Delta Q_B. \end{cases}$$

Let now A be a qubit system in a fully mixed state $\rho^A = \mathbb{1}/2$ and suppose that the evolution brings it to the state $\rho_t^A = |0\rangle\langle 0|$; this process can be interpreted as the erasure of the qubit A : the initial state, fully entangled with the environment, is brought to a default state, independent of the correlations present at the beginning of the protocol. In this setting, one regains exactly the Landauer's bound:

$$\tilde{\Delta}S = S(\rho^A) - S(\rho_t^A) = \log[2] \leq \beta \tilde{\Delta}Q;$$

that is, the heat emitted by a system in order to erase one bit of information is always bigger or equal to $k_B \theta \log[2]$.

The derivation of the second law strongly motivates the identification of the von Neumann entropy with the thermodynamic one, which is at the cornerstone of the foundations of quantum statistical mechanics. Moreover, the Landauer's bound demonstrates some consistency of the formalism introduced above, connecting the abstract definition of heat transferred with the entropy decrease.

⁷For example, one can derive the canonical ensemble from the micro-canonical one only if the interaction energy can be considered to be negligible.

Chapter 2

Open quantum systems

The treatise of Mr. Zermelo "On a Theorem of Dynamics and the Mechanical Heat Theory" shows that my respective works have not been understood [...]. The theorem of Poincaré is obviously correct, its application to the theory of heat is not.

Ludwig Boltzmann, *Reply on the considerations on the Theory of Heat of Zermelo*

In this chapter it will be shown how to derive a dissipative dynamics from the unitary evolution of the universe through an approximation scheme. The case in which the reduced dynamical group is Markovian will be explored [3, 4]; in particular, it will be shown how to get an asymptotic expansion for slowly changing environment. This framework will be applied to the description of a two level system in contact with a black body radiation.

2.1 Introduction

At the core of statistical mechanics there is the faith that the ultimate description of the dynamics of the universe shall be reversible, while the appearing of an arrow of time should be considered only as an emergent phenomenon, true on timescales that, even if astonishingly larger than the lifetime of the universe, are still finite. This subtle argument, initially misinterpreted by the scientific community to the point of considering Loschmidt's and Zermelo's oppositions to Boltzmann's H theorem not as paradoxical conclusions, but as true weaknesses of the kinetic theory, shall always be kept in mind as the key of deriving thermodynamics from the underlying dynamical evolution; in particular, it should be clear that some kind of approximation scheme should always be applied, so to isolate the timescales of interest for the experience.

In quantum thermodynamics the importance of this observation becomes even more evident, thanks to the possibility of consistently defining a concept of entropy for systems out of equilibrium. In analogy to what happens for the H theorem, according to which there is no entropy production for the exact dynamics, likewise the full unitary evolution

preserves the entropy; therefore, as it has been shown in the previous chapter, the first approximation one has to do in order to have some change in the total entropy is the one of neglecting a part of the universe, which will be called in the following environment¹; this argument suggests the convenience of formally defining a dynamical evolution map V_t so that the following diagram commutes:

$$\begin{array}{ccc} \rho_0 = (\rho^S \otimes \rho^E)_0 & \xrightarrow[\text{evolution}]{\text{unitary}} & \rho_t = U_t(\rho^S \otimes \rho^E)_0 U_t^\dagger \\ \downarrow \text{Tr}_E & & \downarrow \text{Tr}_E \\ \rho_0^S & \xrightarrow[\text{evolution}]{\text{dynamical}} & \rho_t^S = V_t \rho_0^S \end{array}$$

Decomposing ρ_0^S and ρ_0^E in a basis as $\rho_0^S = \sum \lambda^i |\psi_i\rangle \langle \psi_i|$ and $\rho_0^E = \sum \mu^\alpha |\phi_\alpha\rangle \langle \phi_\alpha|$, it can further be seen that V_t can be written in the form:

$$\begin{aligned} V_t \rho_0^S &= \text{Tr}_B \left[U_t(\rho^S \otimes \rho^E)_0 U_t^\dagger \right] = \sum_{\alpha, \beta} \mathbb{1}_S \otimes \langle \phi_\alpha | \left[U_t(\rho^S \otimes \mu^\beta |\phi_\beta\rangle \langle \phi_\beta|)_0 U_t^\dagger \right] \mathbb{1}_S \otimes |\phi_\alpha\rangle = \\ &= \sum_{\alpha, \beta} \left[\sqrt{\mu^\beta} \langle \phi_\alpha | U_t | \phi_\beta \rangle \right] \rho_0^S \left[\sqrt{\mu^\beta} \langle \phi_\beta | U_t^\dagger | \phi_\alpha \rangle \right] \equiv \sum_{\alpha, \beta} (W_{\alpha, \beta})_t \rho_0^S (W_{\alpha, \beta}^\dagger)_t. \end{aligned}$$

It should be noticed that the family of operators $\{W_{\alpha, \beta}\}$ satisfies the following completeness relation:

$$\begin{aligned} \sum_{\alpha, \beta} (W_{\alpha, \beta})_t (W_{\alpha, \beta}^\dagger)_t &= \sum_{\alpha, \beta} \langle \phi_\alpha | U_t \mu^\beta | \phi_\beta \rangle \langle \phi_\beta | U_t^\dagger | \phi_\alpha \rangle = \\ &= \text{Tr}[\rho_B] \mathbb{1}_S = \mathbb{1}_S; \end{aligned}$$

this implies, thanks to Kraus decomposition theorem, that any reduced evolution V_t can be characterised as a completely positive, trace preserving map.

It is clear that, without further approximations, there are no simple relations between V_t and $V_{t'}$ for different times t and t' : this follows from the fact that, in principle, timescales of the order of the one of Poincaré recurrence theorem T_{Poin} are included in the theory. Nevertheless, if one restricts himself to observations on timescales T_{obs} :

$$T_{obs} \ll T_{Poin}, \quad (2.1)$$

effects connected to the inversion of the entropy flow can be safely neglected. Moreover, when studying a system in contact with a thermal environment, a second reasonable approximation one can make is the one of only considering observations which cannot resolve timescales under a certain Δ_{coarse} , which is long compared to the decay timescales for the excitations of the bath:

$$\Delta_{coarse} \gg \Delta_{bath}. \quad (2.2)$$

¹The name bath will be used as a synonym, when one wants to underline the fact that the environment is supposed to be in a stationary state.

These two approximations together can be mathematically translated to the Markov condition on the dynamical evolution:

$$V_{t_1} V_{t_2} = V_{t_1+t_2} \quad \forall t_1, t_2 \geq 0,$$

which can be restated as the additional request of V_t to be a dynamical semigroup; this characteristic evolution is called Markovian because the dynamics can be considered to depend only on the instantaneous state of the system. It is important that both the condition (2.1) and (2.2) hold for this formalism to be justified: the first, ensuring that the entropy flows always in the same direction, restores the injectivity of the evolution map; the latter, on the other hand, allows one to neglect stochastic fluctuations due to short memory effects of the environment, justifying a deterministic description of the evolution.

2.2 Microscopic derivation

In the following sections it will be shown how a quantum dynamical semigroup can be derived from the underlying unitary evolution via an approximation scheme, and which role the conditions (2.1) and (2.2) play in this.

Let H be the Hamiltonian of the whole universe, and let it be decomposed as:

$$H = H^S + gH^I + H^B,$$

where H^S and H^B are the free Hamiltonians of the system and bath, and H^I represents the interaction between the two, with g denoting the interaction strength. In order for the Markov approximation to hold, the evolution of the system shouldn't depend on the particular state of the bath or on the correlations present between the two; this corresponds to requiring the density matrix of the universe to be of the form:

$$\rho_t \approx \rho_t^S \otimes \rho_t^B;$$

of course, this condition can faithfully reproduce the effective evolution of the system only in the weak coupling limit, that is for $g \ll 1$ and on times of observation less than a bound somehow proportional to a power of g^{-1} . In this limit, it is useful to write the evolution equation of the universe in the interaction picture²:

$$\dot{\rho}_t = -ig [H_t^I, \rho_t],$$

which can be expressed in the integral form as:

$$\rho_t = \rho_0 - ig \int_0^t ds [H_s^I, \rho_s].$$

²In this picture the interaction Hamiltonian becomes: $H_t^I = e^{i(H^S+H^B)t} H^I e^{-i(H^S+H^B)t}$, and the density matrix is given by: $\rho_t = e^{i(H^S+H^B)t} (e^{-iHt} \rho e^{iHt}) e^{-i(H^S+H^B)t}$.

In order to investigate the effects deriving from the existence of different timescales, it is useful to combine the two previous equations in an integro-differential one, and to trace out the environment:

$$\dot{\rho}_t^S = -ig \text{Tr}_B [[H_t^I, \rho_0]] - g^2 \int_0^t ds \text{Tr}_B [[H_t^I, [H_s^I, \rho_s]]];$$

it should be noticed that, without loss of generality, the first term on the right hand side of the equation can be neglected; in fact, if one writes the interaction Hamiltonian as:

$$H_t^I = \sum_i A_t^i \otimes B_t^i,$$

with A^i and B^i operators with support respectively on the system or on the bath only, one can express this term as:

$$-ig \text{Tr}_B [[H_t^I, \rho_0]] = \sum_i (A_t^i \rho_0^S \text{Tr} [B_t^i \rho_0^B] - \rho_0^S A_t^i \text{Tr} [B_t^i \rho_0^B]);$$

denoting with $\{\epsilon_B\}$ the eigenstates of H_B , and noticing that $\rho_B \equiv \omega_\beta(H^B)$ is diagonal in this basis, one obtains that:

$$\langle B_t^i \rangle_{\rho_B} := \text{Tr} [B_t^i \rho_0^B] = \sum_{\epsilon_B} \langle \epsilon_B | B_t^i | \epsilon_B \rangle \langle \epsilon_B | \rho_B | \epsilon_B \rangle.$$

up to a redefinition of the bath Hamiltonian, the non zero matrix element of each B^i can be considered to be off diagonal, so that it follows that $\langle B_t^i \rangle_{\rho_B} = 0$. This is equivalent to the assumption that the interaction does not produce an average frequency shift [3].

If one only considers observations which cannot resolve phenomena faster than a timescale Δ_{coarse} , which is long compared to the one of the excitations of the bath (condition (2.2)), and that additionally the bath has so many degrees of freedom that it won't be affected by the interaction with the system, the *Born approximation* can be applied and the density matrix of the universe can be written in the form:

$$\rho_t \approx \rho_t^S \otimes \rho^B.$$

Rewriting the evolution equation one gets:

$$\dot{\rho}_t^S = -g^2 \int_0^t ds \text{Tr}_B [[H_t^I, [H_s^I, \rho_s^S \otimes \rho^B]]];$$

as it can be noticed, even if the stochastic fluctuations coming from the excitations of the bath have been smeared out with the Born approximation, the evolution equation still depends on the full history of the system; assuming that the bath completely erases the memory of the system or, equivalently, that the entropy flows in a constant direction (condition (2.1)), the evolution equation can be made local in time via the so called *Markov*

approximation, which corresponds to substituting the full history $\{\rho_s\}$ with the state at the latest time of evaluation ρ_t :

$$\dot{\rho}_t^S = -g^2 \int_0^t ds \operatorname{Tr}_B [[H_t^I, [H_s^I, \rho_t^S \otimes \rho^B]]].$$

It should be noticed that even if now the evolution equation is local in time, it still retains some memory of the initial state; for this reason, an additional approximation is needed, in order to erase any dependence on the initial conditions: this is done sending the lower limit of the integral to $-\infty$. Again, this approximation is justified only in the limit in which the condition (2.2) holds, as a necessary condition for the integral to converge.

The approximations outlined above goes under the name of *Born-Markov scheme*. The equation obtained can be rewritten in the form:

$$\dot{\rho}_t^S = -g^2 \int_0^\infty d\tau \operatorname{Tr}_B [[H_t^I, [H_{t-\tau}^I, \rho_t^S \otimes \rho^B]]],$$

where the change of variables $\tau = t - s$ has been used. Even if the resulting equation is local in time and independent on the initial conditions, this form of the evolution is not in general sufficient to guarantee the existence of a quantum dynamical semigroup; in particular, the evolution map so generated could fail to be completely positive [11]. A further approximation has to be done. In particular, in the next section the *rotating wave approximation* will be presented, which corresponds to an average over rapidly oscillating degrees of freedom, which will lead to the correct Markovian evolution.

2.3 Rotating wave approximation

Before starting to describe this approximation scheme, it is useful to define the eigenoperators of a Hamiltonian. Let A be an operator and $\{|\epsilon_i\rangle\}$ the eigenbasis of the Hamiltonian H with eigenvalues $\{\epsilon_i\}$. For each energy gap $\omega = \epsilon - \epsilon'$, ($\epsilon, \epsilon' \in \{\epsilon_i\}$), define:

$$A(\omega) = \sum_{\substack{\epsilon, \epsilon' \\ \epsilon - \epsilon' = \omega}} \langle \epsilon | A | \epsilon' \rangle |\epsilon\rangle \langle \epsilon'|.$$

This new operators satisfy the completeness relation:

$$\sum_{\omega} A(\omega) = \sum_{\omega} \sum_{\substack{\epsilon, \epsilon' \\ \epsilon - \epsilon' = \omega}} \langle \epsilon | A | \epsilon' \rangle |\epsilon\rangle \langle \epsilon'| = \sum_{\epsilon, \epsilon'} |\epsilon\rangle \langle \epsilon | A | \epsilon' \rangle \langle \epsilon'| = A, \quad (2.3)$$

and the two additional properties:

$$A^\dagger(\omega) = \sum_{\substack{\epsilon, \epsilon' \\ \epsilon - \epsilon' = \omega}} \langle \epsilon' | A | \epsilon \rangle |\epsilon'\rangle \langle \epsilon| = \sum_{\substack{\epsilon, \epsilon' \\ \epsilon' - \epsilon = -\omega}} \langle \epsilon | A | \epsilon' \rangle |\epsilon\rangle \langle \epsilon'| = A(-\omega), \quad (2.4)$$

and:

$$[H, A^\dagger(\omega) B(\omega)] = \sum_{\substack{\epsilon, \epsilon' \\ \epsilon - \epsilon' = \omega}} (\langle \epsilon' | A | \epsilon \rangle \langle \epsilon | B | \epsilon' \rangle) [H, (|\epsilon'\rangle \langle \epsilon'|)] = 0. \quad (2.5)$$

Finally, it should be noticed that $A(\omega)$ has the simple commutation relation:

$$[H, A(\omega)] = \sum_{\substack{\epsilon, \epsilon' \\ \epsilon - \epsilon' = \omega}} \langle \epsilon | A | \epsilon' \rangle ([H | \epsilon \rangle \langle \epsilon'|] - [| \epsilon \rangle \langle \epsilon'| H]) = -\omega A(\omega);$$

this property, which is the one that gives the name to the eigenoperators, ensures a particularly simple time dependency in the Heisenberg picture:

$$\dot{A}_t(\omega) = i [H, A_t(\omega)] = -i\omega A(\omega) \implies A_t(\omega) = e^{-i\omega t} A_0(\omega).$$

Having defined the eigenoperators, one can proceed further with the approximations. It should be firstly noticed that the interaction Hamiltonian can be rewritten as:

$$H^I = \sum_{\alpha} A_{\alpha} \otimes B_{\alpha} \stackrel{(2.3)}{=} \sum_{\alpha, \omega} A_{\alpha}(\omega) \otimes B_{\alpha} \stackrel{(2.4)}{=} \sum_{\alpha, \omega} A_{\alpha}^{\dagger}(\omega) \otimes B_{\alpha},$$

where A_{α} and B_{α} operates only on the system or on the bath respectively, and $A_{\alpha}(\omega)$ are the eigenoperators with respect to H_S . The passage to the interaction picture takes now the particularly simple form:

$$H_t^I = \sum_{\alpha, \omega} e^{-i\omega t} A_{\alpha}(\omega) \otimes B_{\alpha}(t).$$

Plugging this expression back into the evolution equation obtained in the previous section, the following result is obtained:

$$\begin{aligned} \dot{\rho}_t^S &= - \int_0^{\infty} d\tau \text{Tr}_B [H_{t-\tau}^I \rho_t^S \otimes \rho^B H_t^I - H_t^I H_{t-\tau}^I \rho_t^S \otimes \rho^B + h.c.] = \\ &= \sum_{\substack{\alpha, \omega \\ \beta, \omega'}} e^{i(\omega' - \omega)t} [A_{\beta}(\omega) \rho_t^S A_{\alpha}^{\dagger}(\omega') - A_{\alpha}^{\dagger}(\omega') A_{\beta}(\omega) \rho_t^S] \int_0^{\infty} d\tau e^{i\omega\tau} \langle B_{\alpha}^{\dagger}(t) B_{\beta}(t - \tau) \rangle_{\rho_B} \\ &+ h.c. , \end{aligned}$$

where the last integral can be recognised to be the one-sided Fourier transform of the bath correlation functions. Since ρ_B is a stationary state of H_B , i.e. $[H_B, \rho_B] = 0$, it can be easily checked that:

$$\begin{aligned} \langle B_{\alpha}^{\dagger}(t) B_{\beta}(t - \tau) \rangle_{\rho_B} &= \text{Tr} [e^{iH_B t} B_{\alpha}^{\dagger} e^{-iH_B t} e^{iH_B(t-\tau)} B_{\beta} e^{-iH_B(t-\tau)} \rho_B] \\ &= \text{Tr} [e^{iH_B \tau} B_{\alpha}^{\dagger} e^{-iH_B \tau} B_{\beta} \rho_B] = \langle B_{\alpha}^{\dagger}(\tau) B_{\beta}(0) \rangle_{\rho_B}; \end{aligned}$$

so that the integral depends only on ω and not on t ; for this reason the notation $\Gamma_{\alpha\beta}(\omega)$ will be used.

At this point, the final approximation can be made: defining the timescale of the intrinsic evolution of the system τ_S as the typical value of $|\omega - \omega'|^{-1}$, for time of observations $t \gg \tau_S$, all the non secular terms (meaning the terms for which $\omega \neq \omega'$) oscillates rapidly with respect to the resolved timescale of the dynamics, so that it is sensible to average them out; this approximation gives the following evolution equation:

$$\dot{\rho}_t^S = \sum_{\substack{\omega \\ \alpha, \beta}} \Gamma_{\alpha\beta}(\omega) [A_\beta(\omega) \rho_t^S A_\alpha^\dagger(\omega) - A_\alpha^\dagger(\omega) A_\beta(\omega) \rho_t^S] + h.c. .$$

At this point, it is useful for interpretational reasons to divide $\Gamma_{\alpha\beta}(\omega)$ in real and imaginary part, defining:

$$\begin{aligned} \Gamma_{\alpha\beta}(\omega) &= \frac{1}{2} \gamma_{\alpha\beta}(\omega) + i S_{\alpha\beta}(\omega); \\ \gamma_{\alpha\beta}(\omega) &= \Gamma_{\alpha\beta}(\omega) + \Gamma_{\alpha\beta}^*(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \langle B_\alpha^\dagger(\tau) B_\beta(0) \rangle_{\rho_B}; \\ S_{\alpha\beta}(\omega) &= \frac{1}{2i} (\Gamma_{\alpha\beta}(\omega) - \Gamma_{\alpha\beta}^*(\omega)); \end{aligned}$$

it should be noticed in particular that $\gamma_{\alpha\beta}(\omega)$ is a positive matrix, being the real part of the Fourier transform of the matrix $\langle B_\alpha^\dagger(\tau) B_\beta(0) \rangle_{\rho_B}$, which is positive for each τ . With these definitions, the evolution equation can be rewritten as:

$$\begin{aligned} \dot{\rho}_t^S &= -i \left[\sum_{\substack{\omega \\ \alpha, \beta}} S_{\alpha\beta}(\omega) A_\alpha^\dagger(\omega) A_\beta(\omega), \rho_t^S \right] + \\ &+ \sum_{\substack{\omega \\ \alpha, \beta}} \gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_t^S A_\alpha^\dagger(\omega) - \frac{1}{2} \{ A_\alpha^\dagger(\omega) A_\beta(\omega), \rho_t^S \} \right). \end{aligned}$$

The sum inside the commutator is conserved by the free evolution, thanks to the condition (2.5), and for this reason can be interpreted as a simple shift in the energy levels of the unperturbed Hamiltonian, which accounts for the binding energy contained in the interaction with the environment; for its similarity to the fine structure corrections to the spectral lines of atoms, this term is often referred to as Lamb shift Hamiltonian. The superoperator in the second line accounts for the non unitarity of the evolution and for this reason these terms goes under the name of dissipator, and are indicated as $\mathcal{D}(\rho_t^S)$. Since $\gamma_{\alpha\beta}(\omega)$ is a positive matrix, it can be diagonalised, giving the Lindbladian form of the evolution equation:

$$\dot{\rho}_t^S = -i [H_{LS}, \rho_t^S] + \sum_{\omega, k} \gamma_k(\omega) \left(A_k(\omega) \rho_t^S A_k^\dagger(\omega) - \frac{1}{2} \{ A_k^\dagger(\omega) A_k(\omega), \rho_t^S \} \right) =: \mathcal{L} \rho_t^S,$$

where the Lindbladian superoperator has been implicitly defined; it is useful to note for what follows that $\mathcal{L}\rho$ is traceless for any ρ , thanks to the fact that the derivative of a density matrix must be traceless.

This equation can be formally integrated to generate the quantum dynamical semigroup $V_t = \exp \mathcal{L}t$; moreover, it can be shown that any quantum dynamical semigroup can be generated from a Lindbladian superoperator [14]. This concludes the derivation of the effective Markovian evolution from the microscopic dynamics of the system.

A final remark is needed: in this derivation the Hamiltonian of the state is considered to be constant during the evolution whereas, when implementing a thermodynamic protocol, one should have the freedom of changing it in an arbitrary fashion; for this reason, it might seem that this derivation, even if of some interest by itself, won't be relevant in the context of thermodynamics. Nevertheless, comparing the approximation scheme just presented with the one for varying Hamiltonians [1, 8], one can see that the main ideas and the use of the conditions (2.1) and (2.2) are unvaried, while some minor technicalities are added (this similarity is a consequence of the fact stated above, that for any Markovian equation it should be possible to write the evolution in the Lindbladian form). For this reason, it has been preferred to give the derivation just presented, in order to clearly stress the conceptual basis underlying the approximation scheme without getting excessively diverted by technical details.

2.4 Entropy production in open quantum systems

It is interesting to now study how the two procedures of tracing out part of the environment and approximating the reduced dynamics with a Markovian semigroup leads to entropy production in the system. In particular, assuming that the system equilibrates to a full rank density matrix ρ_0 , one can find a Hamiltonian H such that $\rho_0 =: \omega(\tilde{H})$; therefore, in order to measure the dissipation during a thermalisation process, one can study without loss of generality the quantity:

$$\theta S(\rho || \omega_\beta(H)) = F[(\rho, H)_\beta] - F[\omega_\beta(H)]$$

which measure the work one can extract from ρ , using the fact that the system is not in its equilibrium state. Then, for a general reduced dynamical map V_t it is easy to show that the available work can only decrease over time:

$$\begin{aligned} S(V_t \rho || \omega_\beta(H)) &\stackrel{(1)}{=} S(V_t \rho || V_t \omega_\beta(H)) \stackrel{(2)}{=} S(\text{Tr}_B [U_t(\rho^S \otimes \rho^B)U_t^\dagger] || \text{Tr}_B [U_t(\omega_\beta(H) \otimes \rho^B)U_t^\dagger]) \stackrel{(3)}{\leq} \\ &\stackrel{(3)}{\leq} S(U_t(\rho^S \otimes \rho^B)U_t^\dagger || U_t(\omega_\beta(H) \otimes \rho^B)U_t^\dagger) \stackrel{(4)}{=} S(\rho^S \otimes \rho^B || \omega_\beta(H) \otimes \rho^B) \stackrel{(5)}{=} \\ &\stackrel{(5)}{=} S(\rho || \omega_\beta(H)) + \underline{S(\rho_B || \rho_B)}, \end{aligned}$$

where one uses, in order, the stationarity of ω (1), the definition of V_t (2), the fact that the distinguishability can only decrease tracing out part of the system (3) and, finally, the

invariance of the relative entropy under unitary transformations (4) and the distributivity over product states (5).

This result is similar in spirit to the second law demonstrated in the previous chapter, in the sense that it ensures that on any finite interval of time the availability won't rise, but it does not give any information about the monotonicity of the change of entropy; even if it would be tempting to state that for $\rho_{t'}$ evaluated at a later time t' the availability is less or equal to the one at time $t < t'$, this is in fact not true in general: it is sufficient to consider a exactly recurrent system, with periodicity T , for which the availability will first decrease, to only go back to the initial quantity at time T .

Nonetheless, when the Markovian approximation can be applied, one can use the result just shown to prove that:

$$S(V_{t'} \rho || \omega_\beta(H)) = S(V_{t'-t} V_t \rho || \omega_\beta(H)) \leq S(V_t \rho || \omega_\beta(H)) \quad \text{for } t' \geq t.$$

It is now clear how the semigroup property of V_t is crucial to ensure that the entropy has a constant direction. In this case, one can define the entropy production rate as the change of availability over time and, using the previous inequality, one can show that:

$$\begin{aligned} \sigma(\rho_t) &:= -\frac{1}{\theta} \frac{\partial}{\partial t} \Delta F \Big|_{\omega_\beta(H)}^{\rho_t} = -\frac{\partial}{\partial t} S(V_t \rho || \omega_\beta(H)) = \\ &= \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} (S(V_\varepsilon V_t \rho || \omega_\beta(H)) - S(V_t \rho || \omega_\beta(H))) \geq 0, \end{aligned}$$

which clearly states that, as long as the semigroup approximation well approximates the true reduced dynamics, the entropy will increase. Moreover, using the fact that V_t can always be expressed as $V_t = \exp \mathcal{L}t$ and plugging in in the previous definition the expression of $\omega_\beta(H)$, one gets an explicit expression for the entropy production rate:

$$\begin{aligned} \sigma(\rho_t) &= -\text{Tr} [\mathcal{L}(\rho_t) \log [\rho_t]] - \beta \text{Tr} [\mathcal{L}(\rho_t) H] = \\ &= \frac{d}{dt} S(\rho_t) - \frac{1}{\theta} \frac{dQ}{dt}(\rho_t) \geq 0, \end{aligned}$$

obtaining the infinitesimal version of the second law of thermodynamics.

2.5 Slowly varying Lindbladian equation

When one considers a thermodynamical protocol in which some family of parameters of the Hamiltonian $\{\lambda_t\}$ is varied, it is always implicitly assumed that the interaction with the environment, in the limit of an infinitely slow transformation, will bring the system to the instantaneous thermal state defined by $\omega_\beta(H(\{\lambda_t\}))$. This condition mathematically translates to the possibility of defining a family of Lindbladian operators such that for each t one has:

$$\lim_{T \rightarrow \infty} e^{\mathcal{L}_t T} \rho = \omega(H_t),$$

for any initial state ρ^3 . If the protocol is realised in finite time though, some corrections to the evolution of the state must be added: in particular, if the transformation is performed in some long time T , the state can be perturbatively expanded, as it is shown in the paper [6], to which this section is inspired.

Considering a general mixing Lindbladian \mathcal{L} , it is always possible to divide its action on a density matrix ρ as:

$$\mathcal{L}\rho = \mathcal{L}(\mathbb{1}/d) + \mathcal{L}(\hat{\rho}),$$

where the hat indicates the traceless component and d the dimension of the space; in particular, since $\mathcal{L}(\omega) = 0$ by construction, one has that $\mathcal{L}(\mathbb{1}/d) = -\mathcal{L}(\hat{\omega})$. Moreover, since ω , which has by definition unitary trace, is the unique zero eigenvector of the Lindbladian, the action of the superoperator on the traceless subspace will be invertible: therefore, it is possible to define a non singular matrix Λ which describes the action of \mathcal{L} on the subspace of traceless hermitian operators. Hence, considering a thermodynamic protocol as described above, the evolution equation can be rewritten as:

$$\dot{\rho}_t = \mathcal{L}_t(\rho_t) = \Lambda_t(\hat{\rho}_t - \hat{\omega}_t),$$

where t runs from 0 to T . In order to isolate the effects appearing on different timescales, it is useful to rescale the parameter t to the interval $[0, 1]$ and, consequently, the variables of the problem as:

$$\begin{aligned} \tilde{\rho}_\tau &:= \rho_{\tau T} & \tau \in [0, 1]; \\ \tilde{\Lambda}_\tau &:= \Lambda_{\tau T} \end{aligned}$$

plugging in the redefined variables in the Lindbladian equation, one gets:

$$\dot{\tilde{\rho}}_\tau = \dot{\rho}_{\tau T} = T\tilde{\mathcal{L}}_\tau \tilde{\rho}_\tau.$$

It should be noticed that, even if $\tilde{\mathcal{L}}_\tau$ will be independent on T (the passage from the first equation to the last being only a reparametrisation of the same trajectory in the space of Lindbladians), this is not the case for $\tilde{\rho}_\tau$, whose derivative explicitly depends on the time of the protocol; for example, as it would be reasonable to expect, for $T \rightarrow \infty$ one has:

$$\lim_{T \rightarrow \infty} \tilde{\mathcal{L}}_\tau \tilde{\rho}_\tau = \lim_{T \rightarrow \infty} \frac{\dot{\tilde{\rho}}_\tau}{T} = 0,$$

so that the solution in the adiabatic limit is exactly the instantaneous steady state trajectory $\tilde{\omega}_\tau$. This remark motivates the expansion in powers of $1/T$:

$$\tilde{\rho}_\tau = \tilde{\rho}_\tau^0 + \frac{1}{T}\tilde{\rho}_\tau^1 + \frac{1}{T^2}\tilde{\rho}_\tau^2 + \dots, \quad (2.6)$$

³This condition is satisfied if each \mathcal{L}_t has a unique zero eigenstate and the real part of every other eigenvalue is negative. This kind of Lindbladian are called mixing or relaxing in the literature [5].

where it can be noticed that in order for $\tilde{\rho}_\tau$ to be a density matrix all the perturbation must be traceless; plugging this ansatz in the evolution equation and matching in powers of $1/T$, one obtains the system of equations:

$$\begin{cases} \tilde{\mathcal{L}}_\tau \tilde{\rho}_\tau^0 = 0 \\ \tilde{\mathcal{L}}_\tau \tilde{\rho}_\tau^{i+1} = \tilde{\Lambda}_\tau \tilde{\rho}_\tau^{i+1} = \dot{\tilde{\rho}}_\tau^i \end{cases} \quad \forall i \in \mathbb{N};$$

as expected, the first equation simply gives $\rho^0 \equiv \omega$. Solving iteratively, one can then derive the following formal series solution:

$$\begin{aligned} \tilde{\rho}_\tau &= \tilde{\omega}_\tau + \frac{1}{T} \left[\tilde{\Lambda}_\tau^{-1} \frac{d}{d\tau} \right] \omega_\tau + \frac{1}{T^2} \left[\tilde{\Lambda}_\tau^{-1} \frac{d}{d\tau} \right]^2 \omega_\tau + \dots \\ &= \frac{1}{1 - \frac{1}{T} \left[\tilde{\Lambda}_\tau^{-1} \frac{d}{d\tau} \right]} \omega_\tau; \end{aligned}$$

ignoring here the mathematical sensibility of the formal resummation, it is worth noticing how the evolution equation is independent on the initial conditions: the expansion in (2.6) is therefore equivalent to neglect exponentially decaying transients, which are the only memory of the initial conditions; in any case, in fact, the initial state shouldn't affect the dynamics of the system which is, by construction, Markovian.

Finally, it is interesting to express the entropy production in this case⁴:

$$\begin{aligned} \sigma(\rho_t) &= -\text{Tr} [\mathcal{L}(\rho_t) \log [\rho_t]] - \beta \text{Tr} [\mathcal{L}(\rho_t) H_t] \stackrel{(2.6)}{=} \\ &\stackrel{(2.6)}{=} \left(-\text{Tr} [\mathcal{L}(\rho_t) \log [\omega_t]] - \frac{1}{T} \text{Tr} [\mathcal{L}(\rho_t) \mathcal{J}_{\omega_t}^{-1} [\rho_t^1]] + \mathcal{O} \left(\frac{1}{T^2} \right) \mathcal{O} (\mathcal{L}(\rho_t)) \right) - \beta \text{Tr} [\mathcal{L}(\rho_t) H_t] = \\ &= -\frac{1}{T^2} \text{Tr} \left[\frac{d}{dt} \omega_t \mathcal{J}_{\omega_t}^{-1} \left[\Lambda_t^{-1} \frac{d}{dt} \omega_t \right] \right] + \mathcal{O} \left(\frac{1}{T^3} \right) \\ &=_{\mathcal{O}(\frac{1}{T^3})} -\frac{\beta^2}{T^2} \text{Tr} \left[\dot{H}_t \left(\Lambda_t^{-1} \mathcal{J}_{\omega_t} \left[\dot{H}_t - \langle \dot{H}_t \rangle_{\omega_t} \right] \right) \right] \geq 0; \end{aligned} \quad (2.7)$$

it should be noticed that, even if the quadratic dependence on $1/T$ does not come as a surprise, the β dependence could seem counterintuitive. A way of understanding this scaling is to consider the infinite temperature limit and the zero temperature one: in the first case, all the ω_t will collapse to the single point $\mathbb{1}/d$ and for this reason, after an exponentially short transient, changing the parameters of the Hamiltonian won't affect the state and, therefore, won't produce dissipation; in the opposite limit, ω_t will collapse to the instantaneous ground state, and therefore changing the Hamiltonian parameters (not considering transformations which preserves the ground states) will continuously bring the system out of equilibrium, producing an increase in entropy.

⁴For simplicity of notation from now on all the tildes will be dropped and the interval of t will always be $[0, 1]$.

2.6 Two level system in a radiation field

In order to better illustrate the behaviour of a system under dissipative evolution, an overview on the dynamics of a two level system coupled to a radiative bath will be given and the results from the previous section will be numerically verified in this context.

A two level system can be described by the Hamiltonian:

$$H = \frac{\hbar}{2} \omega_0 \sigma_z,$$

where $\hbar\omega_0$ denotes the energy spacing and ω_0 the transition frequency. It is easy to verify that the matrices σ_{\pm} are eigenoperators of H with eigenvalues $\mp\omega_0$. Then, the Lindbladian equation of such a system coupled to a bosonic bath, which can be thought as the radiation of a black body, is given by [4]:

$$\dot{\rho}_t = \gamma_0(N+1) \left(\sigma_- \rho_t \sigma_+ - \frac{1}{2} \{ \sigma_+ \sigma_-, \rho_t \} \right) + \gamma_0 N \left(\sigma_+ \rho_t \sigma_- - \frac{1}{2} \{ \sigma_- \sigma_+, \rho_t \} \right), \quad (2.8)$$

where γ_0 is the spontaneous emission rate and N is the Planck distribution for the transition frequency; this two quantities can be explicitly expressed as:

$$\gamma_0 = \frac{4\omega_0^3 |\vec{d}|^2}{3\hbar c^3}, \quad N(\omega_0) = \frac{1}{e^{\beta\hbar\omega_0} - 1},$$

where \vec{d} indicates the electric dipole of the system. For simplicity, the Lamb shift Hamiltonian has been ignored. Interpreting the Lindbladian equation, the first parenthesis accounts for the emission of a quantum of energy, while the second is the absorption part; then, it can be seen that the system will undergo spontaneous emission with rate γ_0 , and will have a thermally induced emission and absorption with rate $\gamma_0 N$. For what follows, it is useful to define the total transition rate to be:

$$\gamma = \gamma_0 (2N + 1).$$

Using the Stokes coordinates to parametrise 2x2 Hermitian matrices with trace one:

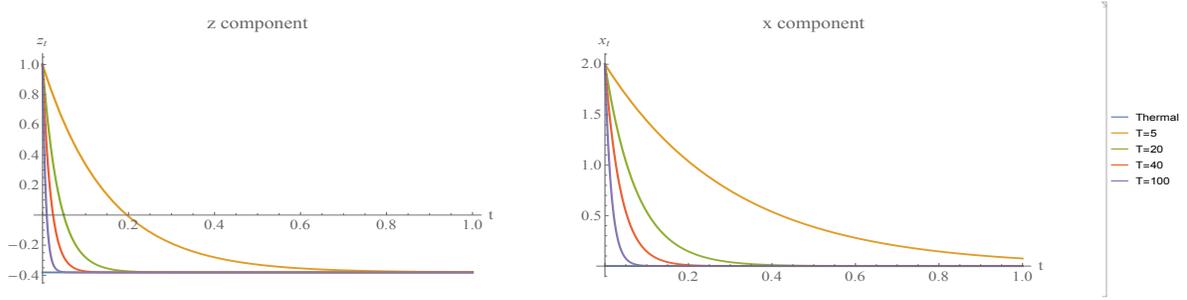
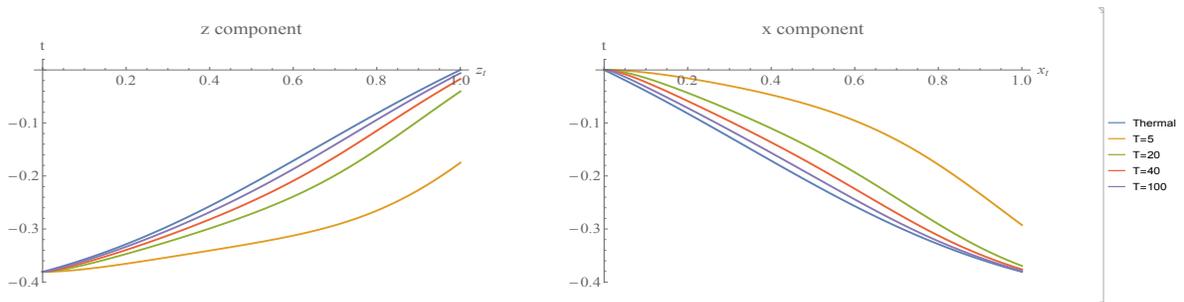
$$\rho = \begin{bmatrix} \frac{1}{2} + z & x + iy \\ x - iy & \frac{1}{2} - z \end{bmatrix} = \frac{\mathbb{1}}{2} + x\sigma_x + y\sigma_y + z\sigma_z,$$

and recalling that the action of the Lindbladian on a density matrix can be completely expressed looking at the traceless subspace only, one can then rewrite the evolution equation above as:

$$\begin{pmatrix} \dot{x}_t \\ \dot{y}_t \\ \dot{z}_t \end{pmatrix} = \Lambda(\hat{\rho}_t - \hat{\omega}_t) = \begin{bmatrix} -\frac{\gamma}{2} & 0 & 0 \\ 0 & -\frac{\gamma}{2} & 0 \\ 0 & 0 & -\gamma \end{bmatrix} \begin{pmatrix} x_t \\ y_t \\ z_t \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ \frac{\gamma_0}{2} \end{pmatrix}$$

Thus, it is easy to verify that the steady state $\mathcal{L}\rho_{steady} \equiv 0$ is given by:

$$\rho_{steady} = \frac{1}{2}\mathbb{1} - \frac{\gamma_0}{2\gamma}\sigma_z = \frac{1}{2} \left(\mathbb{1} + \frac{1 - e^{\beta\hbar\omega_0}}{1 + e^{\beta\hbar\omega_0}} \sigma_z \right) = \begin{bmatrix} \frac{1}{1+e^{\beta\hbar\omega_0}} & 0 \\ 0 & \frac{e^{\beta\hbar\omega_0}}{1+e^{\beta\hbar\omega_0}} \end{bmatrix} \equiv \omega(H),$$

Figure 2.1: Evolution of z_t and x_t with T renormalized to $[0, 1]$.Figure 2.2: The evolution of the system tends to be in the instantaneous thermal states for $T \gg 1$, the system instantaneously thermalizes to $\tilde{\omega}_\tau = \tilde{\omega}((1 - \tau) \sigma_z + \tau \sigma_x)$.

which corresponds exactly to the thermal state for H .

In the case of a fixed Lindbladian the equation can be explicitly integrated, giving:

$$\rho_t = \frac{1}{2}\mathbb{1} + \hat{\rho}_t = \frac{1}{2}\mathbb{1} + e^{\Lambda t}(\hat{\rho}_0 - \hat{\omega}) + \hat{\omega};$$

as it can be seen any state exponentially decays to the thermal one. The evolution for some arbitrary chosen initial conditions are shown in figure 2.1.

One can now illustrate the results of the previous section, choosing a family of Lindbladians such that the instantaneous thermal state is given by:

$$\omega((1 - t) \sigma_z + t \sigma_x).$$

In particular, comparing the trajectories in figure 2.2 and in figure 2.3 it can be noticed that the initial conditions account only for an exponentially short transient, as it was argued in the previous section. Moreover, in picture 2.4 it is shown how the asymptotic trajectory is better approximated by the first approximation trajectory than from the thermal state, as an additional evidence of the validity of the perturbative expansion.

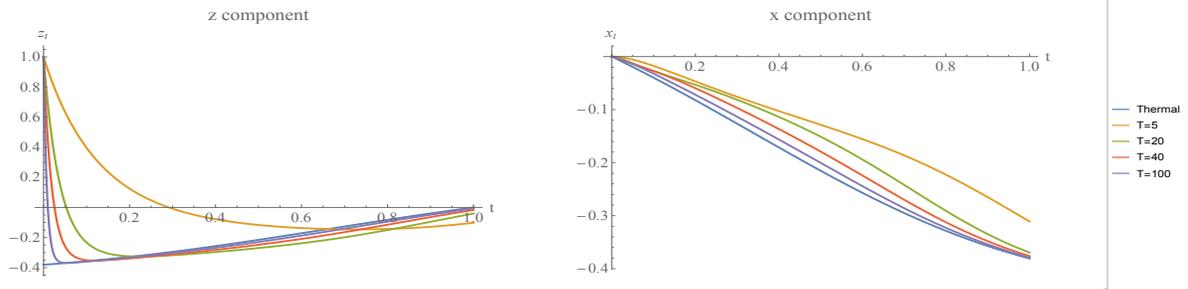


Figure 2.3: The initial conditions only affect an exponentially short part of the trajectory; compare with figure 2.2.

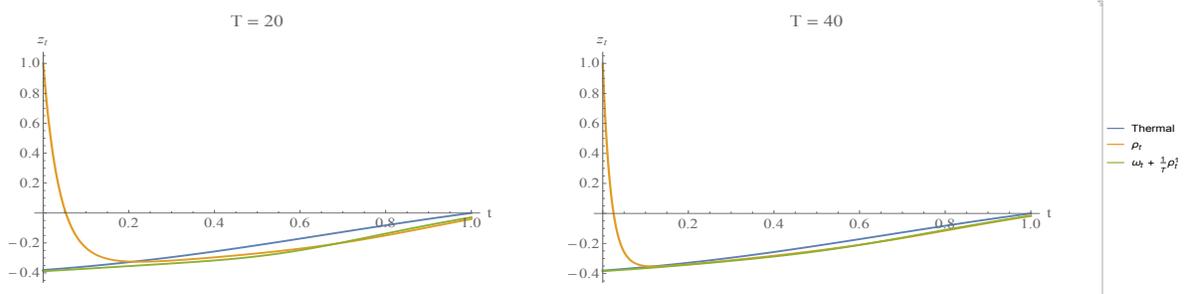


Figure 2.4: After an initial transient depending on the initial conditions, the first order expansion well approximates the real evolution.

Chapter 3

Work extraction and thermodynamic length

There cannot be a greater mistake than that of looking superciliously upon the practical applications of science.

William Thomson, *Popular Lectures*

In this chapter it will be shown how the definition of a metric on the space of density matrices naturally emerges in the context of maximisation of work extraction in the quasi-isothermal limit. It will be first shown how one can derive this concept in classical thermodynamics, and how the derivation given in that setting can be replicated in the quantum framework, extending the formalism to systems out of equilibrium. The two limit cases of a discrete step process between thermal states and of a continuous evolution in finite time will be explored for a two level system. The results presented here fall into a line of geometrisation of quantum mechanics present in the literature: on the one hand, the results about quantum Fisher information and generalised covariance have been already studied from a mathematical point of view in a number of papers [12, 23, 25, 24, 33]; on the other, application of Wootters' distance and Bures metric to quantum thermodynamics have recently appeared, for example in [9, 10, 18]. Then, on the one hand this work connects the studies about the generalised covariance metric to the entropy production rate, on the other it shows how the Bures metric is not the only sensible choice in quantum thermodynamics.

3.1 Classical results

Thermodynamics has evolved to be one of the most comprehensive frameworks of modern physics: it has a range of application which goes from the scale of atoms to black holes, it can be used to analyse living systems and emergent phenomena, and the ideas which have blossomed in this setting find applications in abstract areas, as information theory

and theoretical informatics. Despite the incredible abstraction this theory has experienced from the original problems which it was devised to tackle, it should always be kept in mind the importance of the connection between entropy production and dissipation, and the possibility, or better, the equivalence, of characterising one through the other: it is indeed a fact that nowadays the prejudice of considering on a less noble stance the theories which find a direct technological application is widespread in theoretical physics, and it is hard to believe that many won't consider finding optimal protocols for thermal engines more of an engineering work than a fundamental quest; nonetheless, it is important to remember that whatever can be proven in this more trivial setting, will find its application to all the problems which thermodynamics can be applied to, and that identifying intrinsic limitations can shed light on the foundations of thermodynamics itself. On the other hand, it is important to keep in mind what is proper for a pure science and what for engineering; for this reason, in the following, the concepts will be underlined and the general tools will be presented, but the details of the actual implementation will usually be skipped.

The formalism presented in this chapter in the quantum scenario has been treated in the setting of classical thermodynamics in [2, 7, 21, 30, 31, 37, 38, 39] and the work done here can be considered as the generalisation of these studies to the case in which the observables do not necessarily commute. For this reason it is useful, in order to better grasp the main ideas of the derivation, to first describe how the concept of a thermodynamic length emerges in classical thermodynamics.

A classical thermodynamical system in equilibrium is defined by an inverse temperature β and a Hamiltonian H , which is rewritten in the form:

$$\beta H(q; p | \{\lambda^i\}) = \lambda^i X_i(q; p),$$

where $\{X_i\}$ are arbitrary functions of the phase space coordinates, denominated collective variables, and $\{\lambda^i\}$ are real numbers, denominated conjugate generalised forces¹. This splitting is done so that the $\{\lambda^i\}$ can be considered to be experimentally controllable parameters of the system: for example, a Hamiltonian of the form:

$$H(q; p) = H^{free}(q; p) + V^{con}(q),$$

can be casted in the so called isothermal-isobaric form, in which the collective variables are the energy and the total volume of the system, or more precisely the free Hamiltonian and the confining potential ($X = \{U, V\}$), and the conjugate forces, which control the average value of their respective collective variables, are the inverse temperature and the pressure ($\lambda = \{\beta, \beta p\}$). Clearly then, there is a one-to-one correspondence between thermodynamical protocols and paths in the parameter space $\{\lambda^i(t)\}$. For this reason, the entropy production rate during a thermodynamical transformation can be implicitly defined as:

$$\sigma(\{\lambda^i(t)\})dt = dS - \frac{1}{\theta} dQ,$$

¹In the following, the sum on repeated indices is implied.

which, according to the second law of thermodynamics, is a positive definite quantity for any irreversible transformation. Thus, thanks to the first law, one can express the work produced by a system as:

$$W = \Delta Q - \Delta U = -(\Delta U - \theta \Delta S) - \theta \int_{\{\lambda^i(t)\}} dt \sigma(\{\lambda^i(t)\}), \quad (3.1)$$

where one can recognise the terms inside the parenthesis to be the change of free energy evaluated at the endpoints of the process, while the integral accounts for the loss of available work due to irreversibility.

In order to give an explicit expression for the dissipation term, one models a quasi reversible protocol as the continuous limit of a step process in which the parameters $\{\lambda^i(t)\}$ are varied in a discrete manner and for which, after each step, the system is allowed to thermalise until it reaches equilibrium for a time τ before passing to the following step. In this case, the expression of the change of energy and of the work produced during a single step is given by²:

$$\begin{aligned} \beta \Delta U_k &= \lambda_{(k+1)\tau}^i \langle X_i [(k+1)\tau] \rangle - \lambda_{k\tau}^i \langle X_i [k\tau] \rangle \\ \beta W_k &= \lambda_{k\tau}^i \Delta \langle X_i [k\tau] \rangle = \lambda_{k\tau}^i (\langle X_i [k\tau] \rangle - \langle X_i [(k+1)\tau] \rangle), \end{aligned}$$

where the first equality is simply a way of rewriting the Hamiltonian, while the second comes from an extension of the usual definition of work as force times displacement to the case of generalised variables. Hence, applying the first law, one obtains the expression of the heat absorbed by the system as:

$$\Delta Q_k = \Delta U_k + W_k = \theta \langle X_i [(k+1)\tau] \rangle (\lambda_{(k+1)\tau}^i - \lambda_{k\tau}^i).$$

In this setting it is possible to give a closed expression for the entropy production: if one considers, for example, a cyclic process performed in two steps, the first from state A to state B , and second in the opposite direction, then the total heat absorbed during the transformation is given by:

$$\begin{aligned} \Delta Q_{TOT} &= \theta \langle X_i [A] \rangle (\lambda_B^i - \lambda_A^i) - \theta \langle X_i [B] \rangle (\lambda_B^i - \lambda_A^i) = \\ &= \theta \Delta \lambda^j \frac{\Delta \langle X_i \rangle}{\Delta \lambda^j} \Delta \lambda^i. \end{aligned}$$

It is important to notice that, in this case, ΔQ_{TOT} coincides with the entropy produced, because for any cyclic transformation the following identity holds:

$$\Delta Q_{TOT} = \theta \Delta S - \theta \int_{\{\lambda^i(t)\}} dt \sigma(\{\lambda^i(t)\}),$$

²The angle brackets indicates the average with respect to the Gibbs probability distribution:

$$p(q; p | \{\lambda^i\}) = \frac{e^{-\lambda^i X_i(q;p)}}{Z}.$$

thanks to the fact that the entropy is a function of state.

Now, considering a general protocol, if one assumes that the curve $\{\lambda^i(t)\}$ depends smoothly on t (where t , up to a rescaling, can be considered to be contained in the interval $[0, 1]$) then it is possible to apply a similar argument and give an explicit expression of the heat absorbed during the process run first in the forward direction and then reversed, in a total of $2N$ steps:

$$\begin{aligned} \beta \Delta Q_{TOT} &= - \int_{\{\lambda^i(t)\}} dt \sigma(\{\lambda^i(t)\}) = \\ &= \sum_t \Delta \lambda_t^j \frac{\Delta \langle X_i [t] \rangle}{\Delta \lambda_t^j} \Delta \lambda_t^i =_{\mathcal{O}(N^{-2})} \frac{1}{N} \sum_t \frac{1}{N} \dot{\lambda}_t^j \frac{\partial \langle X_i [t] \rangle}{\partial \lambda_t^j} \dot{\lambda}_t^i =_{\mathcal{O}(N^{-2})} \\ &=_{\mathcal{O}(N^{-2})} \frac{1}{N} \int_{\{\lambda^i(t)\}} dt \frac{d\lambda_t^j}{dt} \frac{\partial \langle X_i [t] \rangle}{\partial \lambda_t^j} \frac{d\lambda_t^i}{dt} = -\frac{1}{N} \int_{\{\lambda^i(t)\}} dt \frac{d\lambda_t^j}{dt} \frac{\partial^2 \log [Z_t]}{\partial \lambda_t^i \partial \lambda_t^j} \frac{d\lambda_t^i}{dt}. \end{aligned}$$

In particular, since the expression obtained is quadratic in the velocities $\{\dot{\lambda}^i(t)\}$, the heat absorbed during the forward transformation exactly equals the one for the reversed protocol; for this reason, one can rewrite equation (3.1) in the form:

$$W = -\Delta F - \frac{\theta}{2N} \int_{\{\lambda^i(t)\}} dt \frac{d\lambda_t^j}{dt} \frac{\partial^2 \log [Z_t]}{\partial \lambda_t^i \partial \lambda_t^j} \frac{d\lambda_t^i}{dt}, \quad (3.2)$$

giving an explicit expression of the dissipation which accompanies a thermodynamic transformation close to equilibrium. It is worth to point out some features of this equality: firstly, thanks to the well known identity of classical statistical mechanics:

$$\frac{\partial^2 \log [Z_t]}{\partial \lambda_t^i \partial \lambda_t^j} = \langle (X_i - \langle X_i [t] \rangle) (X_j - \langle X_j [t] \rangle) \rangle_t = \text{Cov}_t(X_i, X_j),$$

this form of expressing the entropy production connects the dissipation during a process with the fluctuations of the collective variables computed with respect to the equilibrium distribution; in this way, this result can be considered to give a similar insight with the one coming from the fluctuation-dissipation theorems. Secondly, since $g_{i,j} := \text{Cov}_t(X_i, X_j)$ is a semidefinite matrix, a semi-Riemannian structure can be defined on the space of parameters. Moreover, recalling the definition of the energy functional of a curve:

$$E(\gamma) := \int_{\gamma} g(\dot{\gamma}, \dot{\gamma}),$$

it is easy to identify this expression with the dissipation integral in equation (3.2). Then, it is clear that the expression of the entropy production rate naturally leads to the introduction of a metric structure on the space of parameters, which allows for an abstract procedure of computing the dissipation for any thermodynamic trajectory $\{\lambda^i(t)\}$; more importantly, though, what really motivates the introduction of a metric structure is that

the problem of finding minimally dissipative protocols can be solved automatically in this formalism, simply by integrating the geodesic equation³ of the metric.

3.2 Isothermal work extraction from a quantum system

The derivation of the entropy production rate just given for the classical case can be reproduced in the quantum framework in an almost identical manner, with the additional freedom of not having to assume full thermalisation at each step.

It is first important to notice that an arbitrary thermodynamical protocol can be thought as the limit of a discrete sequence of the form:

$$(\rho_1; H_1) \longrightarrow (\rho_2; H_2) \longrightarrow \dots \longrightarrow (\rho_N; H_N),$$

where each step is performed in a fixed time $\delta\tau$, and the states and the Hamiltonians are connected by the relation:

$$\lim_{\delta\tau \rightarrow \infty} \rho_i = \omega_\beta(H_i).$$

The work extracted during such a sequence of transformations can be computed according to the definition given in section 1.3 as:

$$W = \sum_{i=1}^{N-1} \text{Tr} [\rho_i (H_i - H_{i+1})],$$

which can be rewritten as:

$$\begin{aligned} W &= \sum_{i=1}^{N-1} \text{Tr} [\rho_i (H_i - k_B\theta S(\rho_i) + k_B\theta S(\rho_i) - H_{i+1})] = \sum_{i=1}^{N-1} [F[(\rho_i, H_i)] - F[(\rho_i, H_{i+1})]] \\ &= F[(\rho_1, H_1)] - \left(\sum_{i=1}^{N-1} [F[(\rho_i, H_{i+1})] - F[(\rho_{i+1}, H_{i+1})]] \right) - F[(\rho_N, H_N)], \end{aligned}$$

where in the first line, adding and subtracting the entropy of each state helps to underline the connection between the work extraction and the change of free energy, while in the second line, one isolates the difference in free energy evaluated at the endpoints from the rest of the sum, which will give the dissipative contributions. This identification can be made more evident, recalling that the free energy out of equilibrium can be connected to the equilibrium one via the identity:

$$F[(\rho, H)] = F[(\omega(H), H)] + \theta S(\rho||\omega),$$

³In general, geodesics only minimise the length and not the energy functional, since the length is invariant under arbitrary reparametrisation, while the energy is not; nonetheless, the two problems will be considered as equivalent for the following, since the solution of the geodesic equation gives an arc-length parametrised curve, which is minimal for the energy functional as well.

and rewriting the work as:

$$\begin{aligned}
W &= F[(\omega_1, H_1)] + \theta S(\rho_1|\omega_1) - F[(\omega_N, H_N)] - \theta S(\rho_N|\omega_N) + \\
&\quad - \sum_{i=1}^{N-1} [F[(\omega_{i+1}, H_{i+1})] + \theta S(\rho_i|\omega_{i+1}) - F[(\omega_{i+1}, H_{i+1})] - \theta S(\rho_{i+1}|\omega_{i+1})] = \\
&= -\Delta F_{eq} + \theta (S(\rho_1|\omega_1) - S(\rho_N|\omega_N)) - \theta \sum_{i=1}^{N-1} [S(\rho_i|\omega_{i+1}) - S(\rho_{i+1}|\omega_{i+1})], \quad (3.3)
\end{aligned}$$

where the first term is the difference in free energy for the equilibrium ensemble, the terms inside the parenthesis account for the non equilibrium contributions evaluated at the endpoints of the transformation, and the terms in the sum can be recognised to be the entropy production rate defined in chapter 2. Therefore, it can be seen how this expression is completely analogous to the one obtained in equation (3.1) for the classical case.

The expansion just obtained is exact, and it is certainly useful for interpretational reasons, in the sense that it helps to isolate and identify the terms which allows the analogy with classical thermodynamics, but, in principle, in the same way in which the exact evolution equation for an open system failed to clearly depict the short time behaviour which are of interest for the experience, this expression is still too general to show a univocal character. In particular, if one is interested only in the case in which the system is always close to a thermal state, an approximation scheme must be applied. Therefore, under the assumption that the state ρ can be written in the form:

$$\rho_i = \omega_i + \varepsilon \rho'_i + \mathcal{O}(\varepsilon^2),$$

it can be shown (appendix C) that the last sum in equation (3.3) can be expanded as:

$$\begin{aligned}
\sum_{i=1}^{N-1} [S(\rho_i|\omega_{i+1}) - S(\rho_{i+1}|\omega_{i+1})] &= \sum_{i=1}^{N-1} \left[\frac{1}{2N^2} \text{Tr} \left[\delta\omega_{i+1} \mathcal{J}_{\omega_{i+1}}^{-1} [\delta\omega_{i+1}] \right] \right] + \mathcal{O}\left(\frac{1}{N^2}\right) + \\
&\quad - \sum_{i=1}^{N-1} \left[\frac{\varepsilon}{N} \text{Tr} \left[\rho'_i \mathcal{J}_{\omega_{i+1}}^{-1} [\delta\omega_{i+1}] \right] \right] + \mathcal{O}(\varepsilon^2). \quad (3.4)
\end{aligned}$$

For the sake of clarity, the two terms obtained here will be considered separately, corresponding to the two limits of discrete perfectly thermalising protocols ($\varepsilon \rightarrow 0$) and of continuous quasi-isothermal ones ($N \rightarrow \infty$).

3.3 Discrete perfectly thermalising processes

The case in which perfect thermalisation is assumed at each step of the protocol completes the analogy between the derivation for the quantum framework and the one obtained in the classical formalism. In the limit in which $\varepsilon \rightarrow 0$ at each step, the protocol is of the form:

$$(\omega_1; H_1) \longrightarrow (\omega_2; H_2) \longrightarrow \dots \longrightarrow (\omega_N; H_N),$$

so that the states and the Hamiltonians are in a one to one correspondence. This allows to identify a trajectory in the state space ω_t with one in the space of traceless Hamiltonians H_t , and vice versa; this identification provides an isomorphism between the two spaces which can be used to see that, thanks to the fact that the space of Hamiltonians is isomorphic to \mathbb{R}^N , the tangent space of the state space is again isomorphic to the space of Hamiltonians. Plugging the expansion stated in chapter 1 into equation (3.4) :

$$\begin{aligned} \delta\omega_i &=_{\mathcal{O}(\frac{1}{N^2})} \lim_{N \rightarrow \infty} N(\omega(H_{i+1}) - \omega(H_i)) = \\ &= \lim_{N \rightarrow \infty} N(\omega(H_{i+1}) - \omega(H_{i+1} - \Delta H_i)) = \beta \mathcal{J}_{\omega_{i+1}} \left[\Delta H_i - \langle \Delta H_i \rangle_{\omega_{i+1}} \right], \end{aligned}$$

where the notation $\Delta H_i := H_{i+1} - H_i$ has been introduced, one obtains the following expression for the entropy production:

$$\sum_{i=1}^{N-1} [S(\rho_i || \omega_{i+1}) - S(\rho_{i+1} || \omega_{i+1})] =_{\mathcal{O}(\frac{1}{N^2})} \frac{\beta^2}{2N^2} \sum_{i=1}^{N-1} \text{Tr} \left[\mathcal{J}_{\omega_{i+1}} \left[\Delta H_i - \langle \Delta H_i \rangle_{\omega_{i+1}} \right] \Delta H_i \right].$$

If $N \gg 1$ one can pass to the continuous limit at the same order of approximation, i.e. it is possible to replace the discrete index $i \in \{1, \dots, N\}$ with a continuous one $t \in [0, 1]$, and one can rewrite:

$$\Delta H_i = H_{i+1} - H_i \stackrel{N \gg 1}{\cong} H_{t+\frac{1}{N}} - H_t =_{\mathcal{O}(\frac{1}{N^2})} \frac{1}{N} \dot{H}_t;$$

then, equation (3.3) takes the form:

$$W =_{\mathcal{O}(\frac{1}{N^2})} -\Delta F_{eq} - \frac{\beta}{2N} \int_0^1 dt \text{cov}_{\omega_t}(\dot{H}_t, \dot{H}_t). \quad (3.5)$$

It should be noticed that this result is formally equivalent to the one obtained for the classical case, where the covariance has been substituted by the generalised covariance; this is in accordance with the general belief that, at least in the weak coupling limit, the results of thermodynamics shouldn't be significantly altered in the quantum regime, up to a redefinition of some quantities to account for the non commutativity of the observables. In fact, even if it could seem that this setting is more general than the classical one, since here H_t is not required to be decomposed in collective variables, the classical framework naturally generalise to the case in which there is perfect experimental control over each parameter of the Hamiltonian, reestablishing the equivalence between the two settings.

It is useful now to show how the semi-Riemannian structure which was found for the classical case can be restricted to a Riemannian one in the quantum framework. Recalling the explicit expression of the generalised covariance:

$$\text{cov}_{\omega}(A, B) := \text{Tr} [A \mathcal{J}_{\omega} [B]] - \langle A \rangle_{\omega} \langle B \rangle_{\omega},$$

the linearity can be verified by inspection, and the symmetry follows from the fact that \mathcal{J}_{ρ} is a self-adjoint operator. For what regards the positive definiteness, it should be recalled that:

$$S(\omega(H + \varepsilon \dot{H}) || \omega(H)) = \frac{\varepsilon^2}{2} \text{cov}_{\omega}(\dot{H}, \dot{H}) \geq 0,$$

with equality if and only if $\omega(H + \varepsilon \dot{H}) \equiv \omega(H)$. Finding the conditions for which the equality holds then corresponds to identify the null-space of the generalised covariance: this happens whenever $\dot{H} \propto \mathbb{1}$, since this would only correspond to a shift of the trace of $e^{-\beta H}$, which is renormalised to one by Z ; this result corresponds to the intuition that a constant shift in the energy won't affect the physics. Therefore, it is sufficient to constrain the space of Hamiltonians to be traceless, for the covariance to be considered positive definite.

Before passing to illustrate the framework presented for the simplified case in which the system is constituted by a qubit, it is interesting to notice that, thanks to the inequality given in [19]:

$$\text{Tr} [H \mathcal{J}_\rho [H]] \leq \text{Tr} [\rho H^2],$$

one can give a bound on the maximum entropy production rate. In fact, examining the integrand in equation (3.5) and applying the inequality just presented, one obtains that:

$$\text{cov}_{\omega_t}(\dot{H}_t, \dot{H}_t) = \text{Tr} \left[\dot{H}_t \mathcal{J}_{\omega_t} [\dot{H}_t] \right] - \left\langle \dot{H}_t \right\rangle_{\omega_t}^2 \leq \left\langle \dot{H}_t^2 \right\rangle_{\omega_t} - \left\langle \dot{H}_t \right\rangle_{\omega_t}^2 =: \text{Var}_t [\dot{H}_t], \quad (3.6)$$

where the classical variance has been defined. This inequality is a stronger version of the fluctuation-dissipation result presented for the classical case, stating that the entropy production rate is always bounded by the variance of the corresponding fluctuating quantity.

3.3.1 An emblematic example: the two level system

It is useful to investigate what kind of structure the metric just defined induces on the space of Hamiltonians, and how the characteristic of the space can be exploited to design optimal protocols. For the sake of concreteness, the case in which the system is a qubit will be studied in the following section.

Preliminary, it should be noticed that the Stokes coordinates:

$$(\tilde{x}, \tilde{y}, \tilde{z}) \longrightarrow H(\tilde{x}, \tilde{y}, \tilde{z}) = \tilde{x} \sigma_x + \tilde{y} \sigma_y + \tilde{z} \sigma_z,$$

give a parametrisation of the traceless component of the space of hermitian 2x2 matrices $\mathcal{M}(\mathbb{C})^{sa}$. The space of Gibbs state can be parametrised in the same fashion as:

$$(x, y, z) \longrightarrow \omega_{(x,y,z)} \equiv \omega_\beta(H(x, y, z));$$

in the following, the coordinates given without a tilde will be used for the base-point, namely the Gibbs state in which the system is, while the one with tildes will denote the coordinates of the tangent space, corresponding to the change in the Hamiltonian.

Since the Pauli matrices give a basis of the tangent space, the metric at the point (x, y, z) is simply given by:

$$g_{i,j}(x, y, z) = \text{cov}_{\omega_{(x,y,z)}}(\sigma_i, \sigma_j) = \int_0^1 d\tau \text{Tr} \left[\omega_{(x,y,z)}^{1-\tau} \sigma_i \omega_{(x,y,z)}^\tau \sigma_j \right] - \langle \sigma_i \rangle_{\omega_{(x,y,z)}} \langle \sigma_j \rangle_{\omega_{(x,y,z)}};$$

the computation of the metric components for a general base-point in this coordinates is lengthy and, as it can be seen, gives little insight on the structure of the problem:

$$g = \begin{pmatrix} \frac{rx^2\beta\text{sech}^2(r\beta) + (y^2+z^2)\tanh(r\beta)}{r^3\beta} & \frac{xy(r\beta\text{sech}^2(r\beta) - \tanh(r\beta))}{r^3\beta} & \frac{xz(r\beta\text{sech}^2(r\beta) - \tanh(r\beta))}{r^3\beta} \\ \frac{xy(r\beta\text{sech}^2(r\beta) - \tanh(r\beta))}{r^3\beta} & \frac{ry^2\beta\text{sech}^2(r\beta) + (x^2+z^2)\tanh(r\beta)}{r^3\beta} & \frac{yz(r\beta\text{sech}^2(r\beta) - \tanh(r\beta))}{r^3\beta} \\ \frac{xz(r\beta\text{sech}^2(r\beta) - \tanh(r\beta))}{r^3\beta} & \frac{yz(r\beta\text{sech}^2(r\beta) - \tanh(r\beta))}{r^3\beta} & \frac{rz^2\beta\text{sech}^2(r\beta) + (x^2+y^2)\tanh(r\beta)}{r^3\beta} \end{pmatrix},$$

where the notation $r^2 = x^2 + y^2 + z^2$ has been introduced. For this reason it is useful to first analyse the case in which the base-point density matrix is diagonal, namely states of the form $\omega_\beta(r\sigma_z)$, and then use the insights one gets from this simplified case to find a better coordinate system to tackle the problem. In this case, the metric takes the simple form:

$$g = \begin{pmatrix} \frac{\tanh(\beta r)}{\beta r} & 0 & 0 \\ 0 & \frac{\tanh(\beta r)}{\beta r} & 0 \\ 0 & 0 & \text{sech}^2(\beta r) \end{pmatrix}$$

There are some interesting properties to be pointed out. First, it should be noticed that there is a unique eigenvalue for the fluctuations which tend to bring the system in a coherent superposition, which will be called off-diagonal directions, and a different eigenvalue for the direction along which the system stays classic, that is the diagonal direction. This difference is lost both at $r = 0$ and for $r \rightarrow \infty$.

At $r = 0$ the metric becomes euclidean, meaning that all the entries are ones. This is a consequence of the fact that the state of the system is given by $\omega_\beta(r\sigma_z)|_{r=0} \equiv \mathbb{1}$, which is diagonal in all the basis and, for this reason, there cannot be difference in the eigenvalues of different eigendirections; more physically, thinking of the system as a spin in a magnetic field, it is clear that for $r = 0$ the system is completely symmetric, while whenever $r > 0$ the spin will have a preferred basis in which to orient, and consequently any measurements along the orthogonal directions will give quantum interference.

On the other hand, for $r \rightarrow \infty$ the metric tends to be degenerate, with zeros in all the entries; this behaviour has a different explanation for the two eigenvalues: for the off-diagonal one it derives from the fact that the Hamiltonian itself won't be much affected by the addition of a small off-diagonal component, since one has that the diagonal component is of order $r \gg 1$; the behaviour of the diagonal eigenvalue, instead, can be understood examining the population in the excited state: in fact, it will be exponentially decaying in the gap between the levels so, in the limit in which the gap is big, changing the Hamiltonian won't affect but an exponentially low part of the population of the state. The two different sources of decay of the eigenvalues reflect in an exponential spacing between the two: the ratio between the off-diagonal component and the diagonal one exponentially diverges for $r \rightarrow \infty$.

Moreover, since the eigenvalues have the same formal dependence on r and on β , the behaviour just described will be identical if one considers the inverse temperature: for

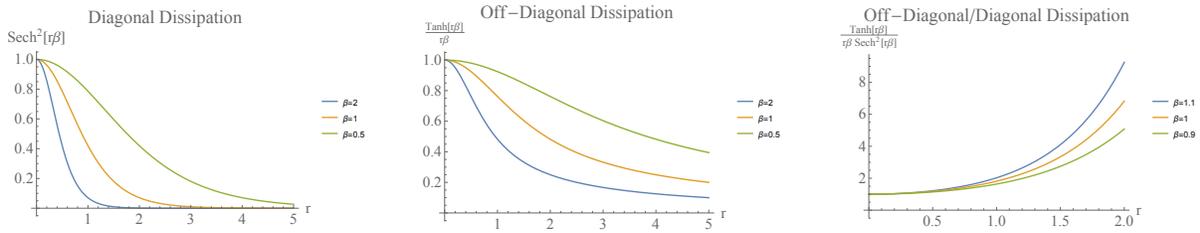


Figure 3.1: Behaviour of the eigenvalues of the covariance metric for different temperatures.

$\beta \rightarrow 0$, the infinite temperature limit, the metric will be euclidean because the two levels will be equally occupied, no matter what the Hamiltonian will look like; while for $\beta \rightarrow \infty$, for any finite r , the same train of thoughts just presented for the off-diagonal and for the diagonal component can be applied again. The facts just described are illustrated in figure 3.1.

It is important to remark that even if there is a direct physical interpretation of the exponential spacing between the eigenvalues of the metric, this is something that couldn't be inferred directly from equation (3.3): this gives important improvement over the naive minimisation, since this method can help to characterise the parameters which will be more dissipative in an automatic way, i.e. independently on any physical intuition on the system. Additionally, it is sensible to expect that the same structure in the eigenvalues will be present in a generic physical system: the covariance metric, in fact, is part of the so called Fisher information metrics, which have been extensively studied for classical systems [27, 28, 35]; in particular, it has been noticed that having a hierarchy of exponentially separated eigenvalues is a generic property for this kind of metrics. If this intuition could be carried through in the quantum case as well, not only the thermodynamic length formalism would give an automatic way of selecting optimal protocols, but it would provide important informations on the physics of the system itself, even thanks to the relation (3.6).

It is now clear that the existence of an eigenvalue in the z direction and one in the perpendicular plane can be seen as a suggestion that spherical coordinates could be a better choice than the Stokes ones; in fact, even if all the systems of coordinates are equal, some are more equal than others, since they automatically implement some symmetry of the system. In particular, it should be noticed that the generalised covariance is invariant under the group $U(n)$, which means that for every $U \in U(n)$ the following relations hold:

$$\begin{aligned} \text{cov}_{\omega(U^\dagger H U)}(A, B) &= \text{Tr} [A \mathcal{J}_{\omega(U^\dagger H U)} [B]] - \langle A \rangle_\omega \langle B \rangle_\omega = \\ &= \text{Tr} [U A U^\dagger A \mathcal{J}_{\omega(H)} [U B U^\dagger]] - \langle A \rangle_\omega \langle B \rangle_\omega = \\ &= \text{cov}_{\omega(H)}(A, B)(U A U^\dagger, U B U^\dagger). \end{aligned}$$

Since $SU(2)$ is in a two to one correspondence with $SO(3)$, passing to the spherical coordinates automatically implements this symmetry. In particular, parametrising the Hamil-

tonian as:

$$(\tilde{r}, \tilde{\theta}, \tilde{\phi}) \longrightarrow H(\tilde{r}, \tilde{\theta}, \tilde{\phi}) = \tilde{r} \cos \tilde{\theta} \sin \tilde{\phi} \sigma_x + \tilde{r} \sin \tilde{\theta} \sin \tilde{\phi} \sigma_y + \tilde{r} \cos \tilde{\phi} \sigma_z,$$

and using the convention above to define coordinates on the space of Gibbs state, one obtains the expression for the metric evaluated at a generic $\omega_{(r,\theta,\phi)}$:

$$\begin{aligned} g &= \begin{pmatrix} \operatorname{sech}^2(\beta r) & 0 & 0 \\ 0 & \frac{r \sin^2(\phi) \tanh(\beta r)}{\beta} & 0 \\ 0 & 0 & \frac{r \tanh(\beta r)}{\beta} \end{pmatrix} = \\ &= \begin{pmatrix} \operatorname{sech}^2(r\beta) & 0 & 0 \\ 0 & \frac{\tanh(r\beta)}{r\beta} & 0 \\ 0 & 0 & \frac{\tanh(r\beta)}{r\beta} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & r^2 \sin^2(\phi) & 0 \\ 0 & 0 & r^2 \end{pmatrix}; \end{aligned}$$

as it can be noticed, the metric can be decomposed as the product of a matrix containing the two eigenvalues (the diagonal one in the radial direction, and the off-diagonal one in the tangential direction) times the euclidean metric in spherical coordinates. Then, thanks to the fact that the metric tensor has this form on all the manifold, it is now clear that the arguments given above are always valid, with the only difference of replacing the z direction with the eigendirection along which the density matrix of the state is diagonal.

3.3.2 Riemannian properties of the covariance metric

It is now interesting to investigate the Riemannian properties induced by this metric. First, it is worth to point out that the radial subspace $Rad_{(\theta_0, \phi_0)} := \{(r, \theta_0, \phi_0) | r \geq 0\}$ is totally geodesic for any (θ_0, ϕ_0) , thanks to the $SO(3)$ symmetry; moreover, similarly to what happens for the geodesics of the sphere, one can also deduce that any plane passing from the origin will be totally geodesic as well. Therefore, in order to completely characterise the behaviour of the geodesics of the manifold, it is sufficient to study the ones which are restricted to a plane, or move only in the radial direction. These two cases are illustrated in figure 3.2.

As it can be seen the optimal trajectories tend to be more and more curved the further away from the origin they are. This can be quantitatively accounted for looking at the scalar curvature, which turns out to depend on the radius alone; its behaviour is illustrated in figure 3.3: as it was suggested by the inspection of the metric, in fact, for $r = 0$ the curvature is zero, so that the space at the origin locally look euclidean⁴; moreover, the scalar curvature is exponentially decreasing in r , accounting for the bigger bending of highly energetic geodesics. It has been conjectured in [25] that the scalar curvature induced by the generalised covariance should be generically monotone in the entropy. This conjecture has been illustrated in figure 3.4. In order to better show this behaviour in the limit of $r \rightarrow \infty$ the population coordinate has been introduced as:

$$p := \frac{1}{2} (1 - \tanh \beta r),$$

⁴The Riemann tensor is quadratic in r at the origin.

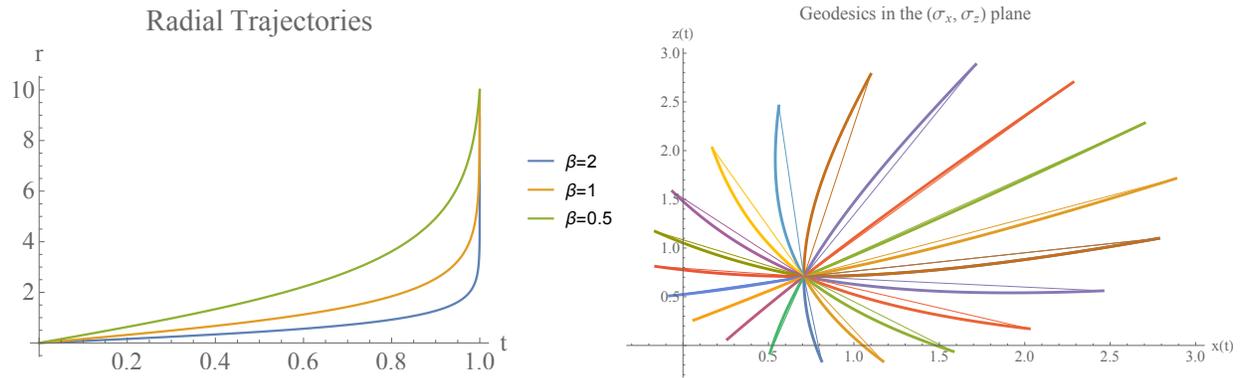


Figure 3.2: Geodesics of the generalised covariance metric: on the left, the behaviour of the geodesics for different temperature is shown; on the right the geodesics of the metric in the (x, z) plane are compared with straight lines.

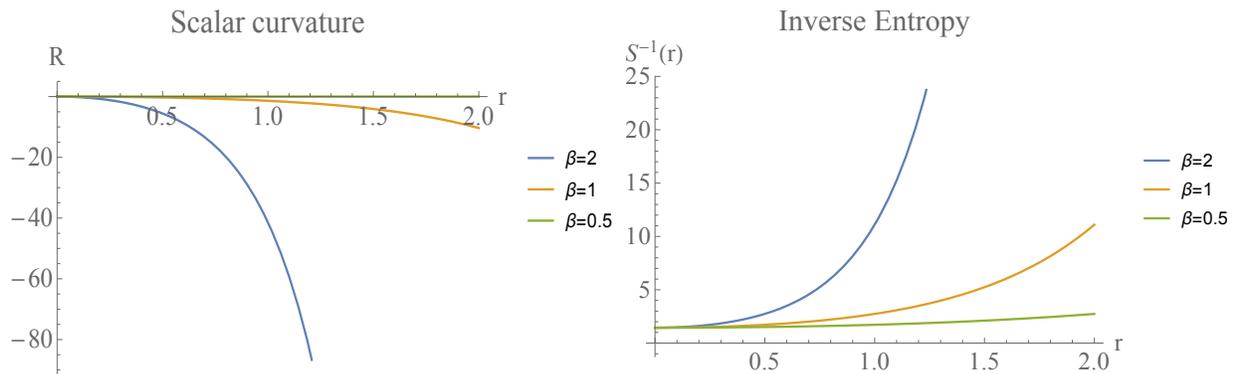


Figure 3.3: Dependence of scalar curvature R and of the inverse entropy $S^{-1}(r)$ on r .

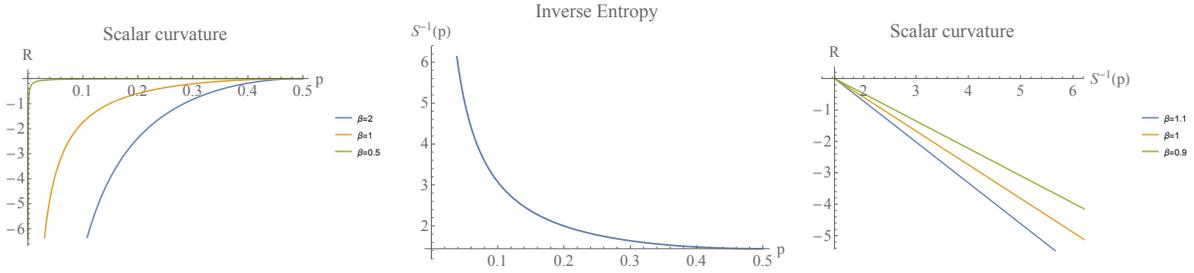


Figure 3.4: Dependence of scalar curvature R and of the inverse entropy on p . In the third plot, it is shown how the two quantities have a linear dependence on each other.

which measure the fraction of the system in the excited state, and it ranges in the interval $[0, \frac{1}{2}]$. Then, examining figure 3.4, it can be seen that the scalar curvature is approximately linear in the inverse of the entropy. This fact agrees with the intuition outlined above and can be understood looking at the two limit cases of an extremely disordered system and an ordered one: in the first case, which formally corresponds to $S^{-1}(\omega) \rightarrow 0$, the absence of a preferred direction will make all the eigenvalues of the metric equal, giving a euclidean character to the space; in the second case, for which $S^{-1}(\omega) \gg 1$, there will exist an exponential spacing in the decay of different eigenvalues of the metric, giving an hyperbolic character to the space. This insight is sustained by the way the temperature influences the scalar curvature: for a high temperature ($\beta \ll 1$) the curvature will stay close to zero even for a high energy difference between the two levels, while in the low temperature limit ($\beta \gg 1$) the system will be really sensitive to changes in the Hamiltonian.

3.3.3 Improvement in the efficiency

As it has been extensively shown, the framework of the thermodynamic length is useful to get insights on the physics of the system, to give fluctuation-dissipation bounds and to automatically provide minimally dissipative trajectories in the space of parameters; nonetheless, if the improvement in the work extraction one would get from implementing a geodesic would be negligible, this formalism would be little more than a theoretical nuance. Therefore it is the aim of this section to show how much the trajectory given by the thermodynamic length significantly outperform the naive choice of connecting two Hamiltonians via a segment. The trajectory chosen to illustrate this fact is defined by the two endpoints $H_0 = 0 \rightarrow H_1 = 10\sigma_z$: in figure 3.5, the euclidean trajectory and optimal trajectories for different values of β are depicted, and the dots along each curve are obtained evaluating each curve at the times $\{\frac{i}{N}\}$; the dots then corresponds to the sequence of Hamiltonians one has to implement when realising the discrete transformation.

Firstly, it has been numerically verified that the dependence of the dissipation on the number of steps decays as N^{-1} regardless of the trajectory performed, in accordance with equation (3.5). To show this behaviour, the quantity:

$$N(-\Delta F_{eq} - W) = \mathcal{O}(1)$$

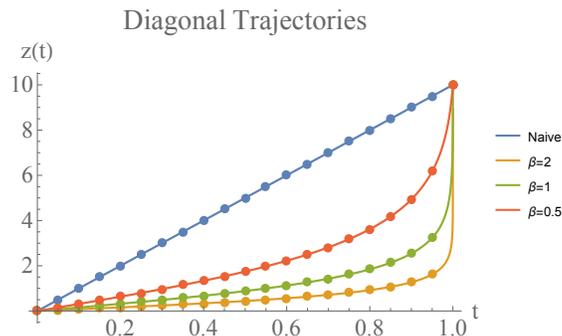


Figure 3.5: Optimal trajectories at fixed endpoints for different temperatures. The blue curve gives the euclidean case, while the dots are equidistant in $t \in [0, 1]$

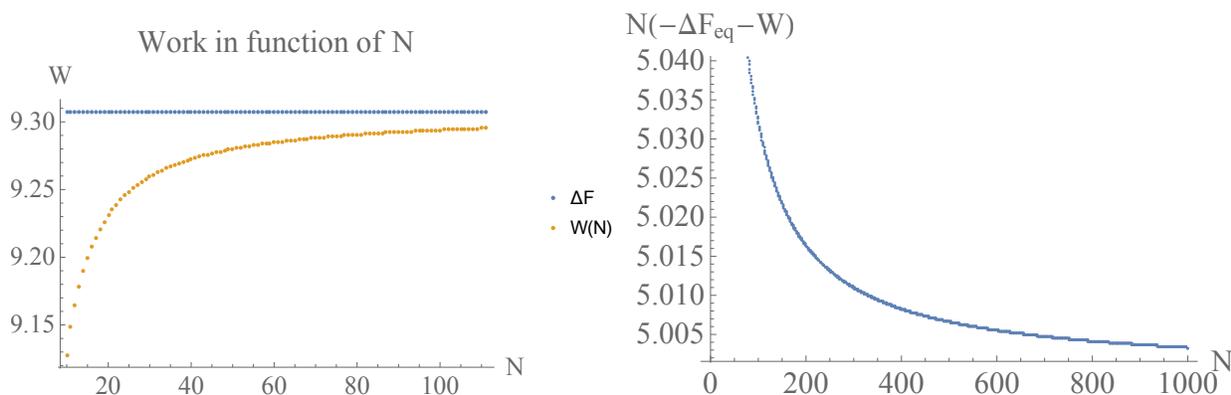


Figure 3.6: For $N \rightarrow \infty$, the work along any trajectory converges to the maximal one, with a correction which scales as $1/N$.

has been plotted in figure 3.6, expecting it to be constant; as it can be seen, though, there is an additional decay: this comes from the resummation of all the other terms in the series expansion, which will give a small shift from the asymptotic constant value. In fact, multiplying again the difference between the free energy and the work by the number of steps, one would obtain an approximately linear scaling, proving the fact that the additional correction is sub-polynomial in N^{-1} . This result sustains the correctness of the approximation scheme applied to obtain equation (3.5).

Successively, the work extracted along the naive protocol has been compared with the one obtains along an optimal trajectory for different temperatures (figure 3.7); it can be seen that not only the improvement is bigger for lower temperatures, as it would be expected from the discussions above, but also the convergence to the maximal work is faster. In fact, after an initial transient for $\beta \ll 1$, the improvement appears to be linear in the inverse temperature (figure 3.8): as it can be seen, already for $\beta = 1$ the optimal protocol is four

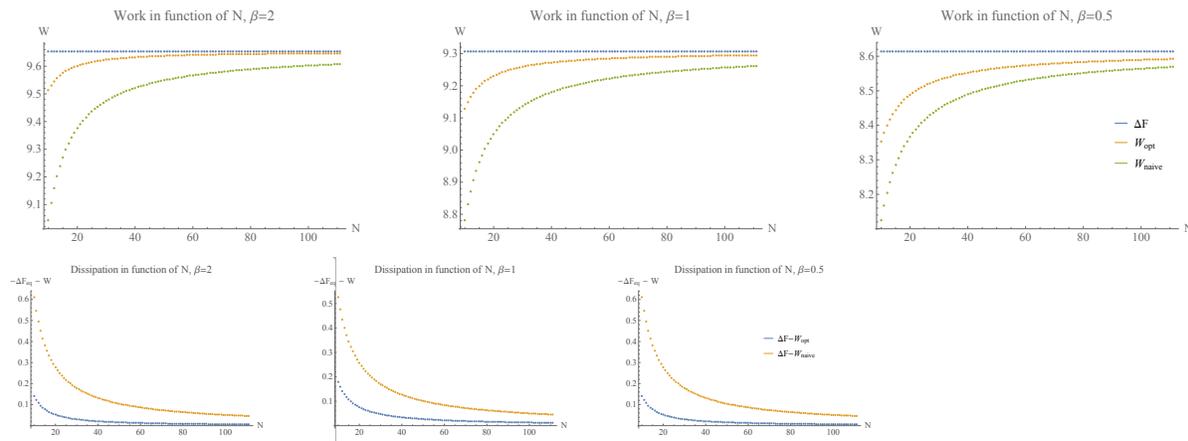


Figure 3.7: The work extracted along the naive trajectory (in green or blue) compared with the optimal protocol (orange).

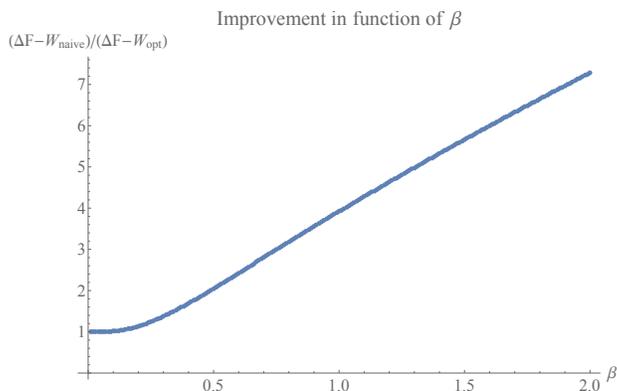


Figure 3.8: The improvement appears to be linear in β . The points of this graph are taken for a fixed number of steps $N = 100$.

times less dissipative than the naive one.

As it can be seen, then, the importance of the thermodynamic length is far from being only theoretical: the improvement in the work extraction is so high that it is sensible from an engineering point of view to implement these protocols, rather than restrict to the naive ones. Two examples of possible applications are treated in appendix D and E, in which it is shown how to give a better bound on the heat released during a Landauer erasure protocol, and in which way Carnot-like quantum cycle can be improved in the strong coupling regime.

3.4 Quasi-isothermal continuous processes

After the study of how to introduce a thermodynamic length on processes for which the state is thermal at each step, it is now time to consider the second term in equation (3.4),

which will give the contributions to the dissipation arising when one considers systems which do not perfectly thermalise at each step⁵.

In analogy to what was done in the previous section, in order to simplify the treatment the limit $N \rightarrow \infty$ will be taken; equation (3.3) and (3.4) can be combined to give:

$$W = -\Delta F_{eq} + \theta (S(\rho_0||\omega_0) - S(\rho_1||\omega_1)) + \theta \varepsilon \int_0^1 dt \text{Tr} [\rho'_t \mathcal{J}_{\omega_t}^{-1} [\dot{\omega}_t]] + \mathcal{O}(\varepsilon^2).$$

Then, inserting the expression of $\dot{\omega}_t$ in the integral, one obtains the following expression:

$$\begin{aligned} \theta \varepsilon \int_0^1 dt \text{Tr} \left[\rho'_t \mathcal{J}_{\omega_t}^{-1} \left[-\beta \mathcal{J}_{\omega_t} \left[\dot{H}_t - \langle \dot{H}_t \rangle_{\omega_t} \right] \right] \right] &= -\varepsilon \int_0^1 dt \text{Tr} [\rho'_t \dot{H}_t] \\ &+ \varepsilon \int_0^1 dt \text{Tr} [\rho'_t \mathcal{J}_{\omega_t}^{-1} [\omega_t]] \langle \dot{H}_t \rangle_{\omega_t}, \end{aligned}$$

where in the second line the fact that $\mathcal{J}_{\omega_t}^{-1} [\omega_t] = \mathbb{1}$ has been used, together with the fact that ρ'_t is traceless, being part of the perturbative expansion of a density matrix. Additionally, if one assumes the expansion:

$$\rho_t = \omega_t + \varepsilon \rho'_t + \mathcal{O}(\varepsilon^2)$$

to hold at all times, it can be noticed that at the same order of approximation one can neglect the non-equilibrium contribution to the free energy:

$$S(\omega_0 + \varepsilon \rho'_0||\omega_0) = \mathcal{O}(\varepsilon^2) = S(\omega_1 + \varepsilon \rho'_1||\omega_1).$$

Putting the two results together, one can then express the work simply as:

$$W = -\Delta F_{eq} - \varepsilon \int_0^1 dt \text{Tr} [\rho'_t \dot{H}_t]. \quad (3.7)$$

It is interesting to notice that this expression could be obtained directly from the definition of work in the continuous case:

$$\begin{aligned} W &= -\int_0^1 dt \text{Tr} [\rho_t \dot{H}_t] = -\left(\int_0^1 dt \text{Tr} [\omega_t \dot{H}_t] + \int_0^1 dt \text{Tr} [\rho'_t \dot{H}_t] \right) = \\ &= \theta \int_0^1 dt \frac{d}{dt} \log [Z_t] - \int_0^1 dt \text{Tr} [\rho'_t \dot{H}_t] = \\ &= -\Delta F_{eq} - \varepsilon \int_0^1 dt \text{Tr} [\rho'_t \dot{H}_t], \end{aligned}$$

reassuring about the compatibility between continuous transformations and discrete ones in the limit in which $N \rightarrow \infty$.

⁵These contributions will also be called finite time effects, because in the limit of a continuous process perfect thermalisation is possible only in the limit in which the time of the process $T \rightarrow \infty$.

In order to define a thermodynamic length in this case, it must be assumed that ρ'_t only depends on ω_t and \dot{H}_t , which is the same as asking the linear response theory to be valid; therefore, the framework which will be now outlined should be expected to hold quite in general. For concreteness and simplicity of exposition, though, the state will be assumed to be described by the expansion given in section 2.5:

$$\rho_t = \omega_t + \frac{1}{T} \Lambda_t^{-1} \frac{d}{dt} [\omega_t]; \quad (3.8)$$

nonetheless, it has to be kept in mind that it should be possible to apply the arguments which will be used to introduce the thermodynamic length to more general perturbation expansions.

Then, plugging the expansion (3.8) into equation (3.7), one gets:

$$\begin{aligned} W &= -\Delta F_{eq} - \frac{1}{T} \int_0^1 dt \operatorname{Tr} \left[\dot{H}_t \Lambda_t^{-1} \frac{d}{dt} [\omega_t] \right] = \\ &= -\Delta F_{eq} + \frac{\beta}{T} \int_0^1 dt \operatorname{Tr} \left[\dot{H}_t \left(\Lambda_t^{-1} \mathcal{J}_{\omega_t} \left[\dot{H}_t - \langle \dot{H}_t \rangle_{\omega_t} \right] \right) \right] \stackrel{(2.7)}{=} \\ &\stackrel{(2.7)}{=} -\Delta F_{eq} - \theta T \int_0^1 dt \sigma(\rho_t), \end{aligned}$$

where the expression of the entropy production rate given in equation (2.7) has been used in the last line. As it can be easily noticed, even in this case the work splits in the difference of free energy at the endpoints minus the integrated entropy production rate.

Then, defining the bilinear map:

$$m_{\omega_t}^\Lambda(A, B) = -\frac{1}{2} \left(\operatorname{Tr} \left[\Lambda_t^{-1} \mathcal{J}_{\omega_t} \left[A - \langle A \rangle_{\omega_t} \right] B \right] + \operatorname{Tr} \left[\Lambda_t^{-1} \mathcal{J}_{\omega_t} \left[B - \langle B \rangle_{\omega_t} \right] A \right] \right),$$

the work can be rewritten in the form:

$$W = \mathcal{O}\left(\frac{1}{T^2}\right) - \Delta F_{eq} - \frac{\beta}{T} \int_0^1 dt m_{\omega_t}^\Lambda(\dot{H}, \dot{H}).$$

Then, thanks to the expression of the second law given in equation (2.7), $m_{\omega_t}^\Lambda$ is a positive map, and since it is trivially linear and symmetric by construction, it can be used to define a semi-Riemannian structure on the space of Hamiltonians; moreover, restricting the domain of $m_{\omega_t}^\Lambda$ to the traceless subspace, it can be made positive definite: in fact, it is the composition of Λ^{-1} , which is non singular on the traceless subspace, with \mathcal{J}_ω , which is positive definite on the same domain.

It can be noticed that all the results given for the covariance metric can be reproduced here for $m_{\omega_t}^\Lambda$. In particular, defining $\lambda_t^{(min)}$ to be the smallest eigenvalues of Λ_t , one can use equation (3.6) to give an analogous bound on the maximum dissipation for a quantum system:

$$m_{\omega_t}^\Lambda(\dot{H}, \dot{H}) \leq (\lambda_t^{(min)})^{-1} \operatorname{cov}_{\omega_t}(\dot{H}_t, \dot{H}_t) \leq (\lambda_t^{(min)})^{-1} \operatorname{Var}_t \left[\dot{H}_t \right].$$

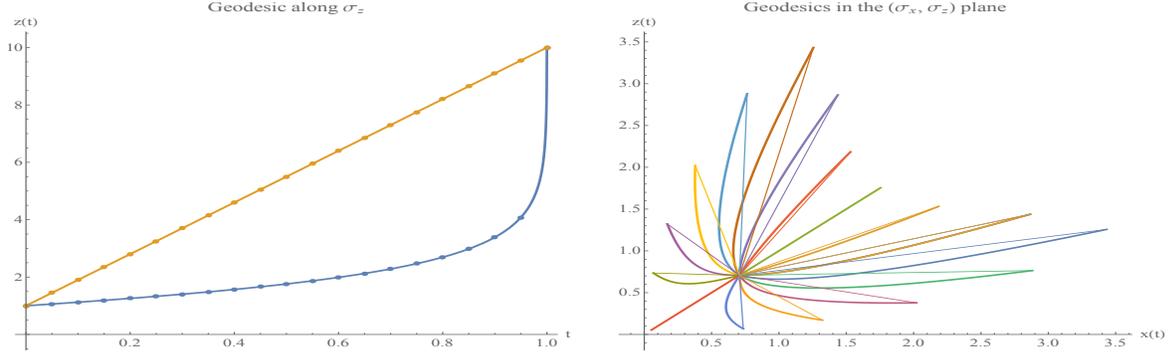


Figure 3.9: Geodesics of m^Λ . The similarity with the one for the generalise covariance should be noticed.

As an example, one can consider the Lindbladian equation in (2.8) describing a qubit in contact with a radiation field. Then, thanks to the fact that the Lindbladian in this case has the same symmetries as the generalised covariance matrix, one can express m^Λ in spherical coordinates for a generic point $\omega_{(r,\theta,\phi)}$ as:

$$\begin{aligned}
 m^\Lambda &= \begin{pmatrix} \frac{\tanh(\beta r) \operatorname{sech}^2(\beta r)}{\gamma} & 0 & 0 \\ 0 & \frac{2r \sin^2(\phi) \tanh^2(\beta r)}{\beta \gamma} & 0 \\ 0 & 0 & \frac{2r \tanh^2(\beta r)}{\beta \gamma} \end{pmatrix} = \\
 &= \frac{\tanh(\beta r)}{\gamma} \begin{pmatrix} \operatorname{sech}^2(\beta r) & 0 & 0 \\ 0 & \frac{2r \sin^2(\phi) \tanh(\beta r)}{\beta} & 0 \\ 0 & 0 & \frac{2r \tanh(\beta r)}{\beta} \end{pmatrix},
 \end{aligned}$$

where the metric has been decomposed to underline the similarity with the covariance metric. In fact, the Riemannian structure which this metric will endow the space of Hamiltonians with is quite similar to the one in the previous section, having an exponentially decreasing non-positive curvature and an analogous structure in the geodesics, as it can be seen from figure 3.9. The main difference comes from the fact that for $r \rightarrow 0$ the metric becomes singular: this is a consequence of the fact that the Lindbladian itself is singular when the energy spacing between the two levels is zero, since in this case the system cannot absorb nor emit photons.

3.5 Conclusions

It is now useful to summarise the results obtained in this chapter. Firstly, it has been shown that the work extracted from a bath can be expressed as:

$$W = -\Delta F_{eq} + \theta (S(\rho_1 || \omega_1) - S(\rho_N || \omega_N)) - \theta \sum_{i=1}^{N-1} [S(\rho_i || \omega_{i+1}) - S(\rho_{i+1} || \omega_{i+1})],$$

which, assuming $N \gg 1$, $T \gg 1$ and that during the transformation the state is always close to a thermal one, can be expressed in the form:

$$W = -\Delta F_{eq} - \frac{\beta}{2N} \int_0^1 dt \text{cov}_{\omega_t}(\dot{H}_t, \dot{H}_t) + \mathcal{O}\left(\frac{1}{N^2}\right) \\ - \frac{\beta}{T} \int_0^1 dt m_{\omega_t}^{\Lambda_t}(\dot{H}, \dot{H}) + \mathcal{O}\left(\frac{\tau_{th}}{NT}\right) + \mathcal{O}\left(\frac{1}{T^2}\right).$$

The two integrands have been recognised to be the entropy production rate, so that this formula has the natural interpretation that the work extracted during a thermodynamical protocol is given by the optimal one, minus the dissipation during the process.

It has been then shown how one can interpret the two integrals as the energy functional of suitable metrics and the Riemannian structure which each of them endows upon the space of Hamiltonians has been separately studied, obtaining optimal protocols which significantly outperforms Euclidean ones. It should be noticed that one can put the two cases together, using the fact that the sum of two scalar products is again a scalar product, obtaining a metric for discrete processes which can be described by the expansion (3.8). For this reason, the formalism presented here not only extends the results of the literature to the quantum setting, but it also generalises the classical framework to the case in which the system is slightly out of equilibrium.

The results given can be extended in many ways: for example, one could wonder how the formalism outlined here can be generalised to the case in which the system is strongly coupled to the environment, a scenario that is of crucial interest for quantum systems; the first steps in this direction have been presented in appendix E, where the generalised covariance metric is treated, and where it is argued how to extend the time-metric to this case, problem which shouldn't be much more than a technical difficulty. Another possible extension is to consider systems which equilibrate to generalised Gibbs ensembles rather than thermal states: even in this case, if one can find a relation between the free energy and the relative entropy along the lines of equation (1.1), it should be possible to reproduce the full derivation without further difficulties. In fact, one of the strength of the thermodynamic length formalism is its versatility, thanks to the ease with which one can extend it to scenarios which weren't initially in the realm of applicability of the framework.

A more fundamental problem is to verify whether the exponentially spaced structure in the eigenvalues of the metric is in fact a generic property: this would imply the existence of a hierarchy in the observables, meaning that only few variables would account for the main features of the system. Then, this would justify the key assumption made in thermodynamics, that a macroscopically large system can be described only by a few parameters, upon restricting the observations to be coarse-grained.

Therefore, it can be seen that the thermodynamic length has all the features a good theoretical framework should have: on the one hand, it has many practical applications and highly simplifies the solution of problems which would be intractable in the present formalism; on the other, it can be used to tackle, and hopefully solve, fundamental questions.

Appendix A

Notations

The notation used throughout the text are listed below:

1. The temperature will be indicated with θ , and the inverse temperature will be indicated with $\beta := (k_B\theta)^{-1}$. As a convention $k_B = 1$.
2. With $=_{\mathcal{O}(f(t))}$ it will be denoted the following equivalence relation:

$$A =_{\mathcal{O}(f(t))} B \iff A = B + \mathcal{O}(f(t)).$$

3. A system at temperature $\theta = \beta^{-1}$ in the state ρ and Hamiltonian H will be indicated with the notation $(\rho; H)_\beta$. The subscript β will be dropped whenever this won't lead to confusions. Moreover, if the state is thermal:

$$\omega_\beta(H) := \frac{e^{-\beta H}}{\text{Tr}[e^{-\beta H}]},$$

the following shorthand will be used:

$$(\omega; H)_\beta := (\omega_\beta(H); H)_\beta.$$

4. The density matrix of a bipartite system AB will be denoted as ρ^{AB} , while the reduced density matrix obtained tracing out part of the system will be denoted by the subscript of the remaining part (e.g. $\rho^A = \text{Tr}_B[\rho^{AB}]$).
5. The average with respect to a state will be denoted with the angle brackets with the state in the subscript:

$$\langle A \rangle_\rho \equiv \text{Tr}[A\rho].$$

6. The operator \mathcal{J}_ρ and its inverse, acting on self-adjoint operators, are defined whenever ρ is a full rank density matrix as:

$$\mathcal{J}_\rho[A] = \int_0^1 d\tau \rho^{1-\tau} A \rho^\tau \quad \mathcal{J}_\rho^{-1}[A] = \int_0^\infty dx (\rho + x)^{-1} A (\rho + x)^{-1}.$$

Additionally, the generalised covariance is given as:

$$\text{cov}_\rho(A, B) := \text{Tr} [A \mathcal{J}_\rho [B]] - \langle A \rangle_\rho \langle B \rangle_\rho = \int_0^1 d\tau \text{Tr} [\rho^{1-\tau} A \rho^\tau B] - \langle A \rangle_\rho \langle B \rangle_\rho;$$

this expression simplifies to the usual covariance whenever A or B commute with ρ .

7. The von Neumann entropy of a state ρ is defined as:

$$S(\rho) = -\text{Tr} [\rho (\log [\rho])].$$

8. The free energy of a state ρ respect to a Hamiltonian H is defined as:

$$F [(\rho; H)_\beta] = \langle H \rangle_\rho - \theta S(\rho).$$

If the free energy is computed on a thermal state $\omega(H)$ with respect to H , the Hamiltonian will be omitted: $F [(\omega(H), H)] \equiv F [\omega_\beta(H)]$.

9. The relative entropy of a state ρ_1 with respect to a state ρ_2 is defined as:

$$S(\rho_1 || \rho_2) = \text{Tr} [\rho_1 (\log [\rho_1] - \log [\rho_2])].$$

10. The mutual information of a bipartite system ρ^{AB} is defined as:

$$I(A|B) := S(\rho^A) + S(\rho^B) - S(\rho^{AB}).$$

11. The Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ are defined as:

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Moreover the two matrices σ_\pm are defined as:

$$\sigma_+ = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \sigma_- = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.$$

where the fact that H_t commutes with e^{H_t} allows to have a well defined differentiation. Since the equality is true for $s = 0$ and the derivatives of the right and the left hand side coincide, the result must hold for all s . In particular, the lemma is regained setting $s = 1$. \square

Recalling the definitions:

$$\mathcal{J}_\rho [A] = \int_0^1 d\tau \rho^{1-\tau} A \rho^\tau \quad \mathcal{J}_\rho^{-1} [A] = \int_0^\infty dx (\rho + x)^{-1} A (\rho + x)^{-1},$$

the expansion of the exponential and of the logarithm can be given:

Theorem 1. *Given H_t and ρ_t a smooth family of hermitian matrices and of full rank density matrices respectively, the following expansions hold to cubic order:*

(i). *The expansion of e^{H_t} is given by:*

$$\begin{aligned} e^{H_t} = & \mathcal{O}(t^3) e^{H_0} + t \mathcal{J}_{e^{H_0}} [H'_0] + \frac{t^2}{2} \mathcal{J}_{e^{H_0}} [H''_0] + \\ & + \frac{t^2}{2} \int_0^1 d\tau \left[\int_0^{1-\tau} d\eta (e^{(1-(\tau+\eta))H_0} H'_0 e^{\eta H_0} H'_0 e^{\tau H_0}) + \right. \\ & \left. + \int_{1-\tau}^1 d\eta (e^{(1-\tau)H_0} H'_0 e^{(\eta+\tau-1)H_0} H'_0 e^{(1-\eta)H_0}) \right]; \end{aligned}$$

(ii). *The expansion of $\log [\rho_t]$ is given by:*

$$\begin{aligned} \log [\rho_t] = & \mathcal{O}(t^3) \log [\rho_0] + t \mathcal{J}_{\rho_0}^{-1} [\rho'_0] + \frac{t^2}{2} \mathcal{J}_{\rho_0}^{-1} [\rho''_0] + \\ & - \frac{t^2}{2} \mathcal{J}_{\rho_0}^{-1} \left[\int_0^1 d\tau \left[\int_0^{1-\tau} d\eta \left(\rho_0^{1-(\tau+\eta)} \mathcal{J}_{\rho_0}^{-1} [\rho'_0] \rho_0^\eta \mathcal{J}_{\rho_0}^{-1} [\rho'_0] \rho_0^\tau \right) + \right. \right. \\ & \left. \left. + \int_{1-\tau}^1 d\eta \left(\rho_0^{(1-\tau)} \mathcal{J}_{\rho_0}^{-1} [\rho'_0] \rho_0^{(\eta+\tau-1)} \mathcal{J}_{\rho_0}^{-1} [\rho'_0] \rho_0^{1-\eta} \right) \right] \right]. \end{aligned}$$

Proof. (i). The term of order t has been computed in the lemma above. The second derivative follows easily, applying again the result in the proof of the lemma, and with a change of coordinates in the second integration.

(ii). The second term is obtained from the formal expansion:

$$\log [\rho_t] = \mathcal{O}(t^3) A + t B + \frac{t^2}{2} C$$

together with the approximate equality:

$$\rho_t = \mathcal{O}(t^3) \rho_0 + t \rho'_0 + \frac{t^2}{2} \rho''_0 = \mathcal{O}(t^3) e^{A+tB+\frac{t^2}{2}C} = \mathcal{O}(t^3) e^{\log[\rho_t]}.$$

For the equality to hold at $t = 0$ one has $A \equiv \log[\rho_0]$; moreover, it follows easily, expanding the exponential and equating the terms in t , that:

$$\mathcal{J}_{\rho_0}[B] \equiv \rho'_0,$$

so that even the term of order t in the expansion is obtained as well. Inserting B in the second derivative of the exponential and repeating the same procedure, one finally obtains the result. \square

These two fundamental expansions can be used to obtain the following:

Theorem 2. *Given H_t and ρ_t a smooth family of hermitian matrices and of full rank density matrices respectively, the following expansion holds to cubic order:*

(i). *The expansion of $Z_t = \text{Tr}[e^{-\beta H_t}]$ is given by:*

$$Z_t = \mathcal{O}(t^3) Z_0 \left[1 - \beta t \langle H'_0 \rangle_0 + \frac{\beta^2 t^2}{2} \left[\text{cov}_0(H'_0, H'_0) + \langle H'_0 \rangle_0^2 - \theta \langle H''_0 \rangle_0 \right] \right];$$

(ii). *The relative entropy $S(\rho_0 || \rho_t)$ can be expanded as:*

$$S(\rho_0 || \rho_t) = \mathcal{O}(t^3) \frac{t^2}{2} \int_0^\infty dx \text{Tr} [\rho'_0(\rho_0 + x)^{-1} \rho'_0(\rho_0 + x)^{-1}].$$

Proof. Before starting, it should be noticed that the two following two relations hold:

$$\text{Tr}[\mathcal{J}_A[B]] \equiv \text{Tr}[AB] \qquad \text{Tr}[\mathcal{J}_A^{-1}[B]] \equiv \text{Tr}[A^{-1}B],$$

thanks to the cyclicity of the trace.

(i). From the first lemma one has:

$$\begin{aligned} \frac{\partial}{\partial t} \text{Tr}[e^{-\beta H_t}] &= -\beta \text{Tr}[\mathcal{J}_{e^{-\beta H_t}}[H'_t]] = \text{Tr}[e^{-\beta H_t} H'_t] \\ \frac{\partial^2}{\partial t^2} \text{Tr}[e^{-\beta H_t}] &= -\beta \frac{\partial}{\partial t} \text{Tr}[e^{-\beta H_t} H'_t] = -\beta \text{Tr}[e^{-\beta H_t} H''_t] + \beta^2 \text{Tr}[\mathcal{J}_{e^{-\beta H_t}}[H'_t] H'_t]; \end{aligned}$$

additionally, this last term can be easily rewritten as:

$$\text{Tr}[\mathcal{J}_{e^{-\beta H_t}}[H'_t] H'_t] = \int_0^1 d\tau \text{Tr}[e^{-\beta(1-\tau)H_t} H'_t e^{-\beta\tau H_t} H'_t] = Z_t \left(\text{cov}_{\omega_t}(H'_t, H'_t) + \langle H'_t \rangle_t^2 \right).$$

Then, the result is simply the Taylor expansion of Z_t . It is useful to point out that expanding the exponential first, one get the following useful relation:

$$\begin{aligned} \text{Tr} \left[\int_0^1 d\tau \left[\int_0^{1-\tau} d\eta (e^{(1-(\tau+\eta))H_t} H'_t e^{\eta H_t} H'_t e^{\tau H_t}) + \right. \right. \\ \left. \left. + \int_{1-\tau}^1 d\eta (e^{(1-\tau)H_t} H'_t e^{((\eta+\tau)-1)H_t} H'_t e^{(1-\eta)H_t}) \right] \right] = \text{Tr}[\mathcal{J}_{e^{-\beta H_t}}[H'_t] H'_t]. \end{aligned}$$

For sake of bookkeeping the quantity in the first trace will be denoted by $\widetilde{\text{cov}}_{e^{H_t}}(H'_t, H'_t)$.

(ii). Expanding ρ_t to second order one has:

$$\begin{aligned} S(\rho_0||\rho_t) &=_{\mathcal{O}(t^3)} \text{Tr} \left[\rho_0 \left(\log [\rho_0] - \log \left[\rho_0 + t \rho'_0 + \frac{t^2}{2} \rho''_0 \right] \right) \right] =_{\mathcal{O}(t^3)} \\ &=_{\mathcal{O}(t^3)} \text{Tr} \left[\rho_0 \left(\log [\rho_0] - \log [\rho_0] - t \mathcal{J}_{\rho_0}^{-1} [\rho'_0] - \frac{t^2}{2} \mathcal{J}_{\rho_0}^{-1} [\rho''_0] \right. \right. \\ &\quad \left. \left. + \frac{t^2}{2} \mathcal{J}_{\rho_0}^{-1} [\text{cov}_{\rho_0}(\mathcal{J}_{\rho_0}^{-1} [\rho'_0], \mathcal{J}_{\rho_0}^{-1} [\rho'_0])] \right) \right]; \end{aligned}$$

since $\mathcal{J}_{\rho_0}^{-1}$ commutes with ρ_0 , and ρ'_0 and ρ''_0 are traceless, one has:

$$\begin{aligned} S(\rho_0||\rho_t) &=_{\mathcal{O}(t^3)} \text{Tr} \left[\rho_0 \left(-t \mathcal{J}_{\rho_0}^{-1} [\rho'_0] - \frac{t^2}{2} \mathcal{J}_{\rho_0}^{-1} [\rho''_0] + \frac{t^2}{2} \mathcal{J}_{\rho_0}^{-1} [\text{cov}_{\rho_0}(\mathcal{J}_{\rho_0}^{-1} [\rho'_0], \mathcal{J}_{\rho_0}^{-1} [\rho'_0])] \right) \right] = \\ &= -\text{Tr} \left[\cancel{\rho_0 \rho_0^{-1} (t \rho'_0 + \frac{t^2}{2} \rho''_0)} \right] + \frac{t^2}{2} \text{Tr} [\rho_0 \rho_0^{-1} \text{cov}_{\rho_0}(\mathcal{J}_{\rho_0}^{-1} [\rho'_0], \mathcal{J}_{\rho_0}^{-1} [\rho'_0])] = \\ &= \frac{t^2}{2} \text{Tr} [\mathcal{J}_{\rho_0} [\mathcal{J}_{\rho_0}^{-1} [\rho'_0]] \mathcal{J}_{\rho_0}^{-1} [\rho'_0]] = \frac{t^2}{2} \int_0^\infty dx \text{Tr} [\rho'_0 (\rho_0 + x)^{-1} \rho'_0 (\rho_0 + x)^{-1}]. \end{aligned}$$

□

A natural consequence of the last two theorems is the following:

Lemma 3. *Let $\omega_t := \omega_\beta(H_t)$ be a smooth family of Gibbs state; then the following expansion holds:*

$$\omega_t =_{\mathcal{O}(t^2)} \omega_0 + t \omega'_0 = \omega_0 \left(\mathbb{1} - \beta t \left[\omega_0^{-1} \mathcal{J}_{\omega_0} [H'_0] - \langle H'_0 \rangle_{\omega_0} \right] \right).$$

Proof. It is sufficient to note that: $\omega_t = \frac{e^{-\beta H_t}}{Z_t}$, and apply the two theorems above to the numerator and the denominator. □

Finally, two important properties of the relative entropy can be now given.

Corollary 1. *The relative entropy is symmetric to cubic order:*

$$S(\rho_0||\rho_t) =_{\mathcal{O}(t^3)} S(\rho_t||\rho_0).$$

Proof. Noticing that ρ_0 can be expanded around ρ_t as: $\rho_0 =_{\mathcal{O}(t^2)} \rho_t - t \rho'_0$, and applying the theorem above, one obtains the result. This is a consequence of the fact that the first contribution to the relative entropy quadratic, and therefore invariant under the change $\rho'_0 \rightarrow -\rho'_0$. □

Corollary 2. *Let $\omega_t := \omega_\beta(H_t)$ be a smooth family of Gibbs state; then one can expand the relative entropy as:*

$$S(\omega_t||\omega_0) =_{\mathcal{O}(t^3)} \frac{t^2}{2} \left(\text{Tr} [H'_0 \mathcal{J}_{\omega_0} [H'_0]] - \langle H'_0 \rangle_{\omega_0}^2 \right) = \text{cov}_{\omega_0}(H'_0, H'_0)$$

Proof. Plugging in the expansion of the thermal state in the expression of the relative entropy, one obtains the result straightaway. □

Appendix C

Quasi-isothermal expansion of the entropy production rate

In order to study protocols in which the system is always close to the equilibrium it is useful to give the expansion of the integrated entropy production rate:

$$\mathcal{Z} := \sum_{i=1}^{N-1} [S(\rho_i || \omega_{i+1}) - S(\rho_{i+1} || \omega_{i+1})],$$

in the case in which the state at each step can be expressed in the form:

$$\rho_i = \omega_i + \varepsilon \rho'_i + \mathcal{O}(\varepsilon^2).$$

Plugging this expression in \mathcal{Z} and using the identity presented in equation 1.2:

$$S(\rho + \varepsilon \rho' || \rho) =_{\mathcal{O}(\varepsilon^3)} \frac{\varepsilon^2}{2} \text{Tr} [\rho' \mathcal{J}_\rho^{-1} [\rho']]$$

one obtains the first step of the derivation:

$$\mathcal{Z} =_{\mathcal{O}(\varepsilon^3)} \sum_{i=1}^{N-1} \left[S(\omega_i + \varepsilon \rho'_i || \omega_{i+1}) - \frac{\varepsilon^2}{2} \text{Tr} [\rho'_{i+1} \mathcal{J}_{\omega_{i+1}}^{-1} [\rho'_{i+1}]] \right];$$

as it can be noticed the first term in the sum cannot be expanded using the expression above without putting additional assumptions on the relation between ω_i and ω_{i+1} : in particular, in the case that the $\{\omega_i\}$ converges to a smooth curve ω_t for $N \rightarrow \infty$, which follows almost by definition of thermodynamic protocol, it is possible to give the expansion:

$$\omega_i =_{\mathcal{O}(\frac{1}{N^2})} \omega_{i+1} - \frac{1}{N} \delta \omega_{i+1},$$

which, plugged in in the previous expression gives:

$$\begin{aligned} \mathcal{Z} &= \sum_{i=1}^{N-1} \left[\frac{1}{2N^2} \text{Tr} \left[\delta\omega_{i+1} \mathcal{J}_{\omega_{i+1}}^{-1} [\delta\omega_{i+1}] \right] \right] + \mathcal{O} \left(\frac{1}{N^2} \right) + \\ &\quad - \sum_{i=1}^{N-1} \left[\frac{\varepsilon}{2N} \text{Tr} \left[\delta\omega_{i+1} \mathcal{J}_{\omega_{i+1}}^{-1} [\rho'_i] \right] + \frac{\varepsilon}{2N} \text{Tr} \left[\rho'_i \mathcal{J}_{\omega_{i+1}}^{-1} [\delta\omega_{i+1}] \right] \right] + \mathcal{O} \left(\frac{\varepsilon^2}{N} \right) \\ &\quad + \frac{\varepsilon^2}{2} \sum_{i=1}^{N-1} \left[\text{Tr} \left[\rho'_i \mathcal{J}_{\omega_{i+1}}^{-1} [\rho'_i] \right] - \text{Tr} \left[\rho'_{i+1} \mathcal{J}_{\omega_{i+1}}^{-1} [\rho'_{i+1}] \right] \right]. \end{aligned}$$

It should be noticed that \mathcal{J}_ρ is self-adjoint with respect to the Hilbert-Schmidt scalar product, which means that for any two self-adjoint matrices A and B the following holds:

$$\text{Tr} [A \mathcal{J}_\rho [B]] = \text{Tr} [\mathcal{J}_\rho [A] B] = \text{Tr} [B \mathcal{J}_\rho [A]].$$

For this reason, one can add together the terms in the second line. For what regards the third line, assuming smoothness in the ρ'_i as well, each of the difference is of order $\mathcal{O} \left(\frac{1}{N} \right)$, so that the whole sum is of order $\mathcal{O} (\varepsilon^2)$. Hence, one can rewrite \mathcal{Z} as:

$$\begin{aligned} \mathcal{Z} &= \sum_{i=1}^{N-1} \left[\frac{1}{2N^2} \text{Tr} \left[\delta\omega_{i+1} \mathcal{J}_{\omega_{i+1}}^{-1} [\delta\omega_{i+1}] \right] \right] + \mathcal{O} \left(\frac{1}{N^2} \right) + \\ &\quad - \sum_{i=1}^{N-1} \left[\frac{\varepsilon}{N} \text{Tr} \left[\rho'_i \mathcal{J}_{\omega_{i+1}}^{-1} [\delta\omega_{i+1}] \right] \right] + \mathcal{O} (\varepsilon^2). \end{aligned}$$

Appendix D

Optimal Landauer erasure

In order to illustrate the improvement one gets from using the thermodynamic length to design optimal protocols, it will be consider how to minimise the heat released during a Landauer erasure procedure performed in N steps.

The system in consideration is given by a particle in a double well potential, which will be modelled as a two level system. The initial potential is taken to be symmetric, and the system is initially started in a completely mixed state (1), corresponding to the physical situation in which the qubit is fully entangled with the environment; the protocol is designed to erase these correlations between system and bath. For this purpose, the energy gap between the two levels is progressively increased in contact with a bath (2), so that all the population will eventually end up in the less energetic state (3); at this point, a quench in the Hamiltonian is performed back to the initial potential (4). In this way, at the end of the protocol the system is in a default pure state $\rho = |0\rangle\langle 0|$. This protocol is depicted in figure D.1.

In the thermodynamical space, the sequence of transformations described above translates to:

$$\left(\frac{\mathbb{1}}{2}; H = 0\right) \xrightarrow[1 \rightarrow 2]{\text{isothermally}} (\omega(r\sigma_z); r\sigma_z) \xrightarrow[2 \rightarrow 3]{r \rightarrow \infty}$$
$$\xrightarrow[2 \rightarrow 3]{r \rightarrow \infty} (|0\rangle\langle 0|; \infty) \xrightarrow[3 \rightarrow 4]{\text{quench}} (|0\rangle\langle 0|; H = 0).$$

As it can be seen, due to the appearance of an infinity in this parametrisation, it is useful to choose another system of coordinates to study the problem. Noticing that the population of the excited state varies from $1/2$ to 0 without presenting any singularities, the coordinates given by:

$$p := \frac{1}{2} (1 - \tanh \beta r),$$

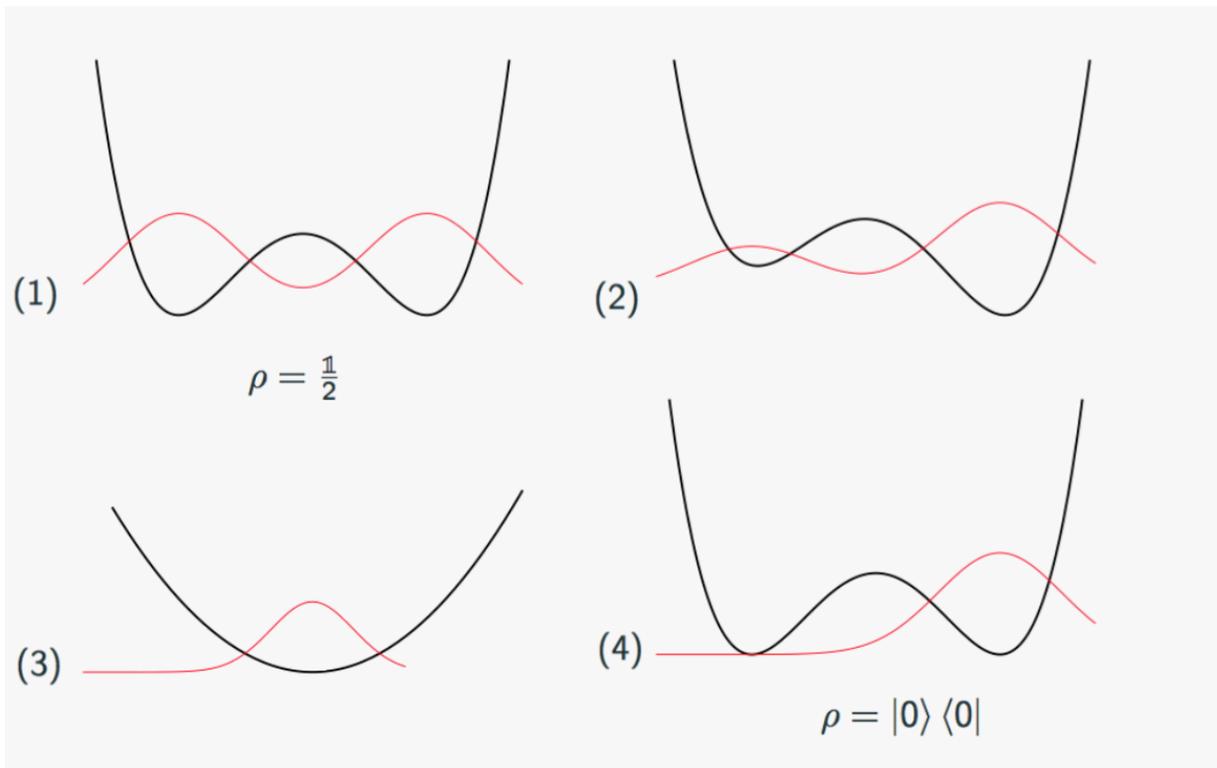


Figure D.1: Schematic depiction of a Landauer Erasure: in black the shape of the potential, in red the population in each well.

is suitable to tackle the problem. In fact, in the coordinates (p, θ, ϕ) , the Christoffel symbol $\Gamma_{p,p}^p$ takes the particularly simple form:

$$\Gamma_{p,p}^p = \frac{(1-2p)}{(2(p-1)p)},$$

suggesting that this choice correctly mirrors the physical structure of the problem. The geodesics equation in this case is analytically solvable and, for the boundary conditions $p_i = 1/2$, $p_f = 0$, there are two possible solutions:

$$\begin{aligned} p_t^a &= \frac{1}{2} \left(\sin \left[\frac{3\pi t}{2} \right] + 1 \right) \\ p_t^b &= \cos^2 \left[\frac{1}{4} \pi (t+1) \right], \end{aligned}$$

plotted in figure D.2. As it can be seen from their graph, the first solution corresponds to a protocol in which one first brings the system Hamiltonian to $-\infty$ (at time $t = 1/3$, for which the population in the excited state is 1) and then to ∞ . This behaviour is a consequence of the compact structure the choice of coordinates endows the system with, and it is similar to what happen on the sphere when a geodesic surpasses the hemisphere and cease to be the global optimal path. This can be verified even looking at the energy functional for the two cases:

$$\begin{aligned} E(p^a) &= \int_{p^a} dt \dot{p}_t^a g_{p,p} \dot{p}_t^a = \frac{9\pi^2}{4\beta^2} \\ E(p^b) &= \int_{p^b} dt \dot{p}_t^b g_{p,p} \dot{p}_t^b = \frac{\pi^2}{4\beta^2}; \end{aligned}$$

as it was suggested by the above intuition, p^b gives the minimum dissipation path. It is now interesting to see how this optimal path compares with the naive choice of changing the population of the excited state linearly, which will be denoted as p^{naive} . The two trajectories are compared in figure D.3.

In order to understand the superiority of the formalism of the thermodynamic length, it is useful to consider the heat released during a Landauer erasure protocol. Using the first law and equation (3.5), one can express the dissipation along an arbitrary protocol as:

$$\begin{aligned} \tilde{\Delta}Q &= -(W + \Delta U) = - \left(-\Delta F_{eq} - \frac{\beta}{2N} \int_0^1 \text{cov}_{\omega_t}(\dot{H}_t, \dot{H}'_t) + \Delta U \right) = \\ &= - \left(-\Delta \mathcal{U} - \theta S(\rho_i) + \theta S(\rho_f) - \frac{\beta}{2N} \int_0^1 \text{cov}_{\omega_t}(\dot{H}_t, \dot{H}_t) + \Delta \mathcal{U} \right) = \\ &= \theta \log [2] + \frac{\beta}{2N} \int_0^1 \text{cov}_{\omega_t}(\dot{H}_t, \dot{H}_t); \end{aligned}$$

in this way, not only the thermodynamic length allows to give an alternative derivation of the Landauer bound, but it additionally provides an expression of the corrections for any

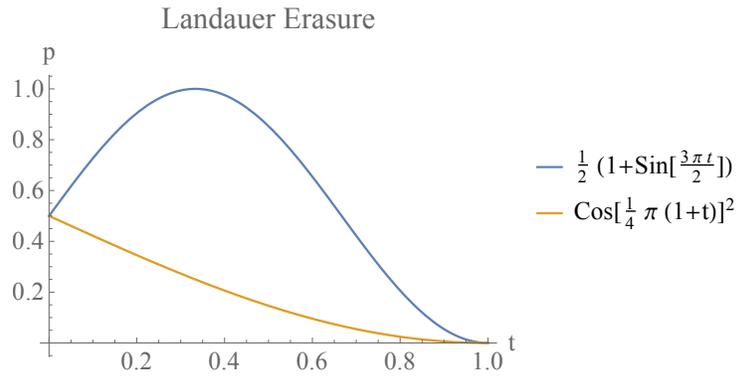


Figure D.2: The two solutions of the geodesics equation for the boundary conditions $p_i = 1/2, p_f = 0$.

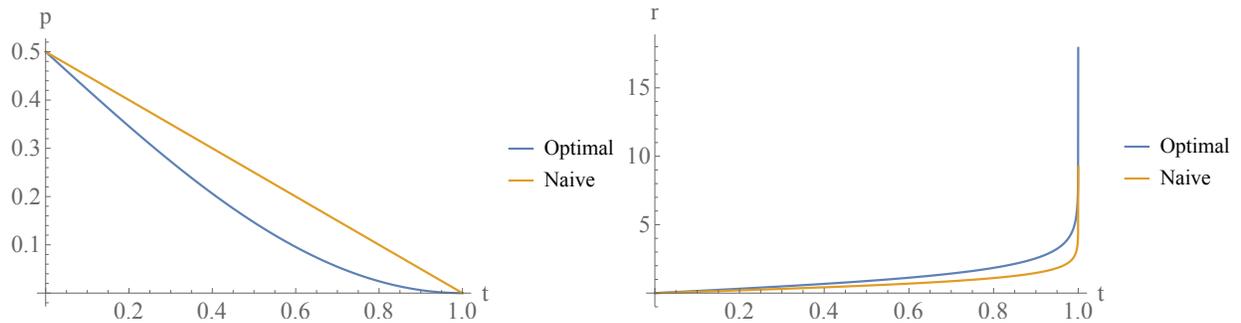


Figure D.3: The optimal trajectory compared with the naive choice of linearly decreasing the population, shown in the coordinates given by p and r .

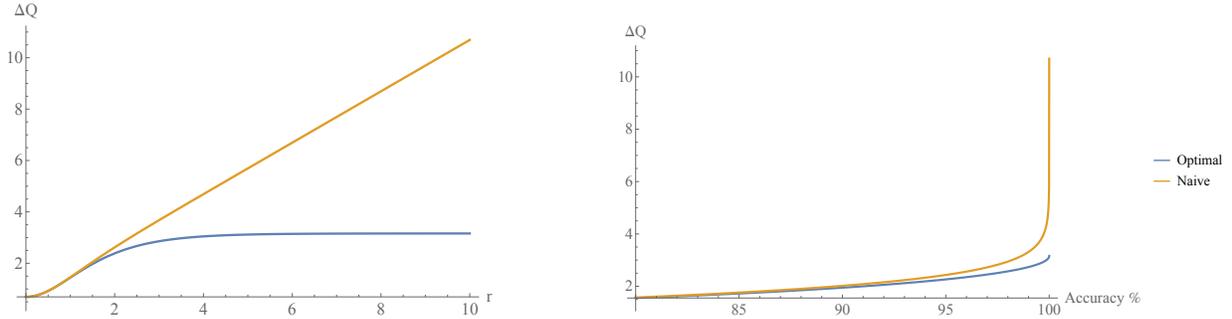


Figure D.4: On the left the heat released in function of the separation between the two levels, on the right in function of the accuracy of the erasure for the naive trajectory and the optimal one. In particular, the accuracy is measured by the percentage of the population present in the ground state at the end of the protocol.

protocol. In particular, recalling the expression of the energy functional of p^b , one can give a tighter Landauer bound for protocols performed discretely in N steps:

$$\tilde{\Delta}Q \geq k_B\theta \left(\log [2] + \frac{\pi^2}{8N} \right).$$

In this way one obtains a lower bound on the heat released; it is interesting to see how the naive trajectory defined above compares with this result. Computing the energy functional $E(p^{naive})$ one gets:

$$E(p^{naive}) = \infty;$$

meaning that, in order to complete the Landauer erasure procedure, an infinite amount of heat must be released in the environment. This result can be understood analysing the energy balance during the protocol: in fact, in order to have a perfect erasure, an infinite amount of energy has to be supplied to the Hamiltonian; in absence of dissipation, this energy is mostly retrieved at the moment of the quench, up to the Landauer cost of bringing the system out of equilibrium ($k_B\theta \log [2]$). On the contrary, when considering dissipation, the energy which is provided to the Hamiltonian can leak to the environment, making it impossible to get it back: in this way, the infinity in the energy functional for the naive protocol can be understood as a consequence of the fact that a finite fraction of the energy provided will be used to complete the procedure; on the other hand, implementing the transformation along an optimal trajectory will bound the dissipation of the system, regardless of the energy supplied.

In particular, it can be seen in figure D.4 that, if one restricts to partial erasure, the heat released performing the naive protocol is finite, albeit diverging as the perfect erasure is approached; on the other hand, for the optimal protocol, the dissipation will be bounded for all precisions. In this way, the improvement achieved using the thermodynamic length will be monotone in the accuracy of the protocol. It is clear then how much the choice of an optimal trajectory can turn out to be favourable.

Appendix E

Optimal work extraction

In this appendix the quantum Carnot cycle will be presented as it is treated in [22], where corrections coming from coupling the system to an environment are considered. The assumption therein will be numerically illustrated and the framework used will be generalised to the case in which the switching on of the interaction is performed in N steps. This gives the possibility of generalising the formalism of thermodynamic length to the strong coupling regime and to show how this approach simplifies the problem of finding an optimal protocol over a naive minimisation procedure.

E.1 The quantum Carnot cycle

In classical thermodynamics the Carnot cycle between two baths at temperatures θ_c and θ_h is defined by the following series of transformations: (i) an adiabatic which brings the system from temperature θ_c to θ_h ; (ii) an isothermal transformation to an arbitrary state c ; (iii) an adiabatic transformation back to temperature θ_c ; and (iv) an isothermal back to the original state. This cycle derives its importance from the relation which connects its efficiency to the absolute temperature of the two baths, with no reference to the underlying structure of the system implementing it¹:

$$\eta_C = \frac{W}{Q_h} = 1 - \frac{Q_c}{Q_h} = 1 - \frac{\theta_c}{\theta_h};$$

moreover, the second law of thermodynamics can be stated as the impossibility of any thermodynamic cycle between two reservoirs at the same temperatures to be more efficient than the Carnot one. Given this equivalence, it is clear that it will be impossible to build a cycle operating exactly at Carnot efficiency, because any real process will involve some dissipation; nonetheless, it will be useful to study near to optimal cases, in order to better understand which mechanisms give rise to entropy production.

Recalling the definition of adiabatic transformation for a quantum system (equation

¹As it is common in the literature, one denotes with Q_h the heat absorbed from the hot bath, while with Q_c the heat released to the cold one. This convention is used so that both quantities will have the same sign.

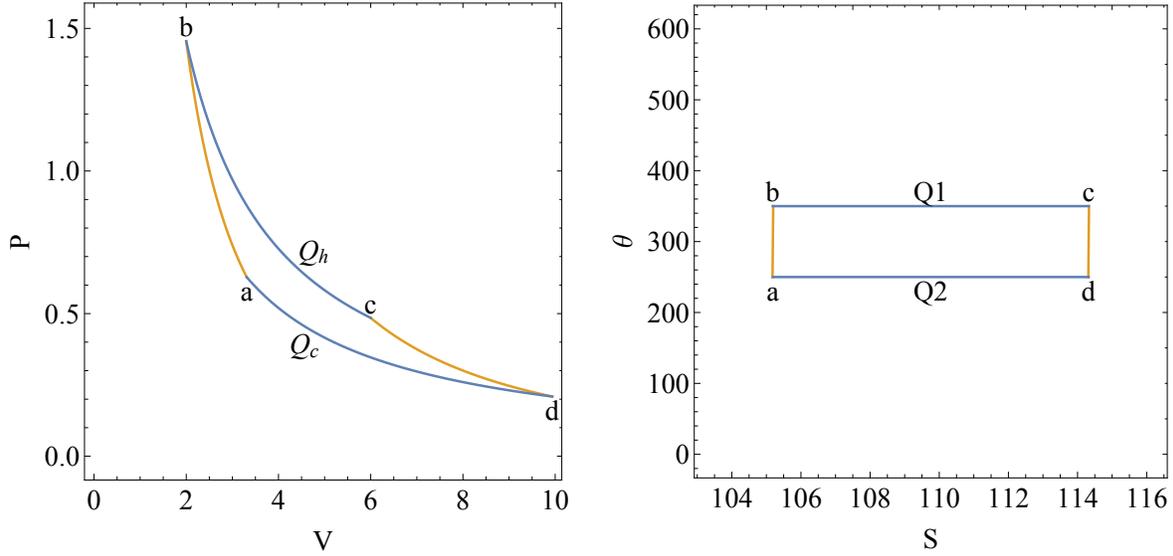


Figure E.1: Depiction of a Carnot cycle for an ideal monoatomic gas in the P-V and θ -S planes.

(1.5)), one can define the quantum Carnot cycle in complete analogy to the classical case as: (i) a series of quenches along the adiabatic set connecting an arbitrary $(\omega; H_A)_{\beta_c}$ to $(\omega; H_B)_{\beta_h} \in \mathcal{A}[(\omega; H_A)_{\beta_c}]$; (ii) an isothermal transformation to an arbitrary state $(\omega; H_C)_{\beta_h}$; (iii) a series of quenches along the adiabatic set of $(\omega; H_C)_{\beta_h}$ to bring the system back to the original temperature; and (iv) an isothermal transformation back to $(\omega; H_A)_{\beta_c}$ in order to close the cycle. The full cycle is presented in the following diagram:

$$\begin{array}{ccc}
 (\omega; H_A)_{\beta_c} & \xrightarrow{\text{adiabatic}} & (\omega; H_B)_{\beta_h} \\
 \uparrow \text{isoth.}\theta_c & & \downarrow \text{isoth.}\theta_h \\
 (\omega; H_D)_{\beta_c} & \xleftarrow{\text{adiabatic}} & (\omega; H_C)_{\beta_h}
 \end{array}$$

It should be noticed that, similarly to what happens in the classical case, asking for (i) and (iii) to be adiabatic transformations leaves only the choice of H_A and H_C unconstrained; in fact, it corresponds to the validity of the two conditions:

$$\begin{cases} \omega_{\beta_c}(H_A) \equiv \omega_{\beta_h}(H_B) \\ \omega_{\beta_h}(H_C) \equiv \omega_{\beta_c}(H_D), \end{cases}$$

which fix H_B and H_D . At this point, one can easily show that the Carnot efficiency has the same functional form in the quantum regime. In particular, since for an ideal isothermal transformation the identity $\Delta Q = \theta \Delta S$ holds, one can express the heat exchanged with

the two baths as:

$$\begin{aligned} Q_h &= \theta_h [S(\omega_{\beta_h}(H_C)) - S(\omega_{\beta_h}(H_B))] = \theta_h [S(\omega_{\beta_h}(H_C)) - S(\omega_{\beta_c}(H_A))] \\ Q_c &= \theta_c [S(\omega_{\beta_c}(H_D)) - S(\omega_{\beta_c}(H_A))] = \theta_c [S(\omega_{\beta_h}(H_C)) - S(\omega_{\beta_c}(H_A))], \end{aligned}$$

which implies that the efficiency is given by:

$$\eta_C = 1 - \frac{\theta_c [S(\omega_{\beta_c}(H_D)) - S(\omega_{\beta_c}(H_A))]}{\theta_h [S(\omega_{\beta_h}(H_C)) - S(\omega_{\beta_c}(H_A))]} = 1 - \frac{\theta_c}{\theta_h}.$$

In the following sections it will be shown how the Carnot efficiency can be approached in quasi-ideal cycles: in particular, assuming the possibility of perfectly realising the adiabatic quenches, the focus will be on how to carry out the isothermal transformations, and which role the non-zero interaction with the bath plays in the entropy production. Thanks to the duality between the heat and the work given by the first law of thermodynamics, this study will be equivalent to the one of finding optimal work extraction protocols for finite coupling strength; this approach will be the one taken here, in analogy to the work in [22].

E.2 Work extraction from a bath in the strong coupling regime

The treatment of the work extraction protocols given in the main text implicitly assumed that the interaction between the system and the bath wouldn't significantly alter the state of the system; this approximation is true only for a vanishingly small interaction strength g . In realistic settings, though, this approximation is usually not justified for quantum systems, since the volume of the boundary can be comparable to the one of the bulk, and, therefore, a generalisation of the framework developed is needed.

Before starting with the derivation, it is convenient to slightly change the notation: in the following, $(\rho; H^S)_g$ indicates a point in the thermodynamic space corresponding to the case in which the density matrix of the universe is given by ρ , and the Hamiltonian is given by $H^S + gV + H^B$, where H^S acts only on the system, H^B is a fixed bath Hamiltonian and V is the interaction between the two². This notation has been chosen thinking of a realistic experimental setting, in which one has control only on the Hamiltonian of the system and on the intensity of the coupling, tuned by allowing the system and the bath to interact more or less (corresponding to increasing or decreasing g), without actually modifying the interaction Hamiltonian: for example, for a distance dependent interaction, the only experimental control on the coupling it is sensible to assume is the possibility of bringing closer or further apart the system and the bath.

Then, an isothermal transformation can be thought as consistent of three parts:

²Since in this section the temperature of the bath will be considered fixed at $\theta = \beta^{-1}$, this notation won't lead to confusion: for example, $(\omega; H^S)_g$ will mean that the density matrix of the universe is given by $\omega_\beta(H^S + gV + H^B)$.

1. Switching on of the interaction. In which the interaction strength is brought from $g = 0$ to a fixed value $g = \tilde{g}$ in N_1 steps:

$$(\rho_1^1; H_A^S)_0 \longrightarrow (\rho_2^1; H_A^S)_{g_1^1} \longrightarrow \dots \longrightarrow (\rho_{N_1}^1; H_A^S)_{\tilde{g}};$$

2. Isothermal transformation in contact with the bath. Performed at fixed interaction strength in N_2 steps changing the system Hamiltonian from H_A^S to H_B^S :

$$(\rho_1^2; H_A^S)_{\tilde{g}} \longrightarrow (\rho_2^2; H_B^S)_{\tilde{g}} \longrightarrow \dots \longrightarrow (\rho_{N_2}^2; H_B^S)_{\tilde{g}};$$

3. Switching off of the interaction. In which the interaction strength is brought from $g = \tilde{g}$ to a fixed value $g = 0$ in N_3 steps:

$$(\rho_1^3; H_B^S)_{\tilde{g}} \longrightarrow (\rho_2^3; H_B^S)_{g_2^3} \longrightarrow \dots \longrightarrow (\rho_{N_3}^3; H_B^S)_0.$$

Recalling the expression for the work extraction given in section 3.2, it can be noticed that the derivation outlined for weakly coupled systems naturally extends to the context of finite interaction strength, giving a formally equal result, upon interpreting each density matrix as representing the state of the entire universe, instead that of the system alone; then, the expression for the work extracted during an arbitrary protocol performed in N steps is given by:

$$W = -\Delta F_{eq} + \theta (S(\rho_1 || \omega_1) - S(\rho_N || \omega_N)) - \theta \sum_{i=1}^{N-1} [S(\rho_i || \omega_{i+1}) - S(\rho_{i+1} || \omega_{i+1})].$$

Applying this formula to each of the stage of the strongly coupled isothermal described above, one obtains:

$$\begin{aligned} W_{TOT} = & F[\omega_\beta(H_A^S)] - F[\omega_\beta(H_B^S)] + \theta (S(\rho_1^1 || \omega_\beta(H_A^S)) - S(\rho_{N_3}^3 || \omega_\beta(H_B^S))) + \\ & - \theta \left(\sum_{i=1}^{N_1-1} [S(\rho_i^1 || \omega_{i+1}^1) - S(\rho_{i+1}^1 || \omega_{i+1}^1)] + \sum_{i=1}^{N_2-1} [S(\rho_i^2 || \omega_{i+1}^2) - S(\rho_{i+1}^2 || \omega_{i+1}^2)] + \right. \\ & \left. + \sum_{i=1}^{N_3-1} [S(\rho_i^3 || \omega_{i+1}^3) - S(\rho_{i+1}^3 || \omega_{i+1}^3)] \right), \end{aligned}$$

where one can recognise in the first line the difference in free energy evaluated at the endpoints plus the difference in non-equilibrium content of the initial and final state, and in the second and third line the entropy produced during the three different parts of the protocol.

It is worth noticing that in the case in which the system thermalises at each step and N_1 , N_2 and N_3 goes to infinity, one regains the ideal limit:

$$W_{TOT} = -\Delta F_{eq};$$

this result implies that for any interaction strength there exists a number of total steps N for which the work extracted is arbitrary close to the ideal case or, to put it with other words, that the presence of a finite coupling strength doesn't intrinsically limit the possibility of attaining maximum work.

E.2.1 Naive minimisation

In order to better understand the contribution to the dissipation coming from the operation of switching on or off the interaction, it is useful to first study the simplified case in which the system is assumed to thermalise at each step and the isothermal is performed continuously ($N_2 \rightarrow \infty$). Additionally, the naive choice of increasing or decreasing the coupling strength linearly is made:

$$\begin{cases} g_i^1 = \frac{i}{N} \tilde{g}; \\ g_i^3 = \tilde{g} - \frac{i}{N} \tilde{g}. \end{cases}$$

and the minimisation will be performed manoeuvring the system Hamiltonian at each step. Then, under this assumptions, the work extracted during an isothermal is given by:

$$W_{TOT} = -\Delta F_{eq} - \theta \sum_{i=1}^{N_1-1} S(\omega(H_i^1) || \omega(H_{i+1}^1)) - \theta \sum_{i=1}^{N_3-1} S(\omega(H_i^3) || \omega(H_{i+1}^3));$$

in order to use a consistent notation with the one of [22], the two sums will be denoted by $\Delta F^{(irr)}$ and $\Delta F^{(res)}$ respectively, corresponding to the entropy produced during the process of switching on or off the interaction. Then, in order to minimise the dissipation, one has to find a family of $\{H_i^1\}$ and $\{H_i^3\}$ which minimises these functionals with the constraints:

$$\begin{cases} H_1^1 \equiv H_A^S + H^B \\ H_{N_3}^3 \equiv H_B^S + H^B. \end{cases}$$

Before studying the functionals $\Delta F^{(irr)/(res)}$, it is useful to explore in which way the relative entropy $S(\rho || \omega(H))$ can be minimised when one does not have perfect control over the whole density matrix; in particular, in the following ρ is constrained to be of the form $\rho := \omega(H^S + gV + H^B)$, where the only freedom is on the choice of H^S . Let, then, H_t a family of Hamiltonians defined as:

$$H_t = H_0 + tY^S = (X_0^S + gV + H^B) + tY^S.$$

Then, X_0^S minimises $S(\rho || \omega(H))$ if and only if for any Y_S the following holds:

$$\begin{aligned} \left. \frac{d}{dt} S(\omega_t || \omega(H)) \right|_0 &= \left. \frac{d}{dt} \text{Tr} [\omega_t (\log [\omega_t] - \log [\omega(H)])] \right|_0 = \\ &= -\beta \text{Tr} [\dot{\omega}_t (H_t - H)] \Big|_0 - \left(\beta \text{Tr} [\omega_t \dot{H}_t] + \log [Z_t] \right) \Big|_0 = \\ &= \beta^2 \text{cov}_{\omega_0}(Y^S, (H_0 - H)) = 0. \end{aligned}$$

Since Y_S is arbitrary, from the fundamental lemma of calculus of variations, this equality can be rewritten as:

$$\begin{aligned} \text{Tr} [Y_S \mathcal{J}_{\omega_0} [H_0 - H]] &= \text{Tr} [\omega_0 Y_S] \text{Tr} [\omega_0 (H - H_0)] \implies \\ \implies \text{Tr}_B \left[\mathcal{J}_{\omega_0} \left[\frac{H_0 - H}{\langle H_0 - H \rangle_{\omega_0}} \right] \right] &= \text{Tr}_B [\omega_0]. \end{aligned} \tag{E.1}$$

A similar procedure can be applied to minimise $S(\omega(H)||\rho)$ with the same constraints, obtaining the condition:

$$\begin{aligned} \left. \frac{d}{dt} S(\omega(H)||\omega_t) \right|_0 &= \left. \frac{d}{dt} \text{Tr} [\omega(H) (\log [\omega(H)] - \log [\omega_t])] \right|_0 = \\ &= \beta \left(\text{Tr} [\omega(H) \dot{H}_t] - \langle \dot{H}_t \rangle_{\omega_t} \right) \Big|_0 = \\ &= \beta \text{Tr} [Y_S (\omega(H) - \omega_0)] = 0, \end{aligned}$$

from which it immediately follows that:

$$\text{Tr}_B [\omega(H)] = \text{Tr}_B [\omega_0]. \quad (\text{E.2})$$

In this case the interpretation of the result is clear: the minimum is attained when, restricting to observables acting on the system alone, ω_0 is indistinguishable from $\omega(H)$. It is now possible to use these results to minimise $\Delta F^{(irr)}$ with the constraint that $H_1^1 \equiv H_A^S + H^B$. Varying the first unconstrained Hamiltonian (H_2^1), one gets the equation:

$$\begin{aligned} S(\omega(H_1^1)||\omega(H_2^1))' + S(\omega(H_2^1)||\omega(H_3^1))' &= 0 \implies \\ \implies \beta \text{Tr} [Y_1^S (\omega(H_1^1) - \omega(H_2^1))] + \beta^2 \text{cov}_{\omega_2} (Y_1^S, (H_2^1 - H_3^1)) &= 0. \end{aligned}$$

This same procedure can be applied for each Hamiltonian, except for the last one, for which one has:

$$S(\omega(H_{N_1-1}^1)||\omega(H_{N_1}^1))' = 0 \implies \text{Tr}_B [\omega(H_{N_1-1}^1)] = \text{Tr}_B [\omega(H_{N_1}^1)].$$

Grouping together all the conditions so found, one gets the system of equations:

$$\forall \{Y_i^S\} \quad \begin{cases} \text{Tr} [(\omega_i^1 - \omega_{i+1}^1) Y_i^S] = \beta \text{cov}_{i+1} (Y_i^S, (H_{i+2}^1 - H_{i+1}^1)) \\ \text{Tr}_B [\omega(H_{N_1-1}^1)] = \text{Tr}_B [\omega(H_{N_1}^1)], \end{cases}$$

where $\{Y_i^S\}$ is an arbitrary family of $N_1 - 1$ operators acting on the system only. Applying the same procedure to $\Delta F^{(res)}$, one gets a similar system:

$$\forall \{Y_S^i\} \quad \begin{cases} \text{Tr} [(\omega_i^3 - \omega_{i+1}^3) Y_i^S] = \beta \text{cov}_{i+1} (Y_i^S, (H_{i+2}^3 - H_{i+1}^3)) \\ \text{Tr}_B \left[\mathcal{J}_{\omega_1^3} \left[\frac{H_1^3 - H_2^3}{\langle H_1^3 - H_2^3 \rangle_{\omega_1^3}} \right] \right] = \text{Tr}_B [\omega_1^3]. \end{cases}$$

The two systems of equations are closed and, for this reason, in principle they could be solved to minimise the dissipation; nonetheless, in practice, in particular when $N \gg 1$, the minimisation problem does not admit an easy solution: in fact, despite the local character of the equations, the boundary conditions and the first closed equation are on the opposite ends of the system (e.g. the boundary condition in the first case is imposed on H_1^1 and the

first closed equation is the one for $H_{N_1}^1$); this feature introduce a global structure, which makes the problem difficult to be treated numerically.

Nonetheless, some intuition can be derived from the equations obtained: in particular, one can see that the first equation is formally identical for the two systems and therefore, as it is sensible to expect, the switching on and off will be symmetric, at least on a local level. Moreover, it depends only on the local structure of the Hamiltonians and of the states, which could lead one to think that, in the continuous limit, it would be possible to rewrite this condition as a differential equation. In fact, using the expansion given in theorem 1 of appendix B, assuming some smoothness on $\{H_i\}$, one has that:

$$\begin{aligned} \text{Tr} [(\omega_i^1 - \omega_{i+1}^1) Y_i^S] &= \text{cov}_i(Y_i^S, (H_{i+1} - H_i)) = \\ &= \frac{1}{N} \text{cov}_i(Y_i^S, \dot{H}_i) = \frac{1}{N} \text{cov}_{i+1}(Y_i^S, \dot{H}_{i+1}) = \\ &= \text{cov}_{i+1}(Y_i^S, (H_{i+2} - H_{i+1})), \end{aligned}$$

where all the equalities should be considered valid up to order $\mathcal{O}(\frac{1}{N^2})$. The identity appearing in the second line has an interesting interpretation: it tells that, if one has control only over the system Hamiltonian, the projection of the velocity \dot{H}_t , given by tracing out the bath, will be a parallel vector field of H_t ; this property, which is the defining one for geodesic curves, shows the compatibility between the thermodynamic length formalism and the naive minimisation one. At the same time if, on the one hand, this equation can be derived only after some hard work in the latter framework, in the thermodynamic length approach it is a simple consequence of the definition of dissipation, illustrating the simplifying power of this formalism.

In order to get some intuition on the local behaviour of the system, it is useful to now explore the simplified case in which the interaction is switched on and off in one step.

E.2.2 Switching on/off of the interaction in one step

The results shown here are inspired by the paper [22], to which one should refer for an extensive treatment; as an extension of that work, some of the analytical results have been numerically illustrated for a spin chain, where the system has been chosen to be the first spin and the rest of the chain to be the bath. The Hamiltonians used are:

$$\begin{cases} H = H^S + gV + H^B \\ gV = g [g_x \sigma_x^S \sigma_x^1 + g_z \sigma_z^S \sigma_z^1] \\ H^B = [\sum_{i=1}^{\infty} e \sigma_z^i + \sum_{i=1}^{\infty} g_x \sigma_x^i \sigma_x^{i+1} + g_z \sigma_z^i \sigma_z^{i+1}], \end{cases}$$

where H^S is an arbitrary Hermitian operator on the first qubit, and the parameters, when not stated otherwise, have been taken as $g = 1$, $e = 1$, $g_x = 1/2$, $g_z = 1/2$ and $\beta = 1$.

In the case in which $N_1 = N_3 = 1$, the expression of the work reduces to:

$$W_{TOT} = -\Delta F_{eq} - \Delta F^{(irr)} - \Delta F^{(res)},$$

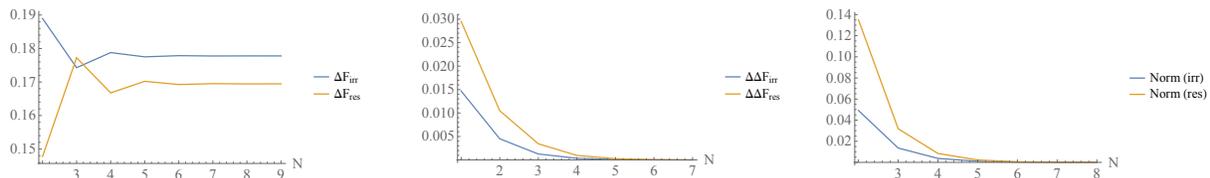


Figure E.2: Convergence of quantities of interest in the size of the bath. In the plot on the left the behaviour of the numerical values of $\Delta F^{(irr)/(res)}$ is shown; the difference for consecutive realisations is shown in the middle; on the right, the convergence of the Frobenius norm of consecutive minimisers \tilde{H}_1^S and \tilde{H}_3^S .

where $\Delta F^{(irr)}$ and $\Delta F^{(res)}$ take the form:

$$\begin{cases} \Delta F^{(irr)} = \theta S(\omega(H_A^S + H^B) || \omega(H_1^S + gV + H^B)) \\ \Delta F^{(res)} = \theta S(\omega(H_3^S + gV + H^B) || \omega(H_B^S + H^B)). \end{cases}$$

Using the results obtained above, the minimisers \tilde{H}_1^S and \tilde{H}_3^S are implicitly given by the equations:

$$\begin{cases} \text{Tr}_B \left[\omega(\tilde{H}_1^S + gV + H^B) \right] = \omega(H_A^S) \\ \text{Tr}_B \left[\omega(\tilde{H}_3^S + gV + H^B) \right] = \text{Tr}_B \left[\mathcal{J}_{\omega(\tilde{H}_3^S + gV + H^B)} \left[\frac{H_3^S + gV - H_B^S}{\langle H_3^S + gV - H_B^S \rangle_{\omega(\tilde{H}_3^S + gV + H^B)}} \right] \right]. \end{cases}$$

It should be noticed that, although a priori the solution will depend on the infinite dimensional bath, due to the locality of the observables of interest it is expected that their value evaluated for a finite bath will converge exponentially fast in the number of degrees of freedom considered [15]. This hypothesis has been checked for the numerically computed minimisers of $\Delta F^{(irr)}$ and $\Delta F^{(res)}$: the convergence has been verified both for the numerical value of the minimum and for the Frobenius norm of the difference between consecutive minimisers of $\Delta F^{(irr)}$ and $\Delta F^{(res)}$; the results obtained are shown in figure E.2. It has been noticed that it is sufficient to take a bath of 9 spins for the error to be of order $\mathcal{O}(10^{-5})$; for this reason, in the following the number of sites N_{sites} will be set to this value.

Then one can go back to the illustration of the validity of the conditions above: in particular, the minimiser \tilde{H}_1^S obtained inverting the implicit equation has been compared with the one given by numerically minimising $\Delta F^{(irr)}$, with an agreement up to order $\mathcal{O}(10^{-6})$ in the Frobenius norm.

It is interesting to now study how the optimal work is affected by the presence of a small interaction. For this purpose, one writes the minimisers of $\Delta F^{(irr)}$ and $\Delta F^{(res)}$ as a function of g :

$$\begin{cases} \tilde{H}_1(g) = \tilde{H}_1^S(g) + gV + H_B \\ \tilde{H}_3(g) = \tilde{H}_3^S(g) + gV + H_B; \end{cases}$$

using again the conditions derived in the previous section, one arrives at the following equations, true at all order in g :

$$\forall Y_S \quad \begin{cases} \text{Tr} \left[Y_S \left(\omega(H_A^S + H^B) - \omega(\tilde{H}_1^S(g) + gV + H^B) \right) \right] = 0 \\ \text{cov}_{\omega(\tilde{H}_3(g))} (Y_S, (H_3^S(g) - H_B^S + gV)) = 0; \end{cases}$$

since this system of equations is derived from an expansion of the relative entropy, one has that for $g = 0$, the minimum is obtained for $\tilde{H}_1^S(0) \equiv \tilde{H}_A^S$ and $\tilde{H}_3^S(0) \equiv H_B^S$. Moreover, if one assumes the dependency on g to be sufficiently smooth, one can formally expand the two minimisers as:

$$\begin{cases} \tilde{H}_1^S(g) = H_A^S + gH_1^{S'} + \mathcal{O}(g^2) \\ \tilde{H}_3^S(g) = H_B^S + gH_3^{S'} + \mathcal{O}(g^2). \end{cases}$$

Plugging this expansion in the condition for the minimum, one obtains, up to order $\mathcal{O}(g^2)$:

$$\forall Y_S \quad \begin{cases} g \text{cov}_{\omega(H_A^S + H^B)} (Y_S, (H_1^{S'} + V)) =_{\mathcal{O}(g^2)} 0 \\ g \text{cov}_{\omega(H_B^S + H^B)} (Y_S, (H_3^{S'} + V)) =_{\mathcal{O}(g^2)} 0, \end{cases}$$

where the expansion of $\omega(\tilde{H}_1^S(g) + gV + H^B)$ has been used to obtain the generalised covariance in the first line. The similarity between the conditions for the minimiser of $\Delta F^{(irr)}$ and of $\Delta F^{(res)}$ is a simple consequence of the approximate symmetry of the relative entropy.

Using once again the arbitrariness of Y_S , one can trace out the bath, arriving to the following conditions:

$$\begin{cases} \text{Tr}_B \left[\mathcal{J}_{\omega(H_A^S + H^B)} \left[H_1^{S'} - \langle H_1^{S'} \rangle_{\omega(H_A^S + H^B)} \right] \right] = -\text{Tr}_B \left[\mathcal{J}_{\omega(H_A^S + H^B)} \left[V - \langle V \rangle_{\omega(H_A^S + H^B)} \right] \right] \\ \text{Tr}_B \left[\mathcal{J}_{\omega(H_B^S + H^B)} \left[H_3^{S'} - \langle H_3^{S'} \rangle_{\omega(H_B^S + H^B)} \right] \right] = -\text{Tr}_B \left[\mathcal{J}_{\omega(H_B^S + H^B)} \left[V - \langle V \rangle_{\omega(H_B^S + H^B)} \right] \right]. \end{cases}$$

On the left hand side of the equations, the trace over the bath can be taken without further complications, since $H_{A/B}^S$ act only on the system; then, defining for bookkeeping the linear operator $L_{\omega(H)}$ as:

$$L_{\omega(H)} [X] := \mathcal{J}_{\omega(H)} \left[X - \langle X \rangle_{\omega(H)} \right],$$

one can rewrite the left hand side as $L_{\omega(H_{A/B}^S)} [H_{1/3}^{S'}]$. In order to apply the same procedure to the right hand side, one has to define the operator $\tilde{V} := -\text{Tr}_B [\omega(H_B) V]$, which is often called the dressed interaction in the literature; then, the conditions above can be compressed in the form:

$$L_{\omega(H_{A/B}^S)} \left[H_{1/3}^{S'} \right] = L_{\omega(H_{A/B}^S)} \left[\tilde{V} \right];$$

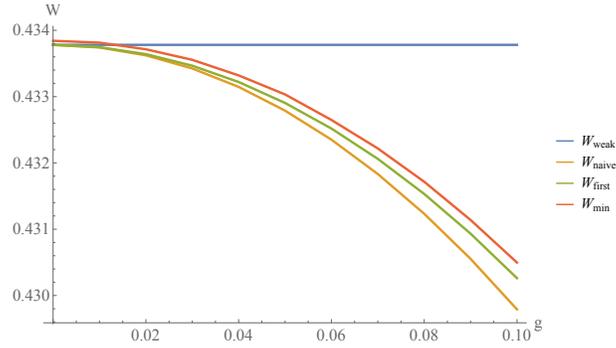


Figure E.3: Work extracted during a cycle in function of the interaction strength for different choices of the system Hamiltonian: H_{min} is the minimizer numerically computed; H_{naive} is the naive choice, that is the zeroth order approximation, and H_{first} is the first order approximation, both given in the text.

since $L_{\omega(H_{A/B}^S)}$ is a linear operator, this equation gives a preliminary expression for the first order of the expansion of $H_{1/3}^S$:

$$H_{1/3}^{S'} \equiv \tilde{V} + M,$$

where M is an arbitrary element of the kernel of $L_{\omega(H_{A/B}^S)}$; this ambiguity could make this result useless: nonetheless, it can be easily checked that any element in the kernel won't contribute to $\Delta F^{(irr)/(res)}$ up to order $\mathcal{O}(g^3)$; therefore, one can set M to zero without affecting the physical results. Then, one can give the expansion of the dissipation terms up to second order in g :

$$\begin{cases} \Delta F_{opt}^{(irr)} = \mathcal{O}(g^3) \frac{\beta g^2}{2} \text{cov}_{\omega(H_A^S)}(\tilde{V}, \tilde{V}) \\ \Delta F_{opt}^{(res)} = \mathcal{O}(g^3) \frac{\beta g^2}{2} \text{cov}_{\omega(H_B^S)}(\tilde{V}, \tilde{V}). \end{cases} \quad (\text{E.3})$$

This expansion has been numerically illustrated for a cycle ($H_A^S = H_B^S$), and the result are plotted in figure E.3. Moreover, a polynomial fit has been realised for the curves in the figure:

$$p(g) = c_0 + c_1 g - c_2 g^2 - c_3 g^3,$$

obtaining a good agreement with the theoretical predictions:

$$\begin{cases} c_0 = \mathcal{O}(10^3) W_{max}; \\ c_1 = \mathcal{O}(10^3) 0; \\ c_2^{naive} > c_2^{first} = \mathcal{O}(10^3) c_2^{min}; \\ c_3^{naive} > c_3^{first} > c_3^{min}. \end{cases}$$

Finally, the value of c_2^{first} has been compared to the one computed directly using the equation (E.3), confirming their equality up to order $\mathcal{O}(10^3)$.

E.2.3 Thermodynamic length in the strong coupling regime

It is now time to see how the formalism of the thermodynamic length can be applied to simplify the evaluation of a minimal protocol in the case in which the number of steps is considerably high ($N \gg 1$). In analogy to what happened for the expression of the work, the derivation that lead to the equation (3.4) naturally generalises to the case in which the system is strongly coupled to the environment; then, applying the approximation:

$$\rho_i = \omega_i + \varepsilon \rho'_i + \mathcal{O}(\varepsilon^2)$$

leads to the same expression of the work:

$$W = -\Delta F_{eq} - \frac{\beta}{2N} \int_0^1 dt \text{cov}_{\omega_t}(\dot{H}_t, \dot{H}_t) - \varepsilon \int_0^1 dt \text{Tr} [\rho'_t \dot{H}_t],$$

with the only difference that now the density matrices which appear in the formula refer to the one for the universe, and not for the system alone.

In the following, for simplicity of exposition the focus will be on the perfectly thermalising case ($\varepsilon \rightarrow 0$). Before starting, though, it is important to clear out some subtleties which might seem to have been overlooked in the derivation above. Firstly, since one is considering the density matrix of the system and bath, it might look necessary to introduce a super-bath which would let the full system thermalise; nonetheless, it turns out that this addition is actually redundant: thanks to the fact that \dot{H} will act only on the system and on the support of the interaction V , which can be reasonably supposed to be local, one does not actually need the full system to be thermal, but only that the density matrix of this smaller region to be approximately Gibbsian³; then, it is clear that the infinite bath is already sufficient to ensure the correctness of the expansion. On the other hand, one might wonder how the quasi-adiabatic expansion could possibly be implemented in the case in which the system is strongly coupled to the bath since, in that scenario, the derivation of the Lindbladian equation given in chapter 2 cannot be applied; in fact, it is sensible to expect that the correlation between the system and bath will become so strong that the correct dynamics should take into account features of the environment as well: for example, it is a well known fact that the asymptotic thermal state of a system strongly coupled to the environment won't simply be $\omega_\beta(H^S)$ but rather:

$$\rho^S = \text{Tr}_B [\omega_\beta(H^S + gV + H^B)].$$

Nonetheless, it can still be argued, as it is often done in the literature, that, despite the strong coupling between the system and the bath, the various sites of the bath will continue to be weakly coupled with one another; thus, it is possible to reduce the strong coupling case to the weakly interacting one simply by considering a big enough buffer region around the system, which can be usually delimited by the support of the interaction. Then, it will

³This condition can be made even weaker: it is sensible to expect that a similar result can be derived when the density matrix only appears to be thermal for what regards the value of the observables of interest, which are usually only a small subset of all the possible observables.

be sufficient to write down the Lindbladian evolution for this bigger region and to consider the reduced density matrix of the system whenever needed.

It will be now shown how one can define a thermodynamic metric in the strong coupling regime: in fact, the thermodynamic manifold has to be modified in order to take into account the fact that one cannot restrict the focus to the system Hamiltonian alone. Nonetheless, the dimension of the manifold will only increase by one: in fact, it is sufficient to specify an element in the space of traceless system Hamiltonians and a real number in the positive real line \mathbb{R}^+ to univocally fix a point in the thermodynamic space:

$$(H^S; g) \longrightarrow (\text{Tr}_B [\omega_\beta(H^S + gV + H^B)]; H^S)_g.$$

Then, thanks to the fact that the thermodynamic space is diffeomorphic to \mathbb{R}^{N+1} , the tangent space will be isomorphic to the space itself. For this reason, in order to give an explicit expression of the metric tensor, it is sufficient to choose a basis of the traceless subspace of hermitian operators acting on the system, which will be denoted as $\{\Sigma_i\}$; then, it is easy to see that one has:

$$\begin{cases} g_{i,j} [(H^S; g)] := \text{cov}_{\omega_\beta(H^S+gV+H^B)}(\Sigma_i, \Sigma_j) \\ g_{i,V} [(H^S; g)] := \text{cov}_{\omega_\beta(H^S+gV+H^B)}(\Sigma_i, V) \\ g_{V,V} [(H^S; g)] := \text{cov}_{\omega_\beta(H^S+gV+H^B)}(V, V). \end{cases}$$

Considering now the isothermal described above, one can give the expression for the total work extracted during the three stages as:

$$\begin{aligned} W_{TOT} = -\Delta F_{eq} - \frac{\beta}{2N} \int_0^1 dt \dot{g}_t^2 \text{cov}_{\omega(H_A^S+g_tV+H^B)}(V, V) - \frac{\beta}{2N} \int_0^1 dt \text{cov}_{\omega(H_t^S+\tilde{g}V+H^B)}(\dot{H}_t, \dot{H}_t) \\ - \frac{\beta}{2N} \int_0^1 dt \dot{g}_t^2 \text{cov}_{\omega(H_B^S+g_tV+H^B)}(V, V), \end{aligned}$$

where, for notation sake, the first and last integral will be denoted as $\Delta F^{(irr)}$ and $\Delta F^{(res)}$, the second as $\Delta F^{(iso)}$. Now, it can be noticed that one can bound $\Delta F^{(irr)}$ (and equivalently $\Delta F^{(res)}$) by:

$$\begin{aligned} \Delta F^{(irr)} = \frac{\beta}{2N} \int_0^1 dt \dot{g}_t^2 \text{cov}_{\omega(H_A^S+g_tV+H^B)}(V, V) \stackrel{(3.6)}{\leq} \frac{\beta}{2N} \int_0^1 dt \dot{g}_t^2 \text{Var}_{\omega(H_A^S+g_tV+H^B)}[V] \leq \\ \leq \max_{g \in [0,1]} \left(\text{Var}_{\omega(H_A^S+gV+H^B)}[V] \right) \frac{\beta}{2N} \int_0^1 dt \dot{g}_t^2, \end{aligned}$$

where the inequality (3.6) has been used in the second step and the definition of classical variance has been recalled:

$$\text{Var}_\rho[A] := \langle A^2 \rangle_\rho - \langle A \rangle_\rho^2.$$

It is clear, then, that minimising the quantity so obtained will give an upper bound on the minimal dissipation: this can be easily done, recalling the boundary conditions $g_0 = 0$ and $g_1 = \tilde{g}$ and defining $\lambda^{(irr)}$ as:

$$\lambda^{(irr)} := \max_{g \in [0,1]} \left(\text{Var}_{\omega(H_A^S+gV+H^B)}[V] \right);$$

it follows that the minimal dissipation during an optimal switching on protocol can be upper bounded by:

$$\Delta F_{opt}^{(irr)} \leq \beta \frac{\lambda^{(irr)} \tilde{g}^2}{2N}$$

One can apply the same kind of argument in order to bound $\Delta F^{(res)}$ and $\Delta F^{(iso)}$, with the additional definition of:

$$\lambda^{(iso)} := \max_{t \in [0,1]} \left(\text{Var}_{\omega(H_t^S + \tilde{g}V + HB)} \left[\dot{H}_t \right] \right).$$

Then, the maximum work extractable during a real isothermal transformation, performed in $3N$ steps and at coupling \tilde{g} , is lower bounded by:

$$W_{TOT}^{opt} \geq -\Delta F_{eq} - \frac{\beta}{2N} (\lambda^{(iso)} + (\lambda^{(irr)} + \lambda^{(res)}) \tilde{g}^2).$$

Remarkably, in order to give this lower bound, the precise form of the metric hasn't been used. In particular, if the structure of the eigenvalues is similar to the one described in the main text, it will be possible to get an exponential improvement on this bound simply by performing the isothermal along the less dissipative direction. Nonetheless, the simplicity with which the bound has been obtained justifies its interest.

E.3 Quasi-ideal Carnot efficiency

It can now be shown how to give corrections to the Carnot efficiency starting from the expression of the maximum work extractable. Let then use the shorthand notation:

$$W = -\Delta F_{eq} - \mathcal{Z},$$

where \mathcal{Z} indicates all the terms accounting for the dissipation. Then, one can express the heat exchanged with the hot and cold reservoir during a Carnot like cycle as:

$$\begin{aligned} Q_h &= \left(\Delta U|_B^C + W_h \right) = -\Delta F_{eq}|_B^C + \Delta U|_B^C - \mathcal{Z}_h = \theta_h \Delta S|_B^C - \mathcal{Z}_h \\ Q_c &= - \left(\Delta U|_D^A + W_c \right) = \Delta F_{eq}|_D^A - \Delta U|_D^A + \mathcal{Z}_c = \theta_c \Delta S|_A^D + \mathcal{Z}_c; \end{aligned}$$

moreover, recalling that $\Delta S|_A^D \equiv \Delta S|_A^C \equiv \Delta S|_B^C =: \Delta S$, one can give the expression of the efficiency of the cycle as:

$$\eta = 1 - \frac{Q_c}{Q_h} = 1 - \frac{\theta_c}{\theta_h} \left[\frac{1 + \frac{\beta_c}{\Delta S} \mathcal{Z}_c}{1 - \frac{\beta_h}{\Delta S} \mathcal{Z}_h} \right],$$

from which it becomes clear how the maximisation of the efficiency is connected with the minimisation of \mathcal{Z} . Plugging in the bound obtained in the previous section, one can give a

lower bound on an optimal Carnot like engine in which the two isothermal are performed in N steps each:

$$\eta_C = 1 - \frac{\theta_c}{\theta_h} \geq \eta_{opt} \geq 1 - \frac{\theta_c}{\theta_h} \left[\frac{1 + \frac{\beta_c^2}{2N\Delta S} \left(\lambda_c^{(iso)} + (\lambda_c^{(irr)} + \lambda_c^{(res)}) \tilde{g}^2 \right)}{1 - \frac{\beta_h^2}{2N\Delta S} \left(\lambda_h^{(iso)} + (\lambda_h^{(irr)} + \lambda_h^{(res)}) \tilde{g}^2 \right)} \right].$$

Thanks to the relations which connects $H_{A/C}$ with $H_{B/D}$, it is expected that there should be some relations between the different λ s of the two isothermals; this possibility, though, won't be investigated here further. Still, it is interesting to see how, in the limit $N \rightarrow \infty$, the lower bound converges to the Carnot efficiency:

$$\begin{aligned} & 1 - \frac{\theta_c}{\theta_h} \left[\frac{1 + \frac{\beta_c^2}{2N\Delta S} \left(\lambda_c^{(iso)} + (\lambda_c^{(irr)} + \lambda_c^{(res)}) \tilde{g}^2 \right)}{1 - \frac{\beta_h^2}{2N\Delta S} \left(\lambda_h^{(iso)} + (\lambda_h^{(irr)} + \lambda_h^{(res)}) \tilde{g}^2 \right)} \right] = \mathcal{O}\left(\frac{1}{N^2}\right) \\ & = \mathcal{O}\left(\frac{1}{N^2}\right) \eta_C - \frac{1}{2N\Delta S} \frac{\theta_c}{\theta_h} \left[\beta_c^2 \left(\lambda_c^{(iso)} + (\lambda_c^{(irr)} + \lambda_c^{(res)}) \tilde{g}^2 \right) - \beta_h^2 \left(\lambda_h^{(iso)} + (\lambda_h^{(irr)} + \lambda_h^{(res)}) \tilde{g}^2 \right) \right]; \end{aligned}$$

therefore, since the optimal efficiency can be upper and lower bounded as $\eta_C - \mathcal{O}\left(\frac{1}{N}\right) \leq \eta_{opt} \leq \eta_C$, it is clear that the Carnot efficiency can be achieved only for $N = \infty$.

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