Thermodynamics and information in linear quantum lattices

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Termodinâmica e informação em redes quânticas lineares

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Abstract

When a quantum system is coupled to several heat baths at different temperatures, it eventually reaches a non-equilibrium steady state (NESS) featuring stationary internal heat currents. From one side, these currents are responsible to cause decoherence and produce entropy in the system. However, their existence also induce correlations between different parts of the system. In this work, we explore this two-folded aspect of NESSs. Using phase-space techniques we calculate the Wigner entropy production on general linear networks of harmonic nodes. Working in the ubiquitous limit of weak internal coupling and weak dissipation, we obtain simple closed-form expressions for the entropic contribution of each individual quasi-probability current. Our analysis also shows that, it is exclusively the (reversible) internal dynamics which maintain the stationary (irreversible) entropy production. From the informational point of view, we address how to quantify the amount of information that disconnected parts of a quantum chain share in a non-equilibrium steady-state. As we show, this is more precisely captured by the conditional mutual information (CMI), a more general quantifier of tripartite correlations than the usual mutual information.

As an application, we apply our framework to the paradigmatic problem of energy transfer through a chain of oscillators subject to self-consistent internal baths that can be used to tune the transport from ballistic to diffusive. We find that the entropy production scales with different power law behaviors in the ballistic and diffusive regimes, hence allowing us to quantify what is the “entropic cost of diffusivity”. We also compute the CMI for arbitrary sizes and thus find the scaling rules connecting information sharing and diffusivity. Finally, we discuss how this new perspective in the characterization of non-equilibrium systems may be applied to understand the issue of local equilibration in non-equilibrium states.

**Keywords:** Wigner entropy NESS; Entropy production NESS; Entropic cost of diffusivity; Information sharing NESS; Conditional Mutual Information NESS.
**Resumo**

Quando um sistema quântico é acoplado à diversos banhos térmicos de diferentes temperaturas, eventualmente um estado estacionário fora do equilíbrio (NESS), caracterizado por correntes internas de calor é atingido. Por um lado, essas correntes são responsáveis por causar decoerência e produzir entropia no sistema. Entretanto, sua existência também induz correlações entre diferentes partes do sistema. Neste trabalho, nós exploramos este duplo aspecto dos NESSs. Usando técnicas do espaço de fase nós calculamos a produção de entropia de Wigner em redes lineares harmônicas. Trabalhando no célebre limite de fraco acoplamento interno e dissipativo, nós obtivemos expressões simples e frechadas para a contribuição de cada corrente de quasi-probabilidade na entropia. Nossa análise também mostra que, a dinâmica interna (reversível) é **exclusivamente** responsável em manter a produção de entropia (irreversível) estacionária. Considerando um ponto de vista informacional, nós trabalhamos no problema de como quantificar a informação compartilhada entre partes desconexas de uma cadeia quântica em um estado estacionário fora do equilíbrio. Nós mostramos então que esta é mais precisamente caracterizada utilizando a informação mútua condicional (CMI), um quantificador mais geral de correlações tripartites do que a usual informação mútua.

Como aplicação, nós utilizamos o paradigmático problema da transferência de energia em uma cadeia de osciladores sujeita a banhos internos auto-consistentes, que podem ser usados para mudar de um transporte balístico para difusivo. Nós encontramos que a produção de entropia escala com diferentes leis de potência nos regimes balístico e difusivo, permitindo então quantificar o “custo entrópico da difusividade”. Nós também computamos a CMI para cadeias de diversos tamanhos e assim encontramos leis de escala relacionando a informação compartilhada com a difusividade. Finalmente nós discutimos como esta nova perspectiva na caracterização de sistemas fora do equilíbrio pode ser aplicada para entender o problema de equilíbrio local em estados fora do equilíbrio.

**Palavras-chave:** Entropia de Wigner NESS; Produção de entropia NESS; Custo entrópico da difusividade; Informação compartilhada NESS; Informação Mútua Condicional NESS.
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Chapter 1

Introduction

Thermodynamics is one of the most reliable theories in physics. It resisted all of the major transformations from the beginning of the XX century - Quantum Mechanics and General Relativity Theory - remaining in its validity. We quote here Einstein’s beliefs on thermodynamics, “It is the only physical theory of universal content, which I am convinced, that within the framework of applicability of its basic concepts will never be overthrown.” One of the reasons for its success and robustness is because it does not rely on any assumption of the microscopic world, but just in recognizing some order and regularity in the macroscopic properties it is able to state general rules and laws [1].

However, its range of applicability is mostly restricted to systems in equilibrium, which seldom is the case of most problems in nature. In order to overcome this problem, Onsager in 1931 and afterwards Prigogini in 1961, have assumed that a non-equilibrium system could be locally approximated by equilibrium ones. Such hypothesis, although somewhat restrictive, allowed them to use the well established notions from equilibrium thermodynamics - heat, energy, entropy, etc. - to describe non-equilibrium systems [2].

This new approach shed light particularly in transport problems from a thermodynamic point of view. We can mention, for instance, the Fourier, Ohm and Fick’s law where a gradient of temperature, electrical potential and concentration generates a current of heat, electrons and particles, respectively\(^1\).

In such problems, after a given time the system eventually reach a steady state, which is characterized by a non-vanishing gradient and a constant current. These states are known as Non-equilibrium steady-states (NESSs). They are easier to be theoretically dealt and yet can bring valuable information of the system in question. For example, looking to the scaling of the

\(^1\)There are also cross effects, as in the case of a thermoelectric material where a gradient of temperature generates a current of particles.
current with the system size, one can determine the kind of transport (ballistic\textsuperscript{2} or diffusive\textsuperscript{3}) the system presents.

With the development of Quantum Mechanics and the recent experimental improvements in controlling quantum systems [3–9], some concepts originally developed in the thermodynamic scenario, are being now extended to the microscopic world.

However, one must now be careful with others phenomena stemming from the quantum nature of the processes involved. For instance, the collapse of the wave function after a measurement or properties like entanglement and discord [10, 11]. The role of measurement, for example, influences the way we characterize the work done in a process [12], or the heat exchanged between two systems [13]. Entanglement, on the other hand, can be interpreted as an available resource on the operation of a thermal machine [10, 11, 14–17]. This field of research is now being called Quantum Thermodynamics.

Interestingly, as well in the classical scenario, most of these experimental setups presents non-equilibrium processes, and again, many ideas developed in the past decades can be applied here. For example, the problem of heat transport naturally appears in a chain of trapped ions. In this case, the phonons are responsible to the propagation of heat and by measuring its mean occupation number in the steady state, one can determine the kind of transport of the system [18]. Another interesting example of transport in quantum systems is the thermoeletric effect, that can be built using fermionic cold atoms coupled with two thermal reservoirs [19]. In fact, NESSs can be obtained using cold atoms in very different ways [20, 21].

Furthermore, NESSs have been used as tools to model systems in several fields of the knowledge. For instance, we can mention systems involving biochemical reactions (as ATP hydrolysis), biomolecular motors and biological cells (as mRNA translation) [22–24].

Quantum thermodynamics is on the frontier between statistical mechanics and quantum information. Particularly, understanding quantum processes from thermodynamics can bring new ideas for tasks in quantum computation and other information processing tasks. The reason is in the similarity between logical operations and thermal machines: in both cases, an input state is transformed, through a certain resource quantity, in an output state [16, 17, 25–27]. Therefore, characterizing the irreversibility or efficiency of such process, will help in the development of new quantum algorithms.

In this dissertation, we consider a quantum system coupled with several reservoirs. The

\textsuperscript{2}Heat current is independent of the system size.

\textsuperscript{3}Heat current is proportional to the inverse of the system size.
temperature gradient will produce heat currents, which has basically two roles. From one side, they are responsible to cause decoherence in the system and thus producing a finite amount of non-equilibrium entropy. However, their existence will also induce correlations between different parts of the system. This competition will eventually reach a NESS, where entropy is constantly being produced and the parts of the systems are correlated in some way.

In chapter 2 we describe the ensuing dissipative dynamics adopting a local master equation\(^4\) [29, 30] and exploiting its simple structure considering a particular quadratic Hamiltonian.

In chapter 4, employing phase-space techniques, we obtain closed-form analytical expressions quantifying the irreversibility of the steady-state, broken down into the elementary contributions corresponding to individual dissipation channels. Thus, one can identify the irreversibility generated by a single bath in a multi-reservoir chain. In addition, we also obtain an expression which neatly illustrates the essential role played by the unitary dynamics in sustaining the irreversibility, by enabling energy transport through the lattice. This is somewhat counter-intuitive, as the unitary part of the dynamics is usually attributed to a reversible contribution. However, within the context of NESSs, that is not true since it is the intra-system interactions which allow for current to flow from one bath to other, hence sustaining the NESS.

Already in chapter 6, we then turn to explore NESSs from the informational point of view. Since information does not satisfies a continuity equation it cannot be quantified in terms of a current. Thus, the question is more appropriately phrased in terms of the amount of information shared between different parts of a quantum chain. For a connected bipartition of the lattice, the natural quantifier is the mutual information (MI). Conversely, motivated by some recent developments in the field of Quantum Markov chains [31–35], we show that for disconnected parts, the appropriate quantifier is actually the conditional mutual information (CMI) [36, 37] \(\mathcal{I}(A : C|B)\), a more general measure of tripartite correlations.

Finally, we apply these two results to the exactly soluble chain presented in chapter 3. Although simplified, in order to get rid unnecessary complications, this model captures the essence of typical quantum transport problems, encompassing ballistic and diffusive regimes. Specifically, the model consists of a one-dimensional bosonic chain subject to two local Lindblad dissipators at the end-points [38–43], plus additional self-consistent reservoirs [44] used to tuned between ballistic and diffusive transport. The main advantages of this model is that the transport regime can be easily changed, the state is Gaussian in both regimes and it can be solved

\(^4\)Which is accurate to lowest order in the inter-node interaction strength [28].
analytically for arbitrary system sizes in the steady state.

Thus, in chapter 5, we could calculate separately the contributions for the irreversibility stemming from the physical and the self-consistent reservoirs. We observe that each contribution scales polynomially with a distinct exponent. This then allow us to unambiguously quantify the irreversible cost of maintaining a diffusivity profile.

In the second part of chapter 6, making use of techniques stemming from Gaussian quantum information theory [45–47], we are able to study the shared information in chains of arbitrary size, including the thermodynamic limit. This allows us to find general scaling laws that reveal how the CMI scales with the system size in both regimes. Conclusively, we show how such a study can be used to shed light on the question of local thermalization of non-equilibrium systems [33, 48].

Lastly, we mention that the results of this dissertation was content for two scientific papers\(^5\) [49, 50].

\(^5\)The paper of Ref. [49] is still in revision process.
Chapter 2

Open quantum system

2.1 Postulates of Quantum Mechanics

Quantum Mechanics is a cinematic theory for microscopic systems. Modernly, we can formulate it in terms of four postulates.

1. **The state** of the system is completely characterized by a density operator $\rho$ acting in a Hilbert space $\mathbb{H}$. Furthermore, the density matrix must be Hermitian ($\rho = \rho^\dagger$), positive semi-definite ($\rho \geq 0$) and normalized $\text{tr}(\rho) = 1$.

2. **Observables** are represented by Hermitian operators of $\mathbb{H}$.

3. A **measurement** can be described by a set of operators $\{M_m\}$ with eigenvalues $m$, acting on $\mathbb{H}$, such that $\sum_m M_m^\dagger M_m = 1$. Performing a measurement in a state $\rho$, the probability of obtaining an outcome $m$ is $P_m = \text{tr} \left( M_m^\dagger M_m \rho \right)$ and the state becomes $\rho \rightarrow \rho_m = \frac{M_m \rho M_m^\dagger}{P_m}$.

If a given measure $M$ can be decomposed in terms of projective measurements $\Pi_m$, such that

$$M = \sum_m m \Pi_m,$$

(2.1)

where $m$ is the eigenvalue associated with $\Pi_m$, $\Pi_m^2 = \Pi_m$, $\Pi_m^\dagger = \Pi_m$ and $\sum_m \Pi_m = 1$, then the mean value of $M$ can be written as,

$$\langle M \rangle = \sum_m m P_m = \sum_m m \text{tr} \left( \Pi_m^\dagger \Pi_m \rho \right) = \sum_m \text{tr} \left( \Pi_m \rho \right) = \text{tr} \left( \sum_m m \Pi_m \right) \rho = \text{tr}(M \rho).$$

(2.2)

---

1We are going to use natural units, $\hbar = c = 1$.

2One can show that the uncertainty principle is a corollary of the third postulate.
4. An isolated system evolves accordingly with the von Neumann equation,

\[ \frac{\partial \rho}{\partial t} = -i[H, \rho], \]  

(2.3)

where $H$ is the Hamiltonian.

As in the classical mechanics, a perfect isolated system does not exist. A system is always interacting with its surrounds. It can be demonstrated that such complicated interactions can be described by a set of measurements being performed on the system. Thus, due the third postulate we should conclude that the simple existence of an environment will change the system. The area of Quantum Mechanics that studies the evolution of subsystems in contact with an environment (that is a set of another quantum subsystems) is common called Open Quantum Systems [51].

### 2.2 Quantum master equation

We consider a linear network of $L$ harmonic oscillators with Hamiltonian $H$ given by,

\[ H := \sum_{k=1}^{L} H_{kk} a_k^\dagger a_k + \sum_{k \neq \ell} H_{k,\ell} a_k^\dagger a_\ell, \]  

(2.4)

where $a_i$ denotes the bosonic annihilation operator of the $i$-th mode. Otherwise, we impose no restrictions on the structure of the network, shaped by the non-zero off-diagonal matrix elements $H_{k,\ell} = H_{\ell,k}^*$ ($H_{kk} = \omega_k$ is the modes’ frequency). We also couple each mode with a thermal reservoir\(^3\).

In this section we will pinpoint the main ideas behind a microscopic derivation of a Quantum Master Equation, i.e., an equation for the time evolution of the density matrix of this linear network. A detailed derivation can be found in Refs. [51, 52].

We start defining the total Hamiltonian $H_T$,

\[ H_T = H + H_E + V, \]  

(2.5)

where $H_E$ is the Hamiltonian of the environment and $V$ encompasses the interactions between the system and environment. Since most widely used baths in experimental setups are the

---

\(^3\)Since our system has $L$ modes, then we will have $L$ baths.
eletromagnetic field and the phonons in a crystal, we will assume that the $\mathcal{H}_E$ is composed by a set of harmonic oscillators,

$$\mathcal{H}_E = \sum_{\alpha=1}^{L} \sum_{k=1}^{\infty} \left\{ \Omega_{\alpha,k} b_{\alpha,k}^{\dagger} b_{\alpha,k} + \nu_{\alpha,k} (b_{\alpha,k} b_{\alpha,k}^{\dagger} + b_{\alpha,k}^{\dagger} b_{\alpha,k}) \right\}, \quad (2.6)$$

where the operators $b_{\alpha,k}$ corresponds to the annihilation operator of the “k-th” mode of the “$\alpha$-th” bath. If $\nu_{\alpha,k} \neq 0$ we say that the bath has squeezing terms.

For the interacting term, we will assume that the system-environment coupling is linear$^4$ in $b_{\alpha,k}$,

$$V = \sum_{\alpha=1}^{L} \sum_{k=1}^{\infty} \gamma_{\alpha} \left( M_{\alpha} b_{\alpha,k}^{\dagger} + M_{\alpha}^{\dagger} b_{\alpha,k} \right), \quad (2.7)$$

where $\gamma_{\alpha} > 0$ captures the dissipation strength and $M_{\alpha}$ are operators of the system. The dynamic of the composite density matrix (system + environment) will be governed by the von-Neumann Eq. (2.3). We will consider that the initial state of the system is uncorrelated with the bath, i.e.,

$$\rho_T(0) = \rho(0) \otimes \rho_E(0), \quad (2.8)$$

where $\rho(0)$ is the state of the linear network and the state of the environment, $\rho_E(0)$, is in the Gibbs thermal state. We will also assume that the dissipation strength is weak, in such a way that the evolved state remains uncorrelated

$$\rho_T(t) \approx \rho(t) \otimes \rho_E(t). \quad (2.9)$$

In order to obtain an equation for the time evolution of $\rho(t) = tr_E(\rho(t))$, it is necessary to make more two approximations. The first one is the Markov approximation and it consists in assume bath correlations decay quickly. The physical motivation behind this approximation consists in the idea that the environment is big and chaotic, such that the excitations induced by the system in the bath will not affect the system again in some time in the future$^5$. The second is the Rotating-wave (secular) approximation, which consists in trow way therms that oscillate very fast. The reason for this approximation lies on remembering that all bath-stuff are fast, whereas system stuff are slow.

$^4$There is two reasons for this choice. First, because many systems used in literature have this kind of couplings and second, it really simplifies the calculus.

$^5$A memoryless environment.
Thus, under these assumptions, one can obtain the following quantum master equation
\[
\frac{d\rho}{dt} = -i[H, \rho] + \sum_{k=1}^{L} L_k(\rho) + \mathcal{O}(\gamma^2),
\]
(2.10)
where \( L_k \) are the Lindblad super-operators in the standard form [53, 54] and \( \gamma := \max\{\gamma_1, \cdots, \gamma_L\} \). Individually, each super operator \( L_k \) is \( \mathcal{O}(\gamma_k) \) and, in general, can act globally on all modes. However, we will make the additional assumption of weak internal coupling between the nodes, which leads to the Local Master Equation (LME)
\[
\frac{d\rho}{dt} = -i[H, \rho] + \sum_{k=1}^{L} \mathcal{D}_k(\rho) + \mathcal{O}(\lambda \gamma),
\]
(2.11)
where the local dissipators are given by\(^6\),
\[
\mathcal{D}_k(\rho) = \gamma_i(N_i + 1)D[a](\rho) + \gamma_iN_iD[a^\dagger](\rho) - \gamma_iM_iB[a^\dagger](\rho) - \gamma_iM_i^*B[a](\rho),
\]
(2.12)
with
\[
D[a](\rho) = a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\} \quad \text{and} \quad B[a](\rho) = a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}.
\]
(2.13)
Here \( N_i \) and \( M_i \) are constants that can be associated to the thermal fluctuations and the degree of squeezing according to,
\[
N_i + \frac{1}{2} = (\bar{n}_i + \frac{1}{2}) \cosh(2r_i), \quad M_i = (\bar{n}_i + \frac{1}{2}) e^{i\theta_i} \sinh(2r_i),
\]
(2.14)
where \( \bar{n}_i \) is the local Bose-Einstein occupation and \( z_i = r_i e^{i\theta_i} \) is the local squeezing value. Moreover, \( \lambda := \max\{H_k, \ell\} \) with \( k \neq \ell \) is the highest internal coupling among all nodes.

Care must be taken when using Eq. (2.11) to describe a multipartite open quantum system, since it is well known that going beyond its range of validity might lead to thermodynamic inconsistencies [28, 30, 55]. The parameter range in which the many approximations underlying both global and local master equations are satisfied have been critically (and extensively) discussed in the literature [29, 52, 56–64]. However, local master equations also arise naturally when considering certain repeated-interaction models [57, 64, 65]. This picture enables a thermodynamically consistent bookkeeping of all energy exchanges occurring in dissipative processes exactly described by Eq. (2.11) [66, 67]. Thus, only within certain parameters range
\(^6\{\cdot, \cdot\}_+\) stands for anti-commutator.
it is correct to say that $\bar{n}_1 - \bar{n}_L (r_1 - r_L)$ represents a gradient of temperature (squeezing).

### 2.3 A simple example: One mode coupled with a bath

Before going through a simple example, let us write the Quantum Master Equation in terms of the expectation value of an operator. In the Schrödinger picture, from Eq. (2.2) we have that

$$\frac{d\langle O \rangle}{dt} = \text{tr} \left\{ \frac{d\rho}{dt} O \right\}. \quad (2.15)$$

Substituting Eq. (2.11) and using the cyclic property of the trace, one can obtain,

$$\frac{d\langle O \rangle}{dt} = i\langle [\mathcal{H}, O] \rangle + \sum_k \langle \dot{\mathcal{D}}[L_k](O) \rangle, \quad (2.16)$$

where

$$\dot{\mathcal{D}}[L_k](O) = \gamma_i (N_i + 1) \tilde{D}[a](O) + \gamma_i N_i \tilde{D}[a^\dagger](O) - \gamma_i M_i \tilde{B}[a^\dagger](O) - \gamma_i M_i^* \tilde{B}[a](O), \quad (2.17)$$

with $\tilde{D}[L_k](O)$ and $\tilde{B}[L_k](O)$ are defined as

$$\tilde{D}[L_k](O) = L_k^\dagger OL_k - \frac{1}{2} \{L_k^\dagger L_k, O\} \quad \text{and} \quad \tilde{B}[L_k](O) = L_k^\dagger OL_k - \frac{1}{2} \{L_k L_k^\dagger, O\}, \quad (2.18)$$

and are common called the adjoint dissipator.

We consider now, as a simple application, a single bosonic node weakly coupled to a bath at inverse-temperature $\beta_1 = T_1^{-1}$ with zero squeezing. The LME can then be written as,

$$\frac{d\rho}{dt} = -i[\mathcal{H}, \rho] + \gamma (\bar{n} + 1) D[a](\rho) + \gamma \bar{n} D[a^\dagger](\rho), \quad (2.19)$$

with the Hamiltonian,

$$\mathcal{H} = \omega a^\dagger a. \quad (2.20)$$

A situation of particular interest is the steady state. The solution in this case is the Gibbs thermal state, $\rho_{\text{TH}} = \frac{e^{-\beta_1 \mathcal{H}}}{\text{tr}(e^{-\beta_1 \mathcal{H}})}$, which can be verified by simple inspection of Eq. (2.19). Moreover, this state is also a fixed point of the dissipator,

$$D[a](\rho_{\text{TH}}) = 0. \quad (2.21)$$
Now, using Eq. (2.16), we can calculate the time evolution of the mean value of the number operator \( O = a\dagger a \)

\[
\frac{d\langle a\dagger a \rangle_t}{dt} = \gamma \left( \bar{n} - \langle a\dagger a \rangle_t \right),
\]

(2.22)

which has by solution an exponential decay,

\[
\langle a\dagger a \rangle_t = \bar{n} + \langle a\dagger a \rangle_0 e^{-\gamma t},
\]

(2.23)

where \( \langle a\dagger a \rangle_0 \) is the initial condition of the occupation number. Furthermore we can define a current of quanta \( J_1 \) as,

\[
J_1(t) := \frac{d\langle a\dagger a \rangle_t}{dt},
\]

(2.24)

thus Eq. (2.22) can be viewed as a continuity equation. In this way, as we expected, if \( \bar{n} > \langle a\dagger a \rangle_t \) the current is positive, meaning that quanta are being injected in the system and if \( \bar{n} < \langle a\dagger a \rangle_t \) the opposite happens.

### 2.4 The Covariance Matrix

We now turn to the general case of \( L \) independent bosonic modes. The algebra is then given by,

\[
[a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i, a_j] = 0 \quad \text{where} \quad i, j = 0, \ldots, L.
\]

(2.25)

It is worth to order these creations and annihilations operators in vector of \( 2L \) dimension\(^7\),

\[
R = (a_1, a_1^\dagger, \ldots, a_L, a_L^\dagger)^\top.
\]

(2.26)

Thus, we can rewrite the algebra in a very compact way

\[
[R_i, R_j^\dagger] = \Sigma_{ij}, \quad \text{with} \quad \Sigma = \bigoplus_{i=1}^{L} \sigma_z,
\]

(2.27)

where \( \sigma_z \) is the Pauli matrix and the symbol \( \bigoplus \) stands for the tensorial sum. In this dissertation we are going to work exclusively with Gaussian states [46], which has the useful property of being completely characterized by the first and second moments [68]. Therefore, we define the

\(^7\)Notation: we are going to write all matrices in bold.
2L × 2L Covariance Matrix (CM) \( \Theta \) and the vector of the means \( \mu \) such that,
\[
\Theta_{ij} = \frac{1}{2} \langle \{ \delta R_i, \delta R_j^\dagger \} \rangle, \quad \mu_i = \langle R_i \rangle, \quad \text{with} \quad i, j = 1, \ldots, 2L, \tag{2.28}
\]
where \( \delta R_i = R_i - \langle R_i \rangle \). To illustrate the form of the CM, we write the case of two modes \( (L = 2) \) and vanishing first moments \( (\mu = 0) \):
\[
\Theta = \begin{pmatrix}
\langle a_1^\dagger a_1 \rangle + 1/2 & \langle a_1 a_1 \rangle & \langle a_1 a_2 \rangle & \langle a_2 a_2 \rangle \\
\langle a_1^\dagger a_2 \rangle & \langle a_1^\dagger a_1 \rangle + 1/2 & \langle a_1^\dagger a_2 \rangle & \langle a_2 a_2 \rangle \\
\langle a_2 a_2 \rangle & \langle a_1 a_2 \rangle & \langle a_2 a_2 \rangle + 1/2 & \langle a_2 a_2 \rangle \\
\langle a_2^\dagger a_2 \rangle & \langle a_2^\dagger a_2 \rangle & \langle a_2^\dagger a_2 \rangle & \langle a_2 a_2 \rangle + 1/2 \\
\end{pmatrix}. \tag{2.29}
\]
This structure for the CM is not the most standard in the literature, which is usually defined in terms of quadrature operators \([46,47]\). However, it turns out to be more useful for the problems we will explore, due to a convenient separation of the dynamics of the two reduced covariance matrices,
\[
C_{ij} = \langle a_j^\dagger a_i \rangle - \langle a_j^\dagger \rangle \langle a_i \rangle, \tag{2.30}
\]
\[
S_{ij} = \langle a_i a_j \rangle - \langle a_i \rangle \langle a_j \rangle, \tag{2.31}
\]
which are \( L \times L \). The relation between \( \Theta \) and \( C, S \) can then be written rather elegantly as
\[
\Theta = \frac{I_{2L}}{2} + C \otimes (\sigma_+ \sigma_-) + C^T \otimes (\sigma_- \sigma_+) + S \otimes \sigma_+ + S^* \otimes \sigma_-, \tag{2.32}
\]
where \( \sigma_i \) are the usual Pauli matrices and \( I_{2L} \) is the \( 2L \times 2L \) identity matrix.

**The Bona Fide relation:** Given any matrix, there is a constraint that it should obey in order to represent a physical state. Let us now briefly derive it. Consider a linear combination of the operators \( \delta R_i \) weighted by some complex numbers \( \beta_i \),
\[
Y = \sum_{i=1}^{L} \delta R_i \beta_i. \tag{2.33}
\]
Since $YY^\dagger$ is a positive semi-definite operator, it follows that,

$$
\langle YY^\dagger \rangle = \sum_{i,j} \beta_i \beta_j^* \langle \delta R_i \delta R_j^\dagger \rangle \geq 0.
$$

(2.34)

Now, using the algebra defined in Eq. (2.27), one may get,

$$
\delta R_i \delta R_j^\dagger = \frac{1}{2} \{\delta R_i, \delta R_j^\dagger\} + \frac{1}{2} \Sigma_{ij}
$$

$$
= \Theta_{ij} + \frac{1}{2} \Sigma_{ij}.
$$

(2.35)

Finally, substituting Eq. (2.35) into Eq. (2.34) we obtain,

$$
\langle YY^\dagger \rangle = \sum_{i,j} \beta_i \beta_j^* \left[ \Theta_{ij} + \frac{1}{2} \Sigma_{ij} \right] \geq 0.
$$

(2.36)

Since this equation is a quadratic form in relation to the matrix $[\Theta_{ij} + \frac{1}{2} \Sigma_{ij}]$, the following constraint should be guaranteed by the CM,

$$
\Theta_{ij} + \frac{1}{2} \Sigma_{ij} \geq 0.
$$

(2.37)

This is the so-called Bona Fide relation. Furthermore, it is also possible to prove that Eq. (2.37) encompasses a generalization of Heisenberg’s uncertainty principle$^8$ [69].

### 2.5 Time evolution of the Covariance Matrix for short range Hamiltonians

We intend here to develop an expression for the time evolution of the CM. We will assume that the system dynamics is governed by Eqs. (2.11-2.12) with the following Hamiltonian (in the interaction picture)$^9$,

$$
\mathcal{H}_I = i\lambda \sum_{i=1}^{L-1} (a_i^+ a_{i+1} - a_{i+1}^+ a_i),
$$

(2.38)

where $\lambda$ is the interaction strength between the modes (taken real for simplicity).

---

$^8$Also known as the Robertson-Schrödinger relation

$^9$We have chosen the frequencies of the modes equals.
Using Eq. (2.16) to calculate the time derivative of CM’s elements, one may obtain a Lyapunov equation,

$$\frac{d\Theta}{dt} = V\Theta + \Theta V^\dagger + G,$$  \hspace{1cm} (2.39)

where

$$V = W \otimes I_2, \quad W_{i,j} = -\frac{\gamma_i}{2}\delta_{i,j} + \lambda(\delta_{i+1,j} - \delta_{i,j+1})$$  \hspace{1cm} (2.40)

and

$$G = \text{diag}(P_1, \ldots, P_L), \quad P_i = \begin{pmatrix} N_i + \frac{1}{2} & M_i \\ M_i & N_i + \frac{1}{2} \end{pmatrix}.$$  \hspace{1cm} (2.41)

Now we can use the fact that the Hamiltonian does not spontaneously generate squeezing to factorize the evolution into two parts, related to the reduced covariance matrices $C$ and $S$ in Eqs. (2.30-2.31),

$$\frac{dC}{dt} = WC + CW^\dagger + F_N,$$  \hspace{1cm} (2.42)

$$\frac{dS}{dt} = WS + SW^\dagger + F_M,$$  \hspace{1cm} (2.43)

where

$$F_N = \text{diag}(\gamma_1 N_1, \ldots, \gamma_L N_L).$$  \hspace{1cm} (2.44)

$$F_M = \text{diag}(\gamma_1 M_1, \ldots, \gamma_L N_L).$$  \hspace{1cm} (2.45)

Note how the two equations (2.42) and (2.43) are now structurally identical, which is a consequence of the form of the Hamiltonian chosen in Eq. (2.38).

For completeness, we mention that the $2L$ block matrix $G$ in Eq (2.41) can be written in terms of the reduced matrices $F_N$ and $F_M$ as

$$G = (F_N + I_L/2) \otimes I_2 + F_M \otimes \sigma_+ + F_N^* \otimes \sigma_-.$$  \hspace{1cm} (2.46)
Chapter 3

Exact solution of a Non-Equilibrium Steady State

3.1 A transport problem

In this chapter we will obtain an analytical solution for the CM in the steady state of $L$ interacting bosonic modes, each one coupled with a different reservoir, modeled by the Master Equation\(^1\) (2.11) and Hamiltonian given by Eq. (2.38).

Now, in order to provide a better understanding of the physics behind this model, we briefly review here some basic notions of typical transport problems stemming from non-equilibrium processes. Consider a NESS established when a system (of “length” $L$) is placed between two reservoirs at different temperatures. This exhibits a stationary heat current which, for small temperature gradients $\Delta T$, can be expressed as

$$J_E = \frac{k}{L^\alpha} \Delta T,$$

(3.1)

where $\alpha$ is an exponent that characterizes the heat flow regime. Whenever $\alpha = 1$ one speaks of diffusive behavior (i.e., Fourier’s heat conduction law). However, low-dimensional (and usually integrable) quantum and classical systems usually present a ballistic heat flow [70–72], characterized by $\alpha = 0$ (that is, by a current that is independent of the size of the system). A diffusive flow usually appears in non-integrable and chaotic systems and may therefore be associated with the informational scrambling of the energy transmitted from one reservoir to the other.

\(^1\)With some particulars parameters choice.
3.2 Solution of the Lyapunov equation in the Non-Equilibrium Steady State

The particular case of a NESS is obtained by setting the left-hand side of Eqs. (2.42) and (2.43) to zero,

\[ WC + CW^\dagger + F_N = 0, \]  
\[ WS + SW^\dagger + F_M = 0. \]

We now focus on Eq. (3.2). Analogous results can be stated for Eq. (3.3) by simply replacing \( N_i \) with \( M_i \), \( i = 1, \ldots, L \). But, if there is no squeezing in all environments \( (z_i = 0) \) then \( F_M = 0 \) and we therefore obtain \( S = 0 \).

A ballistic transport can be obtained setting \( \gamma_1 = \gamma_L = \gamma \) and \( \gamma_i = 0 \), for \( i = 2, \ldots, L-1 \) [42]. The matrices \( W \) and \( F_N \) then become,

\[
W = \begin{pmatrix}
-\gamma/2 & \lambda & 0 & 0 & 0 & \ldots & 0 & 0 \\
-\lambda & 0 & \lambda & 0 & 0 & \ldots & 0 & 0 \\
0 & -\lambda & 0 & \lambda & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & \ldots & 0 & -\lambda & 0 & \lambda & 0 \\
0 & 0 & \ldots & 0 & 0 & -\lambda & 0 & \lambda \\
0 & 0 & \ldots & 0 & 0 & 0 & -\lambda & -\gamma/2
\end{pmatrix}
\]

and \( F_N = \gamma \text{diag}(N_1, 0, \ldots, 0, N_L) \).

To make it diffusive, we add additional reservoirs acting on all sites of the chain [44, 73–77]. However, the temperature of these reservoirs is chosen self-consistently, in such a way that in the NESS the currents flow only to the physical reservoirs. Hence, the self-consistent baths can be viewed as auxiliary baths, which introduce noise in the system with the goal of causing decoherence, but without affecting the energy. In practice, this means we should add to Eq. (3.2) the additional terms,

\[ WC + CW^\dagger + F_N - \Gamma C + \tilde{F}_N = 0 \]  
(3.4)
where $\Gamma$ is the coupling constant to the self-consistent reservoirs and

$$\tilde{F}_N = \Gamma \text{diag}(\tilde{N}_1, \tilde{N}_2, \ldots, \tilde{N}_{L-1}, \tilde{N}_L).$$

Here $\tilde{N}_i$, $i = 1, \ldots, L$, are the thermal occupations of the self-consistent reservoirs, which are chosen as

$$\tilde{N}_i = \langle a_i^\dagger a_i \rangle = C_{ij}.$$

(3.5)

A schematic picture of this model can be seen in Fig. (3.1). Thus, Eq. (3.4) can be written as

$$WC + CW^\dagger + F_N - \Gamma \Delta(C) = 0,$$

(3.6)

where $\Delta(C)$ is the operation of removing all diagonals from $C$:

$$\Delta(C) = C - \text{diag}(C_{1,1}, C_{2,2}, \ldots, C_{LL}).$$

Eq. (3.6) is now formally identical to the model studied in Refs. [40–42], which instead of using self-consistent baths, used dephasing baths of the form

$$\mathcal{K}(\rho) = \frac{\Gamma}{2} \sum_{i=1}^L \left[ a_i^\dagger a_i \rho a_i^\dagger a_i - \frac{1}{2} [(a_i^\dagger a_i)^2, \rho] \right].$$

(3.7)

Even though both models lead to the same equation for the covariances, it turns out that the steady-states themselves are different. The reason is that the dephasing model - Eq. (3.7) - does not preserve Gaussianity since the Lindblad generators are quadratic, instead of linear, in the creation and annihilation operators. The NESS of the self-consistent reservoirs is Gaussian, but that of the dephasing model is not.

We also mention that the self-consistent model can be readily extended for the case of squeezing, whereas the dephasing model cannot, since a dissipator such as in Eq. (3.7) preserves the number of particles, but does not preserve the level of squeezing.

The solution of Eq. (3.6) is then identical to that studied in Ref. [40–42]. The matrix $C$ is
Figure 3.1: Schematic picture of the model studied. A one-dimensional chain containing $L$ bosonic modes is put in contact with two reservoirs at each end, each kept at occupations $\bar{n}_1$ and $\bar{n}_L$. The NESS of this system would have a ballistic current. To induce diffusivity the system is augmented with $L$ self-consistent reservoirs, one for each site of the chain. The temperature of these reservoirs is chosen so that in the NESS no current flows to them, but only to the physical reservoirs.

tridiagonal, of the form

$$
C = \begin{pmatrix}
A_1 & x & 0 & 0 & 0 & \ldots & 0 \\
x & A_2 & x & 0 & 0 & \ldots & 0 \\
0 & x & A_3 & x & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & \ldots & 0 & x & A_{L-2} & x & 0 \\
0 & \ldots & 0 & 0 & x & A_{L-1} & x \\
0 & \ldots & 0 & 0 & 0 & x & A_L
\end{pmatrix},
$$

(3.8)

where

$$
A_i = \langle a_i^\dagger a_i \rangle = \frac{N_1 + N_L}{2} + \frac{1}{2} \frac{\gamma(N_1 - N_L)}{4\lambda^2 + \gamma^2 + \gamma \Gamma(L-1)} \Gamma(L - 2i + 1)
$$

$$
+ \frac{1}{2} \frac{\gamma^2(N_1 - N_L)}{4\lambda^2 + \gamma^2 + \gamma \Gamma(L-1)} (\delta_{i,1} - \delta_{i,L}),
$$

(3.9)

$$
x = \langle a_i^\dagger a_{i+1} \rangle = \frac{\gamma \lambda}{4\lambda^2 + \gamma^2 + \gamma \Gamma(L-1)} (N_L - N_i).
$$

(3.10)
3.3 The current

In this section, we will motivate an expression for the current, using a continuity equation for the quanta (quasi-particles)\(^2\). Let us start calculating the following time derivative,

\[
\frac{d}{dt} \left( \sum_{k=1}^{L} a_k^\dagger a_k \right) = \sum_{k=1}^{L} \text{tr} \left\{ a_k^\dagger a_k \frac{d\rho}{dt} \right\} = -i \sum_{k=1}^{L} \text{tr} \left\{ a_k^\dagger a_k [\mathcal{H}_f, \rho] \right\} + \sum_{j=1}^{L} \text{tr} \left\{ a_k^\dagger a_k D_j(\rho) \right\},
\]

(3.11)

where we have used the Master Eq. (2.11) with \(\mathcal{H}_f\) being given by Eq. (2.38). Working in the unitary term of the above equation, one may obtain

\[
-i \sum_{k}^{L} \text{tr} \left\{ a_k^\dagger a_k [\mathcal{H}_f, \rho] \right\} = \sum_{k=2}^{L-1} \lambda (a_{k-1}^\dagger a_k + a_k^\dagger a_{k-1}) - \lambda (a_k^\dagger a_{k+1} + a_{k+1}^\dagger a_k) = \sum_{k=2}^{L-1} \mathcal{J}_{k,k-1} - \mathcal{J}_{k,k+1},
\]

(3.12)

where we have defined the particle current between the sites \(k\) and \(k + 1\) as \([41, 42, 78]\),

\[
\mathcal{J}_{k,k+1} = \lambda (a_k^\dagger a_{k+1} + a_{k+1}^\dagger a_k), \quad k = 2, \ldots, L - 1.
\]

(3.13)

Now, looking to the dissipative term of Eq. (3.11), we get

\[
\sum_{k,j=1}^{L} \text{tr} \left\{ a_k^\dagger a_k D_j(\rho) \right\} = \gamma \left( N_1 - \langle a_1^\dagger a_1 \rangle \right) + \gamma \left( N_L - \langle a_L^\dagger a_L \rangle \right) + \gamma \sum_{k=1}^{L} \left( \bar{N}_k - \langle a_k^\dagger a_k \rangle \right)
\]

(3.14)

\[
= \gamma \left( N_1 - \langle a_1^\dagger a_1 \rangle \right) + \gamma \left( N_L - \langle a_L^\dagger a_L \rangle \right) = \mathcal{J}_{B,1} + \mathcal{J}_{L,B},
\]

(3.15)

from Eq. (3.14) to Eq. (3.15) we have used the self-consistent condition (see Eq. (3.5)). We also have defined the currents from the physical bath to the first oscillator (\(\mathcal{J}_{B,1}\)) and from the last oscillator to the other physical bath (\(\mathcal{J}_{L,B}\)) as

\[
\mathcal{J}_{B,1} = \gamma \left( N_1 - \langle a_1^\dagger a_1 \rangle \right) \quad \text{and} \quad \mathcal{J}_{L,B} = \gamma \left( N_L - \langle a_L^\dagger a_L \rangle \right).
\]

(3.16)

Note that, due to the self-consistent condition, there is no particle current from the system to the auxiliary baths, corroborating to the idea that they can be seen just as a smart\(^3\) way to induce noise in a harmonic chain coupled with two reservoirs in the ends. Finally, substituting

---

\(^2\)For notation simplicity, we will refer to the “quasi-particles” by simple “particles”.

\(^3\)Because preserves gaussianity.
Eqs. (3.12) and (3.15) into Eq. (3.11), we obtain
\[
\frac{d}{dt} \left( \sum_{k=1}^{L} a_{k}^\dagger a_{k} \right) = \mathcal{J}_{B,1} + \mathcal{J}_{L,B} + \sum_{k=2}^{L-1} \mathcal{J}_{k-1,k} - \mathcal{J}_{k,k+1}. \tag{3.17}
\]

In the particular case of a NESS, \( \frac{d}{dt} \left( \sum_{k=1}^{L} a_{k}^\dagger a_{k} \right) = 0 \) and due to the particles are a conservative quantity, the current that enters the system is the same that leaves, \( \mathcal{J}_{B,1} = -\mathcal{J}_{L,B} \). Nay, the current from the \( k \)-th mode to the \( k + 1 \)-th is equal to the current from the \( k - 1 \)-th to the \( k \)-th,
\[
\mathcal{J}_{k,k+1} = \mathcal{J}_{k-1,k} \equiv \mathcal{J}. \tag{3.18}
\]

Thus, as we expected for a NESS, Eq. (3.17) vanishes.

Similar schemes could be developed to describe a current of energy. However, recently it has been shown that there is also an alternative interpretation in terms of the method of repeated interactions \[79\]. This method can be used to generate local master equations from a physically consistent model \[65, 80\] where the environment is described by the sequential interactions with a series of “environmental units”, which are then discarded after each stroke. Within this framework, it is possible to reconcile local master equations with thermodynamics by identifying a work cost associated with turning the interactions with the units on and off. Once this work term is identified, it turns out (for the specific case of a bosonic chain) that the current of Eq. (3.18) will also correspond to the heat current to the baths, up to a constant \( \omega \).

Thus, to summarize, if one interprets the master Eq. (2.11) as stemming from the method of repeated interactions, the current \( \mathcal{J} \) represents both the particle and heat currents. If not, then \( \mathcal{J} \) is to be interpreted solely as the current of particles.

Finally, substituting Eq. (3.10) into Eq. (3.13), we obtain an expression for the current of the model we are studying,
\[
\mathcal{J} = 2\lambda x = \frac{2\gamma \lambda^2}{4\lambda^2 + \gamma^2 + \gamma \Gamma (L - 1)} (N_L - N_1), \tag{3.19}
\]
that is, up to a constant, the quantity \( x \). It is worth noting that the current depends on the gradient of the occupation number, as in Eq. 3.1 it depends on the temperature gradient. The behavior with \( L \) we will explore in the next section, when we will consider the two kind of transports - ballistic and diffusive - separately.

\[\text{The signal is due to the currents direction.}\]
3.4 Ballistic vs. diffusive transport

Considering the CM given by Eqs. (3.9-3.10), if we set $\Gamma \to 0$ we obtain a ballistic model, where

$$A_i = \langle a_i^\dagger a_i \rangle = \frac{N_1 + N_L}{2} + \frac{1}{2} \frac{\gamma^2 (N_1 - N_L)}{4L^2 + \gamma^2} (\delta_{i,1} - \delta_{i,L}), \quad (3.20)$$

$$\mathcal{J} = 2\lambda \langle a_i^\dagger a_{i+1} \rangle = \frac{2\gamma \lambda^2}{4L^2 + \gamma^2} (N_L - N_1). \quad (3.21)$$

In this case the occupation profile is flat inside the chain, except at the end-points. This is illustrated in Fig. (3.2 a). Moreover, in this case the current is independent of $L$.

Conversely, if $\Gamma \neq 0$, then for a sufficiently large $L$ we obtain

$$A_i = \langle a_i^\dagger a_i \rangle = \frac{(L - i)N_1 + (i - 1)N_L}{L - 1} + \frac{\gamma}{2\Gamma} \frac{(N_1 - N_L)}{L - 1} (\delta_{i,1} - \delta_{i,L}), \quad (3.22)$$

$$\mathcal{J} = 2\lambda \langle a_i^\dagger a_{i+1} \rangle = \frac{2\gamma \lambda^2}{\Gamma} \frac{N_L - N_1}{L}. \quad (3.23)$$

Except for small end-point corrections, we see that in this case $\langle a_i^\dagger a_i \rangle$ interpolates linearly between $N_1$ and $N_L$ (see Fig. (3.2 b-d)). Moreover, the current becomes inversely proportional to $L$, which is the hallmark of a diffusive behavior obeying Fourier’s law. Hence $\Gamma$ can also be interpreted as an additional noise source responsible for changing the flow from ballistic to diffusive.

We also mention that a proposal to simulate this model in trapped ions was given in [18].

3.5 General NESS covariance matrix with squeezing

Finally, if we introduce squeezing in the reservoirs, then Eq. (3.3) will give a non-vanishing solution for $S$. This solution is identical to that for $C$, with $N_i$ replaced by $M_i$. Thus, in the
Figure 3.2: Occupation profile $\langle a_i^{\dagger} a_i \rangle$ as a function of the location $k$ of the site on the chain for various parameters. (a) Ballistic profile for $\Gamma = 0$ and varying $\lambda$. (b) Diffusive profile for $\Gamma = 10^{-6}$. (c) Same as (b) but for different values of $\Gamma$, with fixed $\lambda = 10^{-5}$. (d) Profile for different chain sizes $L$, with fixed $\lambda = 10^{-5}$ and $\Gamma = 10^{-6}$. In all panels $\gamma = 10^{-5}$. In (a)–(c) $L = 10$. 
NESS with squeezing, $S$ would also be tridiagonal, with

$$B_i := \langle a_i a_i \rangle = \frac{M_1 + M_L}{2} + \frac{1}{2} \frac{\gamma (M_1 - M_L)}{4 \lambda^2 + \gamma^2 + \gamma \Gamma (L - 1)} \Gamma (L - 2i + 1)$$

$$+ \frac{1}{2} \frac{\gamma^2 (M_1 - M_L)}{4 \lambda^2 + \gamma^2 + \gamma \Gamma (L - 1)} (\delta_{i,1} - \delta_{i,L}), \quad (3.24)$$

$$y := \langle a_i a_{i+1} \rangle = \frac{\gamma \lambda}{4 \lambda^2 + \gamma^2 + \gamma \Gamma (L - 1)} (M_L - M_1). \quad (3.25)$$

From $C$ and $S$ we can then reconstruct the full CM $\Theta$ using Eq. (2.32). We then find that $\Theta$ will be block tridiagonal, of the form

$$\Theta = \begin{pmatrix}
Q_1 & Z & 0 & 0 & 0 & \ldots & 0 & 0 \\
Z & Q_2 & Z & 0 & 0 & \ldots & 0 & 0 \\
0 & Z & Q_3 & Z & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & \ldots & Z & 0 \\
0 & 0 & 0 & 0 & 0 & \ldots & Z & Q_L
\end{pmatrix}, \quad (3.26)$$

where,

$$Q_i = \begin{pmatrix}
A_i + \frac{1}{2} & B_i \\
B_i^* & A_i + \frac{1}{2}
\end{pmatrix} \quad \text{and} \quad Z = \begin{pmatrix}
x & y \\
y^* & x
\end{pmatrix}. \quad (3.27)$$
Chapter 4

Wigner entropy production in linear quantum lattices

4.1 Entropy production/flux rate

Entropy is known to play a fundamental role in both thermodynamics and information theory. One peculiarity of this quantity is that, unlike energy, it does not satisfy a continuity equation: in addition to the exchange of entropy with the environment, as time passes, entropy can also be produced within the system. This additional contribution is known as the entropy production and serves to quantify the degree of irreversibility of a physical process [81, 82]. In symbols, we can write the following balance equation for the entropy $S(t)$\footnote{Do not confuse with the matrix $S$ defined in Eq. (2.31). Bear in mind that all matrices are in bold.} of the system

$$\frac{dS(t)}{dt} = \Pi(t) - \Phi(t),$$

(4.1)

where $\Pi(t)$ is the entropy production rate and $\Phi(t)$ the entropy flux rate from the system to the environment. The entropy production rate is always non-negative and is zero if and only if the system is in equilibrium, which is a consequence of the second law of thermodynamics. When the system is allowed to relax in contact with a single reservoir, it will in general reach thermal equilibrium where $dS/dt = \Pi = \Phi = 0$. However, when the system is connected to multiple reservoirs kept at different temperatures, it will instead reach a Non-Equilibrium Steady-State (NESS) where $dS/dt = 0$ but $\Pi = \Phi \geq 0$. The NESS is therefore characterized by a finite entropy production rate $\Pi$, which is constantly being converted into an entropy flux $\Phi$ that is...
dumped into the environment.

The theory of entropy production is formulated differently depending on the type of stochastic process at hand. For classical systems, widely used approaches are based on Onsager’s theory of chemical kinetics [83–85], classical master equations [86, 87], or Fokker-Planck equations [88–92]. Conversely, for quantum systems the problem is usually formulated in terms of Lindblad master equations [93, 94], repeated interactions, quantum trajectories [95] and fluctuation theorems [96, 97], among others.

More recently, an alternative formulation based on quantum phase space methods and quantum Fokker-Planck equations [8, 98–100] has appeared. This approach has been put forward for more general reservoirs, such as squeezed, dephasing or even zero temperature environments. More importantly, this framework allows one to identify irreversible quasi-probability currents in phase space, which have an interesting physical interpretation as the ultimate microscopic responsible for the emergence of irreversibility at the quantum level.

The developments in Refs. [8, 98–100] have so far focused exclusively on single systems connected to single reservoirs, and have not addressed explicitly the phenomenology of NESS.

In this chapter, we fill this gap and address the case of a multipartite bosonic system coupled to multiple reservoirs, described by means of local quantum master equations. Employing phase-space techniques, we then obtain two main results: first, we show that it is possible to access the local contribution of each dissipation channel to the entropy production, which are found to be related to the local quasi-probability currents generated from the contact with the environments.

Second, we obtain an expression which pinpoints the essential role played by the unitary dynamics in the entropy production, particularly in NESS. This is somewhat counterintuitive, as the unitary part of the dynamics is usually attributed to a reversible contribution. However, within the context of NESSs, that is not true since it is the intra-system interactions which allow for current to flow from one bath to the other, hence sustaining the NESS. Within our phase-space formulation, we are able to obtain expressions which clearly illustrate this interplay between irreversible quasi-probability currents, stemming from the contact with the reservoirs, and unitary currents, stemming from the internal system interactions.

As an application, we dedicate the next chapter to study the transport of heat in a one-dimensional bosonic chain coupled to two reservoirs at each end [38,41,42,101], more precisely the model described in chapter 3. In this case, we employ our framework to address the problem
of quantifying the *entropic cost of diffusivity*, i.e. how irreversible is a diffusive dynamics, when compared to a ballistic one. We are then able to quantify the individual contributions to irreversibility stemming from the physical reservoirs, and that stemming solely from the self-consistent baths.

### 4.2 Phase space: the Wigner function

We consider here a gaussian quantum system described by the Local Master Equation (2.11) and the quadratic Hamiltonian of Eq. (2.4). For simplicity, we are going to assume all reservoirs without squeezing, that is, $M_i = 0$ for all $i$ in the dissipators (Eq. (2.12)).

We now move to quantum phase space by defining the Wigner function [102],

$$W(\xi) = \frac{1}{\pi^{2L}} \int d\lambda e^{-\sum_{i=1}^{2L}(\lambda_i \alpha_i^\dagger - \lambda^*_i \alpha_i)} \text{tr}\left\{\rho e^{\sum_{i=1}^{2L}(\lambda_i \alpha_i^\dagger - \lambda^*_i \alpha_i)}\right\}, \quad (4.2)$$

where $\xi$ is a $2L$-dimensional complex vector composed by the phase-space variables,

$$\xi = (\alpha_1, \alpha_1^*, \ldots, \alpha_L, \alpha_L^*)^T. \quad (4.3)$$

If the state of the system is Gaussian, then the Wigner function (4.2) is completely determined by the CM and the vector of the means $\mu$,

$$W(\xi) = \frac{1}{\pi^L \sqrt{|\Theta|}} \exp\left\{-\frac{1}{2}(\xi - \mu)^\dagger \Theta^{-1}(\xi - \mu)\right\}, \quad (4.4)$$

where $|\Theta|$ denotes the determinant of the CM.

*En passant*, it may be convenient to note that in light of the factorization (2.32), the matrix $\Theta^{-1}$ may also be written as

$$\Theta^{-1} = B \otimes \sigma_+ \sigma_- + B^T \otimes \sigma_- \sigma_+ + P \otimes \sigma_+ + P^* \otimes \sigma_- , \quad (4.5)$$

where

$$B = (C - S(C^{-1})^T S^*)^{-1}, \quad (4.6)$$

$$P = -C^{-1} S B^T. \quad (4.7)$$

---

2Here we are considering a more general Hamiltonian than Eq. (2.38).
In particular, if $S = 0$ then we simply get $B = C^{-1}$.

### 4.3 Quantum Fokker Planck equation

Now, we are going to study the time evolution of the Wigner function. Using standard correspondence tables [102], one can turn the Lindblad Master Equation (2.11) in a quantum Fokker-Planck equation

$$\partial_t W = U(W) + \sum_{k=1}^{L} D_k(W),$$

(4.8)

where $U(W)$ represents the unitary part and $D_k(W)$ the dissipative. The latter, in particular, may be written as a divergence in the complex plane:

$$D_k(W) = \partial_k J_k(W) + \partial^*_k J^*_k(W),$$

(4.9)

where $\partial_k = \partial/\partial \alpha_k$ ($\partial^*_k = \partial/\partial \alpha^*_k$) and

$$J_k(W) = \frac{\gamma_k}{2} \left( \alpha_k W + (\bar{n}_k + 1/2) \partial^*_k W \right).$$

(4.10)

Hence, the quantum Fokker-Planck Equation (4.8) may be interpreted as a continuity equation for $W$, with the quantities $J_k(W)$ representing quasi-probability (microscopic) currents in phase space. This interpretation is corroborated by the fact that the currents are zero if and only if each mode is in local equilibrium. That is $J_k(W_{eq}) = 0$ if and only if $W$ is in the state

$$W_{eq}(\xi) = \prod_k W_{eq}^{(k)}(\alpha_k, \alpha^*_k),$$

where $W_{eq}^{(k)}(\alpha_k, \alpha^*_k) = e^{-|\alpha_k|^2/(\bar{n}_k + 1/2)}/\pi(\bar{n}_k + 1/2)$.  

(4.11)

Equilibrium can thus be defined as the state for which the microscopic currents vanish identically [98].

In a similar spirit, the unitary part $U(W)$ in Eq. (4.8) may also be cast in the form of a continuity equation,

$$U(W) = \sum_{k=1}^{L} \left[ \partial_k A_k(W) + \partial^*_k A^*_k(W) \right],$$

(4.12)

where $A_k(W)$ represent the reversible quasi-probability current generated by the unitary inter-
action,\
\[ a_k(W) = i \sum_{\ell=1}^{L} H_{k \ell}(\alpha_{\ell}) W, \]  
(4.13)

which afford an intuitive interpretation: the currents generated locally in mode \( k \) stem from the interaction between \( k \) and other modes \( \ell \).

### 4.4 Wigner entropy production of each dissipation channel

We now formulate the problem of how to construct the entropy production for the quantum Fokker-Planck Eq. (4.8). The standard approach involves the von Neumann entropy. However, as shown in Refs. [8,98–100], for Gaussian systems an entirely equivalent formulation may be constructed in terms of the Wigner entropy

\[ S(W) = - \int d\xi \ W(\xi) \ln W(\xi), \]  
(4.14)

which, as we shall review below, offers several advantages over the standard formulation. Differentiating with respect to time and using the Fokker-Planck equation (4.8) one finds

\[ \frac{dS(W)}{dt} = - \sum_{k} \int [\partial_{k} \mathcal{J}_{k}(W) + \partial^{*}_{k} \mathcal{J}^{*}_{k}(W)] \ln W \ d\xi, \]  
(4.15)

where the part related to the unitary dynamics vanishes identically.

Integrating by parts in each variable and noticing that the boundary terms vanish due to the Gaussianity of the state, one may obtain that

\[ \frac{dS}{dt} = \sum_{k} \int [\mathcal{J}_{k}(W) \partial_{k} \ln W + \mathcal{J}^{*}_{k}(W) \partial^{*}_{k} \ln W] \ d\xi. \]  
(4.16)

Next, we write the currents of Eq. (4.10) in terms of the equilibrium state (Eq. (4.11)),

\[ \mathcal{J}_{k}(W) = \frac{\gamma_{k}}{2}(\bar{n}_{k} + 1/2) W \left[ \partial_{k} \ln(W) - \partial^{*}_{k} \ln(W_{eq}) \right]. \]  
(4.17)

Through simple mathematical manipulation, we can rewrite this equation as,

\[ \partial^{*}_{k} \ln(W) = \frac{2}{\gamma_{k}(\bar{n}_{k} + 1/2)} \frac{\mathcal{J}_{k}(W)}{W} + \partial^{*}_{k} \ln(W_{eq}). \]  
(4.18)
Finally, substituting Eq. (4.18) into Eq. (4.16), we can make the desirable separation between the entropy production rate and flux of each mode,

\[
\frac{dS}{dt} = \Pi - \Phi = \sum_k (\Pi_k - \Phi_k),
\]

(4.19)

where

\[
\Pi_k = \frac{4}{\gamma_k(\bar{n}_k + 1/2)} \int \frac{|J_k(W)|^2}{W} d\xi,
\]

(4.20)

\[
\Phi_k = \int \left\{ J_k \partial_k \ln \mathcal{W}_{eq} + J_k^* \partial_k^* \ln \mathcal{W}_{eq} \right\} d\xi.
\]

(4.21)

The identification of these two basic terms as an entropy production rate and an entropy flux rate is based on several corroborating arguments and has been extensively debated in the past, both in the quantum [98] and classical [88, 92] contexts. First, and foremost, the entropy production rate is clearly seen to be always non-negative and zero if and only if the currents themselves are always zero, which only occurs in equilibrium. Second, entropy production rate is seen to be an even function of the irreversible currents, whereas the entropy flux rate is found to be an odd function, as found in other studies of Fokker-Planck equations [88]. And, perhaps most importantly, it can be shown that within a stochastic trajectories framework these expressions for the entropy production satisfy integral fluctuation theorems [89, 98].

The most important feature of Eqs. (4.20) and (4.21), however, is that we can now also identify the individual contribution of each dissipation channel to the total entropy production rate and entropy flux. The entropy production rate (4.20), in particular, acquires an interesting and rich physical interpretation due to its connection to the microscopic irreversible currents \( J_k(W) \). In fact, following the classical approach [92] one sees that Eq. (4.20) may be interpreted as an average of phase space velocities \( J_k(W)/W \). Hence, we see that the \( J_k(W) \) behaves as the microscopic entities ultimately responsible for the emergence of irreversibility, with the entropy production functioning as a sort of average over phase space of these microscopic currents.

As for the entropy flux rate, making use of the identity

\[
\int a_k^* a_\ell \mathcal{W} d\xi = \langle a_k^* a_\ell \rangle + \delta_{k,\ell}/2,
\]

(4.22)
one may rewrite the entropy flux rate in Eq. (4.21) as

\[ \Phi_k = \frac{\gamma_k}{\bar{n}_k + 1/2} \left( \langle a_k^\dagger a_k \rangle - \bar{n}_k \right), \]  

which is therefore seen to be related to the difference between the occupation of the \( k \)-th mode at any given time and the bath-imposed occupation \( \bar{n}_k \). If the mode has a higher occupation than the environment we get \( \Phi_k > 0 \), meaning entropy flows from the system to the environment. Conversely, if \( \langle a_k^\dagger a_k \rangle < \bar{n}_k \) then \( \Phi_k < 0 \) and entropy will flow from the environment to the system.

The entropy production rate (4.20) may also be expressed in terms of the covariance matrix of the system, similarly to the flux (4.23), although the expression is not as simple. We begin by substituting explicitly the current in Eq. (4.17) into Eq. (4.20), for which one finds,

\[ \Pi_k = \Phi_k - \gamma_k + \gamma_k (\bar{n}_k + 1/2) \int W |\partial_k \ln(W)|^2 d\xi. \]  

Next we substitute in the logarithm the explicit formula for the Gaussian Wigner function of Eq.(4.4). Carrying out the remaining integrals we then finally obtain

\[ \Pi_k = \Phi_k - \gamma_k + \gamma_k (\bar{n}_k + 1/2)(\Theta^{-1})_{2k,2k}, \]  

which is the desired expressions, yielding the entropy production rate directly in terms of the CM.

4.5 Role of the unitary dynamics in maintaining a non-equilibrium steady-state

The expression for the entropy production rate in Eq. (4.20) may also be written, after some rearrangements, as

\[ \Pi = - \sum_{k=1}^{L} \int D_k(W) \ln \left( \frac{W}{W_{eq}} \right) d\xi. \]  

Let us consider now the Wigner relative entropy (or Kullback-Leibler divergence),

\[ S(W||W_{eq}) := \int W \ln \left( \frac{W}{W_{eq}} \right) d\xi. \]  

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Differentiating it with respect to time and using the Fokker-Planck Eq. (4.8), one may obtain that,

$$\frac{dS(W\|W_{eq})}{dt} = \int U(W) \ln \left( \frac{W}{W_{eq}} \right) d\xi + \sum_{k=1}^{L} \int D_k(W) \ln \left( \frac{W}{W_{eq}} \right) d\xi,$$  \hspace{1cm} (4.28)

where the second term can be identified with Eq. (4.26). Furthermore, the integral \( \int U(W) \ln(W) \) vanishes. Hence, we conclude that the entropy production rate may be written as

$$\Pi = -\frac{dS(W\|W_{eq})}{dt} - \int U(W) \ln W_{eq} d\xi \hspace{1cm} (4.29)$$

$$= \Pi_{\text{trans}} + \Pi_{\text{NESS}}.$$ \hspace{1cm} (4.30)

This is one of our main results. Since the unitary dynamics is reversible, it is a common place to associate irreversibility with the dissipative contribution. The first term, \( \Pi_{\text{trans}} \), due a transient, can be found in many studies on entropy production [51,93,98,100,103,104] and usually entails to \( \Pi \) an interpretation in terms of the rate at which the system approaches equilibrium (with the relative entropy playing the role of a distance between the present state and the equilibrium state). However, this is only true if the system is connected to a single reservoir or if the different sub-systems do not interact. When they do, the system will instead reach a NESS where the first term is zero, but the second term notwithstanding remains. Hence, Eq. (4.29) puts in evidence the essential role that the unitary interactions have in allowing currents to flow from one bath to another, maintaining the NESS and a finite entropy production rate.

### 4.6 Recovering Onsager’s theory of irreversible thermodynamics

Using the unitary currents of the Wigner space (see Eq. (4.12)) and the moments of the Wigner function (see Eq.(4.22)), we can rewrite the last term in Eq. (4.29) as,

$$\Pi_{\text{NESS}} = -i \sum_{k \neq \ell} \frac{1}{\bar{n}_k + 1/2} \left( H_{k,\ell}\langle a_k^\dagger a_\ell \rangle - H_{\ell,k}\langle a_\ell^\dagger a_k \rangle \right)$$ \hspace{1cm} (4.31)

$$= \sum_{k \neq \ell} \frac{2}{\bar{n}_k + 1/2} \Im \{ H_{k,\ell}\langle a_k^\dagger a_\ell \rangle \}.$$ \hspace{1cm} (4.32)
We point to the fact that this result has no contribution from the diagonal elements $H_{k,k}$, emphasizing the role of the interactions.

Following the same way we have done in section (3.3), we can define here a more general heat current\(^3\),

$$\frac{d\langle a_k^\dagger a_k \rangle}{dt} = i\langle [\mathcal{H}, a_k^\dagger a_k] \rangle = \sum_{\ell \neq k} j_{k,\ell},$$

where

$$j_{k,\ell} = -iH_{k,\ell} \left[ \langle a_{k} a_{\ell} \rangle - \langle a_{k}^2 \rangle \right] = -j_{\ell,k}.$$  \hspace{1cm} (4.34)

which allows to cast Eq. (4.31) in a more symmetric form

$$\Pi_{\text{NESS}} = \frac{1}{2} \sum_{k,\ell} j_{k,\ell} \left( \frac{1}{\bar{n}_k + 1/2} - \frac{1}{\bar{n}_\ell + 1/2} \right).$$

This result can be interpreted from the point of view of Onsager’s theory of irreversible thermodynamics [81, 83]. Within this framework, the entropy production is defined as the product of fluxes times affinities (also called generalized forces). For instance, the current of energy is related to the affinity $1/T$, so that in a classical scenario the Onsager entropy production between two bodies kept at temperatures $T_A$ and $T_B$ would be given by

$$\Pi = j_{AB} \left( \frac{1}{T_A} - \frac{1}{T_B} \right),$$

where $j_{AB}$ would be the current of energy from $B$ to $A$. We see that Eq. (4.35) has the exact same mathematical structure as Onsager’s formula, providing a strong physical justification for the use of the Wigner entropy production rate. Moreover, we also see that precisely due to the fact that we are using the Wigner entropy production rate, the thermodynamic affinity related to the current is not the temperature, but rather the Bose-Einstein occupation $\bar{n} + 1/2$. For high temperatures $\bar{n} + 1/2 \propto T$ so that both frameworks coincide. However, our result holds even in the limit of vanishingly small temperature, where $\bar{n} \to 0$ but the factor of $1/2$ nonetheless remains.

We also call attention to the fact that Onsager’s formula (4.36) is valid only for systems close to equilibrium (linear response theory), whereas Eq. (4.35) is true for states arbitrarily far from equilibrium. This is a consequence of the Gaussianity of the problem in question.

The non-negativity of the entropy production rate is reinforced by the fact that the current always flows from hot to cold, so that the sign of $j_{AB}$ will always be the same as $T_A^{-1} - T_B^{-1}$.

\(^3\text{It is more general because we are considering the Hamiltonian of Eq. (2.4), which allows no local correlations.}\)
Chapter 5

Quantifying the entropic cost of diffusivity

5.1 Total entropy production rate of a chain in NESS

We now illustrate the usefulness of our framework for the Wigner entropy production within the model solved in chapter 3. For simplicity, we will consider zero squeezing in the reservoirs. As we have mentioned, this model captures the essence of typical transport problems, presenting a ballistic or diffusive flow depending on parameters choice. Given that the diffusive regime emerges when noise is added to the system (for instance, by mean of self-consistent reservoirs), we address in this chapter the question of quantifying the irreversible cost of diffusivity.

Let us begin by calculating the total entropy production rate, which may be readily computed from Eq. (4.35). As the currents in Eq. (3.19) are translation invariant, all inner terms in the sum entering Eq. (4.35) vanish and we are left with

\[ \Pi_{\text{NESS}} = \frac{2 \lambda^2 \gamma (\bar{n}_L - \bar{n}_1)}{4 \lambda^2 + \gamma^2 + \gamma \Gamma (L - 1)} \left( \frac{1}{\bar{n}_1 + \frac{1}{2}} - \frac{1}{\bar{n}_L + \frac{1}{2}} \right). \] (5.1)

The entropy production rate is thus manifestly always non-negative and zero if and only if \( \bar{n}_1 = \bar{n}_L \), in which case there is no current flowing through the chain. We also remark the fact that \( \Pi_{\text{NESS}} \) does not depend on \( \bar{n}_k \), which is an important consistency check, as it is precisely the goal of the self-consistent reservoirs to make sure that no current flows through them. Concerning the ballistic vs. diffusive, we see that the entropy production rate behaves exactly like the current, being independent of \( L \) if \( \Gamma = 0 \) and of order \( 1/L \) for \( \Gamma \neq 0 \). It is also noteworthy that, fixing the temperature gradient, the ballistic irreversible entropy-production rate \( \Pi_{\text{NESS}}(\gamma, \Gamma = 0) \) is larger than the diffusive one \( \Pi_{\text{NESS}}(\gamma, \Gamma > 0) \). The reason for this behavior will be elucidate in section 39.
(6.5), where we show that the diffusive regime tends to a local equilibrium state and the ballistic doesn’t.

5.2 Entropy production rate from the physical and the self-consistent reservoirs

We now turn to what is one of the main advantages of our framework, namely that we are able to separate the contributions of the entropy production rate from each dissipation channel. More specifically, we separate the total entropy production rate into two contributions, one stemming from the real reservoirs at the boundaries \( \Pi_r \) and another from the auxiliary self-consistent reservoirs \( \Pi_{sc} \); viz.,

\[
\Pi = \Pi_r + \Pi_{sc}. \tag{5.2}
\]

From Eq. (4.20) we find that the contribution from the physical reservoirs, 1 and \( L \) reads

\[
\Pi_r = \frac{4}{\gamma(\bar{n}_1 + 1/2)} \int \frac{|\mathcal{J}_1(W)|^2}{W} \, d\xi + \frac{4}{\gamma(\bar{n}_L + 1/2)} \int \frac{|\mathcal{J}_L(W)|^2}{W} \, d\xi, \tag{5.3}
\]

where,

\[
\mathcal{J}_1(W) = \gamma \left[ \alpha_1 + (\bar{n}_1 + 1/2) \hat{\alpha}_1 W \right]. \tag{5.4}
\]

Similarly, the entropy production from the self-consistent reservoirs reads

\[
\Pi_{sc} = \sum_k \frac{4}{\Gamma(\langle a_k^\dagger a_k \rangle + 1/2)} \int \frac{|\mathcal{J}_k(W)|^2}{W} \, d\xi, \tag{5.5}
\]

with,

\[
\mathcal{J}_k(W) = \frac{\Gamma}{2} \left[ \alpha_k + (\langle a_k^\dagger a_k \rangle + 1/2) \hat{\alpha}_k W \right]. \tag{5.6}
\]

where we already used the fact that the occupations of the self-consistent reservoirs are \( \tilde{n}_k = \langle a_k^\dagger a_k \rangle \) [Eq. (3.9)].

Lastly, to facilitate the computation of Eqs. (5.3) and (5.5) we write the entropy production rate for the real and the self-consistent reservoirs in the terms of the covariance matrix. This is readily accomplished using Eq. (4.25). All we need to do is to adapt the notation to comply with the separation of the physical from the auxiliary baths. For the contribution to the real reservoir,
Eq. (5.3), we write it as $\Pi_r = \Pi_1 + \Pi_k$ where

$$\Pi_k = \Phi_k - \gamma + \gamma(\bar{n}_k + 1/2)(\Theta^{-1})_{2k,2k}, \quad k = 1, L,$$

(5.7)

where the entropy flux $\Phi_k$ is given by Eq. (4.23). Similarly, for the entropy production rate due to the self-consistent reservoirs, Eq. (5.5), we write $\Pi_{sc} = \sum_k \bar{\Pi}_k$ where

$$\bar{\Pi}_k = -\Gamma + \Gamma((\langle a_k^\dagger a_k \rangle + 1/2)(\Theta^{-1})_{2k,2k}), \quad k = 1, \ldots, L.$$

(5.8)

Here we already used the fact that the occupations number of the self-consistent reservoirs are cast to be $\bar{n}_k = \langle a_k^\dagger a_k \rangle$, so the entropy flux of the self-consistent reservoirs $\bar{\Phi}_k$, vanishes.

In Fig. (5.1) we plot $\Pi_r$ and $\Pi_{sc}$ as a function of $L$ in a logarithmic scale. Interestingly, we see that the irreversibility associated with the physical reservoirs is dominant only for small system size. As the chain is scaled up $\Pi_{sc}$ quickly surpasses $\Pi_r$ and adopts a distinct power-law-like decay $\Pi_{sc} \sim 1/L$ for large $L$. On the other hand—and also in the thermodynamic limit—we observe that the contribution from the real baths to the total steady-state irreversibility decays as $\Pi_r \sim 1/L^2$. The dependence on both $\gamma$ and $\Gamma$, although not explicit in Eqs. (5.3) and (5.5), arises from $W_{NESS}$.

We have thus seen that combining the ease of calculation of the Wigner entropy production for Gaussian states with our simple harmonic model to mimic diffusive heat conduction, provides valuable insights into the relative weight of the individual irreversible processes in the thermodynamic limit.

![Figure 5.1: The separate contributions of the entropy production rate from the real reservoirs ($\Pi_r$) and the self-consistent reservoirs ($\Pi_{sc}$), as a function of the system size $L$, for fixed $\gamma = 10^{-6}$, $\Gamma = 10^{-7}$, $\lambda = 3.10^{-7}$, $\bar{n}_1 = 1$ and $\bar{n}_L = 2$.](image)
Chapter 6

Quantifying shared information in Non-Equilibrium Steady States

6.1 Motivation

One aspect which still remains largely unexplored of Non-Equilibrium Steady States is the connection between transport of excitation and the correlations. After all, the existence of a heat current implies that the excitations moving through the system correlates one part to the other.

Since information does not satisfy a continuity equation we cannot define an information current. Instead, the question is more appropriately phrased in terms of the amount of information shared between different parts of a quantum chain. This shared information is mediated by the heat currents. However, the same reservoirs producing these currents will also in general cause decoherence, which tends to reduce correlations. This competition between heat currents and decoherence will eventually produce a NESS where different parts of the chain share a certain amount of information with each other (for an example, see Ref. [105]). The main goal of this chapter is to address how to quantify this amount of shared information. For a connected bipartition of the chain, the natural quantifier is the mutual information (MI). Conversely, motivated by some recent developments in the field of Quantum Markov chains [31–35], we show that for disconnected parts, the appropriate quantifier is actually the conditional mutual information (CMI) [36, 37] \( I(A : C|B) \), a more general measure of tripartite correlations.

It is worth pointing out that although there is an existing body of work on quantum state transfer in many-body systems [106–110], the NESS scenario that we focus here is fundament-
ally different. In quantum state transfer, the natural figure of merit is the fidelity between the initial sender state and the receiver state at some given time. In contrast, in a NESS scenario correlations appears due to a competition of two effects. On the one hand, the environments tend to cause decoherence [51]. On the other hand, a gradient of temperature (or any other excitation) will tend to induce currents, which is the cause of such correlations. This competition will lead to a NESS in which the different parts share some information (for an example, see Ref. [105]). Thus, we see that unlike in quantum state transfer, in the NESS context information transport cannot be characterized by any type of continuity equation. Instead, it must be characterized by the ability of one part to communicate information to another through the currents.

Finally, we apply these ideas to understand how the shared information within the chain is affected by different heat conduction regimes, using for it the soluble quantum lattice described in chapter 3.

6.2 Quantifying the information sharing:

We consider the NESS generated in a boundary-driven one-dimensional quantum chain, such as that depicted in Fig. (6.1 a).

![Diagram](image)

Figure 6.1: (a) A boundary-driven one-dimensional quantum chain subject to two thermal reservoirs at each end. (b) The information shared between $A$ and $C$, through a middle partition $B$, can be quantified using the conditional mutual information $I(A:C|B)$ defined in Eq. (6.3).

The basic assumptions are that the reservoirs act only locally on the end-points and the interaction Hamiltonian is short-ranged. We define $\mathcal{S} = \{1, \ldots, L\}$ as the set of sites of the chain and $\rho_{\mathcal{S}}$ as the global density matrix in the NESS. Moreover, given any subset $A \subset \mathcal{S}$ we define the reduced density matrix of that subset as $\rho_A = \text{tr}_{\mathcal{S}\setminus A} \rho_{\mathcal{S}}$, where $\mathcal{S}\setminus A$ stands for the partial trace over all sites that are not in the set $A$. The simplest approach to information sharing is to consider a bipartition of the chain in two halves $A = \{1, \ldots, k\}$ and $B = \{k + 1, \ldots, L\}$.
In this case the total amount of information shared between them is quantified by the mutual information (MI) [111]

\[ \mathcal{I}(A:B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}) \geq 0, \]  

(6.1)

where \( S(\rho) = -\text{tr}(\rho \ln \rho) \) is the von Neumann entropy. This quantity measures the amount of information (quantum and classical) contained in the global state \( \rho_{AB} \equiv \rho_S \), but which is missing in the marginalized state \( \rho_A \otimes \rho_B \). If \( \rho_{AB} \) is a pure state (which is seldom the case for NESSs), this reduces to twice the entanglement entropy. Similarly, if one is interested in multipartite systems, one may quantify the shared information using the so-called total correlations (TC) [112], defined as

\[ \mathcal{F} = \sum_{i=1}^{L} S(\rho_i) - S(\rho_S) \geq 0, \]  

(6.2)

where \( \rho_i \) is the reduced density matrix of site \( i \). This quantity is useful in understanding shared information from a global perspective, irrespective of how this information is locally distributed within the chain.

In this chapter, however, our main focus will be on how to quantify the information shared between two disconnected parts of the chain. That is, considering a tripartition \( ABC \), our goal is to address how to quantify the ability of the currents to mediate information between parts \( A \) and \( C \), passing through \( B \) (see Fig. (6.1 b)). It turns out that, for this task, the mutual information \( \mathcal{I}(A:C) \) is not appropriate. Instead, one should consider the conditional mutual information (CMI), [36, 37]

\[ \mathcal{I}(A:C|B) = S(\rho_{AB}) + S(\rho_{BC}) - S(\rho_{ABC}) - S(\rho_B) \geq 0. \]  

(6.3)

To elucidate why, let us first draw a connection with classical Markov chains [31, 35].

Consider a discrete time chain characterized by three random variables, \( X \to Y \to Z \). This process is called Markovian when there is no information flow from the past (\( X \)) to the future (\( Z \))

\[ P(Z|XY) = P(Z|Y). \]  

(6.4)

If we now calculate the joint probability distribution of \( Z \) and \( X \) given \( Y \), using the products
rule, we obtain


(6.5)

Thus, Eq. (6.5) motivates us to another definition of markovianity, as a process where the past \(X\) and the future \(Z\) are uncorrelated if we have knowledge of the present \(Y\). In this way, if we do not have information about \(Y\), then \(X\) and \(Z\) are correlated,

\[ P(X, Z) = \sum_Y P(X|Y)P(Z|Y)P(Y), \]  

(6.6)

so that, in general, \(I(X : Z) \neq 0\). The reason for this correlation lies solely on their common lack of information about \(Y\) and does not reflect, at all, the ability of \(X\) and \(Z\) to share information. Hence, \(I(X : Z)\) is not a proper quantifier of shared information. Instead, Markovianity is correctly quantified by the conditional mutual information of Eq. (6.3). First, for a Markovian system \(I(X : Z|Y) \equiv 0\) [33]. And second, for multi-step chains \(X_1, X_2, \ldots\), the dependence of the CMI on the size of the middle partition directly quantifies the degree of non-Markovianity [113] as it measures the extent of the chain’s memory.

The situation is entirely analogous to our problem. But instead of a probability distribution \(P(X, Y, Z)\), we now have a multi-site density matrix \(\rho\) of the NESS. Hence, the concept of time in our case is replaced by the site index \(i = 1, \ldots, L\) [31–35] (our chain does not have a well defined causal order). Notwithstanding this difference, the logic remains the same: the ability of the currents in sharing information between \(A\) and \(C\) is correctly captured by the CMI \(I(A : C|B)\) and not the MI. If \(I(A : C|B) = 0\) then no information is shared, while the dependence of \(I(A : C|B)\) on the size of \(B\) quantifies the robustness of the chain in sharing information, despite the noise in the channel. Another perspective to further clarify the meaning of the CMI is by means of the so-called chain rule [37]:

\[ I(A : C|B) = I(AB : C) - I(B : C). \]  

(6.7)

Thus, \(I(A : C|B)\) can be viewed as the difference between the total information shared between \(AB\) and \(C\) and the information that is shared only between \(B\) and \(C\) (or vice-versa).
6.3 Calculation of the entropy

We expose here a simple method to compute the von Neumann entropy for Gaussian states, in terms only of the symplectic eigenvalues [114].

The symplectic eigenvalues of a CM $\Theta$ are defined as

$$\{\nu_k\} = \text{eigs}_+(2\Sigma \Theta),$$  \hspace{1cm} (6.8)

where $\Sigma = I_L \otimes \sigma_z$ is the symplectic form related to our choice of structure for $\Theta$. Here, eigs$_+$ means selecting only the positive eigenvalues. The von Neumann entropy is then [45, 47]

$$S(\rho) = \sum_{k=1}^L \left( \frac{\nu_k + 1}{2} \ln \left( \frac{\nu_k + 1}{2} \right) - \frac{(\nu_k - 1)}{2} \ln \left( \frac{\nu_k - 1}{2} \right) \right).$$  \hspace{1cm} (6.9)

The same approach is used for considering any reduced density matrices. Recall that the reduced density matrix of a Gaussian state is also Gaussian and therefore has a CM which is simply obtained by dropping from $\Theta$ the elements one wishes to trace over.

Alternatively, since we are working with gaussian states, one could use the Rényi-2 entropy [115]$^1$, $S_2(\rho) = -\ln \text{tr}[\rho^2]$ to calculate informational-theoretical quantities. In the appendix A, we show that it can be written in terms of the CM as,

$$S_2(\rho) = L \ln(2) + \frac{1}{2} \ln |\Theta|. \hspace{1cm} (6.10)$$

In appendix B, we consider the particular form of the CM we are going to use as an application in next section and we obtain an analytically closed expression for its determinant for arbitrary L. However, such solution is given in terms of non-trivial functions and we could not simplify them to the point of we can understand its behavior. Thus, we have opted to use the standard and well known von-Neumann entropy.

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$^1$In this reference, Adesso et al. show that the Rényi-2 entropy satisfies the strong subadditivity inequality.
6.4 Analysis of the shared information in a Non-Equilibrium Steady State

We now move on to apply these concepts to the model solved in chapter 3. Let us begin our analysis by computing the mutual information $I(A:B)$ [Eq. (6.1)] for a symmetric bipartition at $L/2$. The results as a function of $L$, for different values of $\Gamma$, are shown in Fig. (6.2 a). As can be seen, $I(A:B)$ is independent of $L$ in the ballistic case ($\Gamma = 0$), but scales as $I(A:B) \sim 1/L^2$ in the diffusive case. In Fig. (6.2 b) we present for comparison the total correlations [Eq. (6.2)]. For ballistic transport the TC is an extensive quantity, scaling as $T \sim L$. Conversely, for diffusive transport we find $T \sim 1/L$. This decay of the amount of correlations as one approaches the thermodynamic limit was also found in Ref. [105] for 2-particle entanglement.

![Figure 6.2: (a) Log-log plot of the Mutual Information (MI) $I(A:B)$ [Eq. (6.1)] between two halves of the chain as a function of $L$, for different values of the self-consistent noise $\Gamma$. (b) Same but for the total correlations $T$ [Eq. (6.2)]. The curve for $\Gamma = 1$ was multiplied by $10^{-3}$ to improve visibility. In all curves we set $N_1 = 2$, $N_L = 1$ and $\gamma = \lambda = 1$.](image)

Next we turn to the CMI, which is summarized in Fig. (6.3). We focus on symmetric tripartitions $ABC$ with $b = |B|$ sites in the middle. As illustrated in Fig. (6.3 a), we find that in both regimes the CMI decays exponentially with $b$, as $I(A:C|B) = 1/R^b$, where $R$ is a constant that depends non-trivially on all parameters of the model. The dependence of the CMI on $L$ is shown in Fig. (6.3 b) for $b = 1$ and in Fig. 6.3(c) for multiple values of $b$. We find that for ballistic transport the CMI is independent of $L$, whereas for diffusive transport it scales as $I(A:C|B) \sim 1/L^{2b+2}$.
Figure 6.3: Conditional mutual information (CMI) $\mathcal{I}(A : C|B)$ [Eq. (6.3)] for a symmetric tripartition with the middle block having size $b = |B|$. (a) Log of the CMI as a function of $b$, for both the ballistic case ($\Gamma = 0$, solid lines) and diffusive case ($\Gamma = 0.1$, dashed lines), with different values of $N_I$ and fixed $L = 40$ and $N_L = 1$. In both cases the CMI behaves as $\mathcal{I}(A : C|B) \sim 1/R^b$, where $R > 1$ is a constant that depends on the temperature gradient. (b) Log-log plot of the CMI as a function of $L$ for $b = 1$. If $\Gamma = 0$ then $\mathcal{I}(A : C|B)$ is independent of $L$, whereas for $\Gamma \neq 0$ we get $\mathcal{I}(A : C|B) \sim 1/L^4$. (c) Log-log plot of the CMI vs. $L$ for different values of $b$ with $N_I = 15$, $N_L = 1$ and $\Gamma = 0.1$. For large $L$ the CMI scales as $\mathcal{I}(A : C|B) \sim 1/L^{2b+2}$. (d) Finite size scaling, Eq. (6.11), for two different values of $N_I$, with $N_L = 1$ and multiple values of $\Gamma$, $L$ and $b$. In all curves we set $\gamma = \lambda = 1$.

From these numerical simulations we therefore propose the following scaling law for the CMI:

$$\mathcal{I}(A : C|B) = \frac{u}{(v + \Gamma L)^{2b+2}},$$

(6.11)

where $u$ and $v$ are constants. The behavior also holds for $b = 0$, in which case one recovers the MI in Eq. (6.1). To confirm this scaling law behavior we present in Fig. (6.3 d) plots of
vs. $\Gamma L$ for different values of $\Gamma$, $L$ and $b$. According to Eq. (6.11), this should lead to a fully collapsed straight line, which is precisely what is observed.

Eq. (6.11) provides a full characterization of the information transport for the bosonic model described in chapter 3. It shows that the transport of information is exponentially suppressed by the size $b$ of the middle partition, for both ballistic and diffusive cases. However, in the diffusive case, this suppression is greatly enhanced by a factor depending on the size $L$ of the chain. Unfortunately, it is not possible to state whether such a scaling behavior is universal. It will quite likely be true for fermionic chains, in view of their similarity with the present model (c.f. Ref. [105]). There are rare situations, however, which could serve as counterexamples. One, for instance, is the spin helix model studied in Ref. [116], where in certain cases the NESS may be in a product state, despite having a non-zero current.

### 6.5 Local equilibration

As first put forth in Ref. [48], the behavior of the CMI can also shed light on questions concerning the Hilbert space tensor structure of the NESS and local equilibration. Motivated by this, we now show that the scaling rule (6.11) for the ballistic and diffusive scenarios can give precise information about how close the NESS is from local equilibrium. To accomplish this, we make use of a recently proved theorem by Kato and Brandão [33]. Let $\mathcal{S}_k$ denote the CMI with a tripartition at position $k$ and only 1 site in the middle. The authors have shown that if $\mathcal{S}_k < \epsilon$ for all $k$, then there exists a local Hamiltonian $H = \sum_i h_{i,i+1}$, acting only on sites $i, i+1$, such that

$$S\left(\rho, \frac{e^{-H}}{\text{tr} e^{-H}}\right) < \epsilon L,$$

(6.12)

where $S(\rho||\sigma) = \text{tr}(\rho \ln \rho - \rho \ln \sigma)$ is the quantum relative entropy. This means that states with vanishingly small $\mathcal{S}_k$ tend to be locally thermal (which includes the possibility of a site-dependent temperature, which we have incorporated into $h_{i,i+1}$).

Based on Eq. (6.11), with $b = 1$, we see that in the ballistic case $\mathcal{S}_k \sim L^0$, so that the NESS will in general be far from local equilibrium. However, in the diffusive case $\mathcal{S}_k \sim 1/L^4$ so that Eq. (6.12) scales as $1/L^3$. Hence, we see that in the diffusive case the NESS tends to a locally thermal state in the thermodynamic limit. This agrees with our macroscopic intuition that even though a system may be out of equilibrium it is still in a local equilibrium state, but with a position-dependent temperature.
This result therefore provides a direct application for the CMI in understanding local properties of NESSs.
Chapter 7

Conclusions

We have addressed the calculation of the irreversible entropy-production rate using a quantum phase-space approach based on the Wigner entropy. In particular, we focused on networks of weakly interacting harmonic nodes with arbitrary connectivity, and coupled to various reservoirs at different temperatures. For this wide class of systems, we were able to obtain simple and useful closed-form expressions for both the Wigner entropy-production rate and the entropy flux, solely in terms of the second-order moments of the system. This is possible since we work with an overall harmonic Hamiltonian, which preserves Gaussianity. In addition, we could split the entropy-production rate and flux into contributions stemming from individual quasi-probability currents associated with each open decay channel, which enables one to identify the irreversibility generated by a single bath in a multi-bath lattice. We also discussed how the internal coherent dynamics plays a central role in generating steady-state irreversibility, as it is the leading mechanism enabling energy transport across the network. Then, we used our framework to better understand the interplay between the various sources of irreversibility at play in diffusive heat conduction through a harmonic chain. We mimicked the anharmonicity required to establish the desired diffusive profile by adding auxiliary (self-consistent) reservoirs to our model. In turn, this allowed us to break down the total steady-state irreversible entropy production into a contribution due to the heat transport across the chain, and another one which can be interpreted as the entropic cost of maintaining a stationary diffusive transport. These results were addressed in the paper of Ref. [50].

We then turn to explore NESSs from an informational point of view. We have put forth a detailed study on the information sharing in non-equilibrium steady-states. First, we have shown that the conditional mutual information appears as a robust quantifier of the ability of
the chain to share information between different parts. We then applied this to the same exactly soluble model used above and obtained how the CMI scales with the system size and other relevant quantities, which is summarized by Eq. (6.11). Finally, we have showed how this type of knowledge may find applications in studies of local thermalization of non-equilibrium states, a topic which touches at the heart of many discussions in many-body and statistical physics. A paper (still in revision process) encompassing this second part also was performed [49].

From our studies, several natural questions emerge. The most basic is the aforementioned universality of the scaling (6.11). Another interesting question is how these results would be affected by anomalous diffusion (that is, in which $J \sim 1/L^\alpha$ for some exponent $\alpha$). By understanding what changes this would introduce in the scaling law (6.11), one could address the question of what is the critical value of $\alpha$ for which local equilibration breaks down.
Appendix A

Rényi-2 entropy for Gaussian systems

For Gaussian systems Rényi-2 entropy satisfies the strong subadditivity inequality [115], being able to be used as a suitable tool to calculate informational-theoretical quantities. In this appendix, we show that it can be directed related with CM’s determinant, which is an analytical advantage over the usual von-Neumann entropy.

Let us start this demonstration by writing the Rényi-2 entropy in terms of the system purity $P$,

$$S_2(\rho) = -\ln[\text{tr}(\rho^2)] = -\ln(P). \quad (A.1)$$

We will separate this demonstration in two steps. First, we obtain an expression that relate the purity with an integral of the Wigner function. Second, we solve this integral considering the particular structure of a Gaussian Wigner function.

A.1 The purity and the Wigner function

We can write the displacement operator of a coherent state in the following compact way,

$$D(\xi) = e^{R^t \Omega \xi}, \quad (A.2)$$

where $R$ is the $2L$ dimensional vector encompassing all bosonic operators (see Eq. (2.26)), $\xi$ the $2L$ dimensional vector of complex variables (see Eq. (4.3)) and $\Omega$ the $2L \times 2L$ symplectic
matrix (see Eq. (2.27)). As an example, for \( L = 2 \), we have that,

\[
\begin{pmatrix}
0 & 1 & 0 & 0 \\
-1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & -1 & 0
\end{pmatrix}
\begin{pmatrix}
\alpha_1 \\
\alpha_1^* \\
\alpha_2 \\
\alpha_2^*
\end{pmatrix}
= a_1^* \alpha_1 - a_1 \alpha_1^* + a_2^* \alpha_2 - a_2 \alpha_2^*, \tag{A.3}
\]

which allow us to write the displacement operator as

\[
D(\xi) = e^{a_1^* \alpha_1 - a_1 \alpha_1^* + a_2^* \alpha_2 - a_2 \alpha_2^*}
= D(\alpha_1)D(\alpha_2), \tag{A.4}
\]

that is nothing but the composition rule for two subsequent displacements.

We now define the Wigner function, as we have done in Eq. (4.2), but here in a more compact way making use of the above displacement operator\(^1\),

\[
W_\rho(\xi) = \frac{1}{\pi^{2L}} \int e^{k^{\dagger} \Omega \xi} \text{tr}[\rho D(k)] \, dk,
\tag{A.5}
\]

where \( k = (k_1, k_1^*, \ldots, k_L, k_L^*)^T \). Let us now introduce the quantity \( P_{12} \):

\[
P_{12} \equiv \pi^L \int W_\rho(\xi)W_\rho(\xi) \, d\xi. \tag{A.6}
\]

Thus, substituting Eq. (A.5) into Eq. (A.6), one may rewrite it in terms of the displacement operator,

\[
P_{12} = \frac{1}{\pi^{2L}} \int dk \, dq \, \text{tr}[\rho_1 D(k)] \text{tr}[\rho_2 D(q)] \int d\xi e^{(k+q)^{\dagger} \Omega \xi}.
\tag{A.7}
\]

Note that the integral over \( \xi \) is the integral representation of the dirac delta function in its complex form,

\[
\int d\xi e^{(k+q)^{\dagger} \Omega \xi} = \pi^{2L} \delta^2(k_1 + q_1) \cdots \delta^2(k_L + q_L),
\tag{A.8}
\]

where \( \delta^2(\alpha) \equiv \delta(\text{Re}[\alpha]) \delta(\text{Im}[\alpha]) \). Thus, Eq. (A.7) becomes,

\[
P_{12} = \frac{1}{\pi^L} \int dk \, dq \, \text{tr}[\rho_1 D(k_1, k_1^*, \ldots, k_L, k_L^*)] \text{tr}[\rho_2 D(q_1, q_1^*, \ldots, q_L, q_L^*)] \delta^2(k_1 + q_1) \cdots \delta^2(k_L + q_L)
= \frac{1}{\pi^L} \int dk \, \text{tr}[\rho_1 D(k)] \text{tr}[\rho_2 D(-k)].
\tag{A.9}
\]

\(^1\)Note that the integral is of over all phase space, \( dk = dk_1 dk_1^* \cdots, dk_L, dk_L^* \).
Furthermore, since we are using a coherent basis, the trace of an operator $\mathcal{O}$ is given by

$$\text{tr} [\mathcal{O}] = \frac{1}{\pi^L} \int d\gamma \langle \gamma_1 \ldots \gamma_L | \mathcal{O} | \gamma_1 \ldots \gamma_L \rangle,$$

(A.10)

where $\gamma = (\gamma_1, \gamma_1', \ldots, \gamma_L, \gamma_L')^2$. In this way, $P_{12}$ becomes

$$P_{12} = \frac{1}{\pi^L} \int dk d\eta \langle \gamma_1 \ldots \gamma_L | \rho_1 D(k) | \gamma_1 \ldots \gamma_L \rangle \langle \eta_1 \ldots \eta_L | \rho_2 D(k)^\dagger | \eta_1 \ldots \eta_L \rangle,$$

(A.11)

and making the integral over the variable $k$,

$$P_{12} = \frac{1}{\pi^L} \int d\gamma \langle \gamma_1 \ldots \gamma_L | \rho_1 \delta^3(\gamma_1 - \eta_1) \ldots \delta^3(\gamma_L - \eta_L) | \rho_2 | \eta_1 \ldots \eta_L \rangle$$

(A.12)

$$= \frac{1}{\pi^L} \int d\gamma \langle \gamma_1 \ldots \gamma_L | \rho_1 \rho_2 | \gamma_1 \ldots \gamma_L \rangle.$$

(A.13)

Finally, using again Eq. (A.10), we have that

$$P_{12} \equiv \pi^L \int W_{\rho_1}(\xi) W_{\rho_2}(\xi) d\xi = \text{tr}[\rho_1 \rho_2].$$

(A.14)

Then, taking $\rho_1 = \rho_2 = \rho$, we obtain an expression to calculate the state purity in terms of the Wigner function,

$$P = \text{tr}[\rho^2] = \pi^L \int W_{\rho}(\xi)^2 d\xi.$$  

(A.15)

### A.2 Purity of Gaussian states

Considering the particular case of Gaussian states, the Wigner function is completely characterized by the CM $\Theta$ and the vector of the means, $\mu$ (see Eq. (4.4)). Thus, the purity of Gaussian states, can be computed substituting Eq. (4.4) into Eq. (A.15) and solving the integral over the phase space,

$$P = \frac{1}{\pi^L |\Theta|} \int e^{-i(\xi - \mu)^\dagger \Theta^{-1}(\xi - \mu)} d\xi.$$

(A.16)

Since the CM is positive semi-definite, it can be decomposed using a triangular matrix $Q$,

$$\Theta = QQ^\dagger.$$  

(A.17)
Now, let us make a change of variables defining a vector $\lambda$ such that

$$Q\lambda = \xi - \mu.$$  \hspace{1cm} (A.18)

The differential then becomes,

$$d\xi = |Q|d\lambda = \sqrt{\Theta}d\lambda,$$  \hspace{1cm} (A.19)

and the purity in Eq. (A.16) turn into

$$P = \frac{1}{\pi^L \sqrt{|\Theta|}} \int d\lambda e^{-\lambda^\dagger \lambda},$$  \hspace{1cm} (A.20)

where, $\lambda^\dagger \lambda = \sum_{i=1}^{2L} |\lambda_i|^2 = 2 \sum_{i=1}^{L} |\lambda_i|^2$. The problem, is then reduced to a simple gaussian integral$^5$,

$$P = \int \frac{d\lambda}{\pi^L \sqrt{|\Theta|}} e^{-2\sum_{i=1}^{N} |\lambda_i|^2} = \frac{1}{\sqrt{|\Theta|}} \left( \frac{1}{\pi} \int e^{-2|\lambda_i|^2} d^2\lambda_i \right)^L = \frac{1}{2^L \sqrt{|\Theta|}}.$$  \hspace{1cm} (A.21)

### A.3 Entropy in term of the covariance matrix

Finally, taking the logarithm of the purity we obtain the desired expression relating the Rényi-2 entropy and the CM,

$$S_2(\Theta) = L \ln(2) + \frac{1}{2} \ln |\Theta|.  $$  \hspace{1cm} (A.22)

We here purposely wrote $S_2(\Theta)$, rather then $S_2(\rho)$, to emphases that a Gaussian system is completely determined by the CM.

Although this expression is very simple to be used, it is not straightforward to obtain a closed expression for CM’s determinant for arbitrary size $L$. We then address this problem in Appendix B, but considering the particular structure of the ballistic/diffusive CM described by Eqs. (3.8 - 3.10).

For simplicity, we will suppose no squeezing in the environments, allowing a full description of the CM in terms of the $C$ matrix (Eq. (2.30)). From Eq. (2.32) we have that,

$$\Theta = \left(C + \frac{I_2}{2} \otimes \sigma_+\sigma_-\right) + \left(C^T + \frac{I_2}{2} \otimes \sigma_-\sigma_+\right).$$  \hspace{1cm} (A.23)

$^5$We remain the notation of the main text, $d^2\lambda_i \equiv d\lambda_i d\lambda_i^*$.  

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which motivates the definitions of a new matrix $\tilde{C}$ as,

$$
\tilde{C} = \frac{I_L}{2} + C.
$$

(A.24)

Considering the particular model we have studied in chapter 3, the new covariance matrix $\tilde{C}$ will also be given by Eqs. (3.8 - 3.10), with exception of the diagonal terms,

$$
\tilde{C}_{ii} = \langle a_i^\dagger a_i \rangle + \frac{1}{2} = \frac{1}{2} + \frac{N_1 + N_L}{2} + \frac{1}{2} \frac{\gamma(N_1 - N_L)}{4\lambda^2 + \gamma^2 + \gamma \Gamma(L - 1)} \Gamma(L - 2i + 1)
$$

$$
+ \frac{1}{2} \frac{\gamma^2(N_1 - N_L)}{4\lambda^2 + \gamma^2 + \gamma \Gamma(L - 1)} (\delta_{i,1} - \delta_{i,L}).
$$

(A.25)

Now, we can write a simple expression to relate the determinant of $\Theta$ with the determinant of $\tilde{C}$,

$$
|\Theta| = |\tilde{C}|^2,
$$

(A.26)

and the Rényi-2 entropy then becomes,

$$
S_2(\tilde{C}) = L \ln(2) + \ln |\tilde{C}|.
$$

(A.27)

Thus, the problem is reduced to find a closed formula for the determinant of the tridiagonal $L \times L$, $\tilde{C}$ matrix.

### A.4 Characterizing correlations in terms of the covariance matrix

Once correlations are always between two or more partitions it is necessary to know how to characterize the state of a subsystem. For Gaussian systems, any subsystem is Gaussian and is given by the correspondent partition of the CM. In practice, it means we have to throw away all the rows and columns that do not belong to the modes in question.

As an example, let us consider a Gaussian system composed by 6 modes,
If one defines a partition $A$ composed by the first two modes and a partition $B$ by the others, the reduced CMs would be written as,

$$\tilde{C}_{1,2} = \begin{pmatrix} a_1 & x & 0 & 0 & 0 & 0 \\ x & a_2 & x & 0 & 0 & 0 \\ 0 & x & a_3 & x & 0 & 0 \\ 0 & 0 & x & a_4 & x & 0 \\ 0 & 0 & 0 & x & a_5 & x \\ 0 & 0 & 0 & 0 & x & a_6 \end{pmatrix}, \quad (A.28)$$

$$\tilde{C}_{3,6} = \begin{pmatrix} a_3 & x & 0 & 0 \\ x & a_4 & x & 0 \\ 0 & x & a_5 & x \\ 0 & 0 & x & a_6 \end{pmatrix}, \quad (A.29)$$

where from now on we will denote $M_{i,j}$ the block of a matrix $M$ composed by the modes $i$ to $j$.

Now, we are in position to redefine the Mutual Information (Eq. (6.1)) and the Conditional Mutual Information (Eq. (6.3)) in terms of the Rényi-2 entropy and consequently to the CM’s determinant. Starting with the MI we have that,

$$I_2(A : B) = S_2(\rho_A) + S_2(\rho_B) - S_2(\rho_{AB}) \geq 0. \quad (A.30)$$

If we consider the partition $A$ is composed by modes $\{1, \ldots, k\}$ and $B$ by $\{k + 1, \ldots, L\}$, using the above notation and Eq. (A.27), one may obtain that,

$$\mathcal{J}_2(A : B) = \ln \left( \frac{|\tilde{C}_{1,k+1,L}|}{|\tilde{C}_{1,k+1,L}|} \right). \quad (A.31)$$
Analogously, we can obtain the following expression for the CMI,

\[ \mathcal{J}_2(A : C | B) = S_2(\rho_{AB}) + S_2(\rho_{BC}) - S_2(\rho_{ABC}) - S_2(\rho_B), \]  

(A.32)

\[ = \ln \left( \frac{|C_{1,l} \parallel C_{k+1,l}|}{|C_{1,l} \parallel C_{k+1,l}|} \right), \]  

(A.33)

where we have partitioned the system in the following way,

\[ A = \{1, \ldots, k\}, \quad B = \{k + 1, \ldots, l\} \quad \text{and} \quad C = \{l + 1, \ldots, L\}. \]  

(A.34)
Appendix B

Tridiagonal matrices’ determinants

In this appendix we will develop analytical expressions for matrix’ determinants for arbitrary size. Motivated by the structure of the ballistic/diffusive CM used in the main text, we will consider only tridiagonal matrices with off-diagonal constant. We will denote them by $D_L$, with the sub-index $L$ being the dimension of the matrix.

For instance, if $L = 5$, we have that

$$D_5 = \begin{pmatrix} a_1 & z & 0 & 0 & 0 \\ z & a_2 & z & 0 & 0 \\ 0 & z & a_3 & z & 0 \\ 0 & 0 & z & a_4 & z \\ 0 & 0 & 0 & z & a_5 \end{pmatrix},$$  \hspace{1cm} (B.1)

where, for now $a_i$ are arbitrary and $z$ a constant. We then can define a new matrix $T_L$, with diagonal elements $b_i = \frac{a_i}{z}$ ($i = 1, \ldots, L$), by placing the off-diagonal as a common factor,

$$D_L = zT_L.$$  \hspace{1cm} (B.2)
Turning back to our example of $L = 5$ we have that,

$$T_5 = \begin{pmatrix}
    b_1 & 1 & 0 & 0 & 0 \\
    1 & b_2 & 1 & 0 & 0 \\
    0 & 1 & b_3 & 1 & 0 \\
    0 & 0 & 1 & b_4 & 1 \\
    0 & 0 & 0 & 1 & b_5 \\
  \end{pmatrix}$$

where $b_i = \frac{a_i}{z}.$  \hfill (B.3)

Furthermore, the following relation for the determinants holds,

$$|D_L| = z^L |T_L|.$$  \hfill (B.4)

Thus, the problem is reduced to find an expression for $|T_L|.$

Let us consider now the Laplace expansion for a determinant,

$$f_n = b_n f_{n-1} - f_{n-2},$$  \hfill (B.5)

where,

$$f_n = |T_n|, \quad f_0 = 1 \quad \text{and} \quad f_1 = \frac{a_1}{z}.$$  \hfill (B.6)

Thus, we propose to figure out the problem by solving the recurrence relation of Eq. (B.5), considering two particular structures. The first is the Toeplitz one (diagonal constant) and the second considering linear diagonal. Less than boundary terms (which we will later consider), they represent the two regime ballistic and diffusive studied in main text.

### B.1 Tridiagonal Toeplitz matrix

We consider here the tridiagonal matrix (as in Eq. (B.3)), but with constant diagonal, $b_i \equiv b.$ Thus, the recurrence relation of Eq. (B.5) becomes,

$$f_n = b f_{n-1} - f_{n-2}.$$  \hfill (B.7)
This is now comparable with the recurrence relation for Chebyshev-U polynomials,

\[ U_{n+1}(x) = 2xU_n(x) - U_{n-1}(x), \quad (B.8) \]

where,

\[ U_1(x) = 2x \quad \text{and} \quad U_0(x) = 1. \quad (B.9) \]

Then, the solution of Eq. (B.7) can be given in terms of the Chebyshev-U polynomials,

\[ f_L = U_L(b/2). \quad (B.10) \]

Fortunately, these polynomials have a closed formula,

\[ f_L \equiv |T_L| = \frac{\sinh((L + 1)\theta)}{\sinh(\theta)}, \quad \text{with} \quad \theta = \text{arcosh}(b/2). \quad (B.11) \]

If one is interested in the thermodynamic limit (large \( L \)), we can expand the hyperbolic sine as,

\[ \sinh((L + 1)\theta) \approx \frac{e^{L\theta}}{2}, \quad (B.12) \]

then, the determinant becomes

\[ |T_L| \approx \frac{e^{L\theta}}{2 \sinh(\theta)}. \quad (B.13) \]

Furthermore, if \( T_L \) is a CM and one is interested to calculate Rényi-2 entropy (Eq. (A.22)) in the thermodynamic limit, a linear scaling is obtained\(^1\),

\[ S_2(T_L) = L \ln(2) + \frac{1}{2} \ln |T_L| \approx \left( \frac{1}{2} \text{arcosh}(b/2) + \ln(2) \right) L. \quad (B.14) \]

## B.2 Linear diagonals

Let us now suppose that the diagonal of \( D_L \) is linear,

\[ a_i = \alpha + \beta i, \quad (B.15) \]

\(^1\)Since we are considering large \( L \) we have neglected the term \( \ln(2 \sinh(\theta)) \).
where $\alpha$ and $\beta$ are constants. Thus, the recurrence Eq. (B.5) becomes,

$$f_n = (A + Bn)f_{n-1} - f_{n-2}, \quad (B.16)$$

where,

$$f_1 = A + B, \quad f_0 = 1, \quad A = \frac{\alpha}{z}, \quad B = \frac{\beta}{z}. \quad (B.17)$$

Recurrence relations of this sort are related to Bessel functions. Indeed, one may verify that,

$$f_L = \pi B \left[ J_{1+L+A/B}(2/B)Y_{A/B}(2/B) - J_{A/B}(2/B)Y_{1+L+A/B}(2/B) \right], \quad (B.18)$$

where $J_n(x)$ and $Y_n(x)$ are the Bessel functions of first and second kind, respectively. In order to simplify the notation, let us define the functional,

$$F(L, A, B) = \pi B \left[ J_{1+L+A/B}(2/B)Y_{A/B}(2/B) - J_{A/B}(2/B)Y_{1+L+A/B}(2/B) \right]. \quad (B.19)$$

Thus, we have that

$$f_L = |T_L| = F(L, A, B) \quad (B.20)$$

### B.3 Dealing with boundary effects

Looking carefully to the diagonal of the CM in Eq. (A.25), we see that there is an extra term in the elements $\tilde{C}_{11}$ and $\tilde{C}_{LL}$. Thus, to apply the results obtained in Eq. (B.11) and Eq. (B.20) to the CM of the ballistic/diffusive model, we need to make some adjusts.

We may then rewrite the recurrence relation of Eq. (B.7) as the “bottom-up Laplace expansion” and the “top-down Laplace expansion”\(^2\),

$$|T_{1,L}| = b_L|T_{1,L-1}| - |T_{1,L-2}|, \quad (B.21)$$

$$|T_{1,L}| = b_1|T_{2,L}| - |T_{3,L}|. \quad (B.22)$$

\(^2\)We will use the notation fixed in the example of Eq. (A.29).
Thus, using Eq. (B.21) and Eq. (B.22), we can find formulas for $|T_{i,f}|$ and $|T_{1,f}|$ respectively,

$$|T_{i,f}| = b_1|T_{2,f}| - |T_{3,f}|, \quad f \neq L,$$

(B.23)

$$|T_{i,L}| = b_L|T_{i,L-1}| - |T_{i,L-2}|, \quad i \neq 1.$$  

(B.24)

Now the matrices $T_{2,f}, T_{3,f}, T_{i,L-1}$ and $T_{i,L-2}$ no longer have boundary terms and their determinants can be expressed in terms of the Chebyshev-U polynomials (Eq. (B.11)) or Bessel functions (Eq. (B.20)). Finally, combining Eq. (B.21) with Eq. (B.22), we obtain the solution for the role matrix $T_{1,L}$,

$$|T_{1,L}| = b_1b_L|T_{2,L-1}| - b_L|T_{3,L-1}| - b_1|T_{2,L-2}| + |T_{3,L-2}|.$$  

(B.25)

It is also worth noting that

$$|D_{i,f}| = z^{f-i+1}|T_{i,f}|, \quad i, f = 1, \ldots, L.$$  

(B.26)

### B.4 Connection with the ballistic and diffusive covariance matrix

Although the model we have considered in chapter 3 can be switched from ballistic to diffusive transport just by changing some parameters, we could have considered here only the solution for linear diagonals (Eq. (B.20)) and deal with the ballistic regime as a particular case. However, because (we think) it is not trivial to obtain the Chebyshev-U polynomials from Bessel functions, we have opted to deal with each case separately.

As we have seen in sections A.3 and A.4, the Rényi-2 entropy, the Mutual Information and the Conditional Mutual Information are given in terms of determinants of $\tilde{C}$ (defined in Eqs. (A.24), (A.25), and (3.10)). Thus, in the following two subsection we obtain these determinants in terms of the Chebyshev-U polynomials or Bessel functions.

#### B.4.1 Ballistic transport

A ballistic transport can be obtained by throwing away the auxiliary self-consistent reservoirs, that is, taking $\Gamma \rightarrow 0$ - see section 3.4 - in the $\tilde{C}$ matrix. Thus, using the solution for Toeplitz
matrices (Eq. (B.11)) and Eqs. (B.23 - B.26), one may obtain the following results,

\[ |\tilde{C}_{i,f}| = x^{f-i+1} U_{f-i+1}(a/2x), \quad 1 < i < f < L, \]  
(B.27)

\[ |\tilde{C}_{1,f}| = x^f \left[ \frac{a_1}{x} U_{f-1}(a/2x) - U_{f-2}(a/2x) \right], \quad f < L, \]  
(B.28)

\[ |\tilde{C}_{i,L}| = x^{L-i+1} \left[ \frac{a_L}{x} U_{L-1}(a/2x) - U_{L-2}(a/2x) \right], \quad i > 1, \]  
(B.29)

\[ |\tilde{C}_{1,L}| = x^L \left[ \frac{a_1 a_L}{x^2} U_{L-2}(a/2x) - \frac{a_1}{x} U_{L-3}(a/2x) + \frac{a_L}{x} U_{L-4}(a/2x) \right], \]  
(B.30)

where,

\[ a_k = \tilde{C}_{kk} = \frac{1}{2} + \frac{N_1 + N_L}{2} + (\delta_{1,k} - \delta_{L,k}) \frac{1}{2} \frac{\gamma^2 (N_1 - N_L)}{4 \lambda^2 + \gamma^2}, \quad k = 1, \ldots, L., \]  
(B.31)

and \( x \) is given by Eq. (3.10).

**B.4.2 Diffusive transport**

Now, considering the general case (\( \Gamma \neq 0 \)), we will use the solution of Eq. (B.20) for the matrix determinant. However, it will be necessary to generalize it to calculate the determinant of blocks, that is,

\[ |T_{i,f}| = F(f - i + 1, A_i, B), \quad 1 < i < f < L, \]  
(B.32)

where \( T_{i,f} \) is a matrix with dimension \( f - i + 1 \) and diagonals \( b_n \),

\[ b_n = \tilde{C}_{n+i-1,n+i-1} = A + Bn, \quad n = 1, \ldots, f - i + 1, \]  
(B.33)

with \( x \) being given by Eq. (3.10). Therefore, using Eq. (A.25), we have that \( A \) is going to depend of \( i \),

\[ A_i = \lambda \Gamma (i - 1) + \left( \frac{1}{2x} + \frac{N_1 + N_L}{2x} - \lambda \Gamma (L + 1) \right), \quad B = \lambda \Gamma. \]  
(B.34)

and \( x \) is given by Eq. (3.10).
Thus, by Eqs. (B.23 - B.26) we obtain,

\[
|\tilde{C}_{i,f}| = x^{f-i+1} F(f - i + 1, A_i, B), \quad 1 < i < f < L, \quad (B.35)
\]

\[
|\tilde{C}_{1,f}| = x^f \left[ \frac{\tilde{C}_{11}}{x} F(f - 1, A_2, B) - F(f - 2, A_3, B) \right], \quad 1 < f < L, \quad (B.36)
\]

\[
|\tilde{C}_{i,L}| = x^{L-i+1} \left[ \frac{\tilde{C}_{LL}}{x} F(L - i, A_i, B) - F(L - i - 1, A_i, B) \right], \quad 1 < i < L, \quad (B.37)
\]

\[
|\tilde{C}_{1,L}| = x^L \left[ \frac{\tilde{C}_{11}}{x^2} F(L - 2, A_2, B) - \frac{\tilde{C}_{LL}}{x} F(L - 3, A_3, B) \right. \\
\left. - \left[ \frac{\tilde{C}_{11}}{x} F(L - 3, A_2, B) - F(L - 4, A_3, B) \right] \right]. \quad (B.38)
\]

**B.5 Entropy, Mutual Information and Conditional Mutual Information**

Finally, we can use Eqs. (B.27-B.30) and Eqs. (B.35-B.38) to write closed expressions for the Rényi-2 entropy (Eq. (A.27)), the Mutual Information (Eq. (A.31)) and the Conditional Mutual Information (Eq. (A.33)). The results are going to be shown in terms of the Chebyshev-U polynomials or Bessel functions. Unfortunately, we could not express the results in terms of trivial functions\(^3\), which motivate us to use the well known Von-Neumann entropy in the main text.

\(^3\)Maybe if one take \(L\) large it is possible to use some asymptotic expressions.
Bibliography


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