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Linear Quantum Entropy and Non-Hermitian Hamiltonians

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Academic Editor: Ignazio Licata

Received: 18 October 2016; Accepted: 13 December 2016; Published: 16 December 2016

Abstract: We consider the description of open quantum systems with probability sinks (or sources) in terms of general non-Hermitian Hamiltonians. Within such a framework, we study novel possible definitions of the quantum linear entropy as an indicator of the flow of information during the dynamics. Such linear entropy functionals are necessary in the case of a partially Wigner-transformed non-Hermitian Hamiltonian (which is typically useful within a mixed quantum-classical representation). Both the case of a system represented by a pure non-Hermitian Hamiltonian as well as that of the case of non-Hermitian dynamics in a classical bath are explicitly considered.

Keywords: non-Hermitian quantum mechanics; quantum entropy; quantum-classical theory

1. Introduction

The study of open quantum systems is one of the fundamental problems of modern physics [1,2]. An open quantum system consists of a region of space where quantum processes take place (and which can be studied by the experimenter) in contact with a decohering and dissipative environment that is typically beyond the control of the experimenter. Various instances of concrete open quantum systems can be found in different areas of physics such as, for example, quantum optics, atomic and mesoscopic physics, biophysics or, at even shorter distances, nuclear physics. The interdisciplinary character of the theory of open quantum systems calls for a variety of different approaches. Here, we are concerned in particular with a formalism that adopts non-Hermitian Hamiltonian operators, a theoretical approach that is routinely called non-Hermitian quantum mechanics [3]. The description of open quantum systems in terms of non-Hermitian Hamiltonians [4] can be rigorously derived, in the case of a localised quantum subsystem coupled to a continuum of scattering states, by means of the Feshbach projection formalism [5–7]. Such an approach has been successfully employed to illustrate the complexities of exceptional points, which do occur when resonances coalesce in a non-avoided crossing [4]. When one uses the full non-Hermitian Hamiltonian, left and right eigenvectors [8–10] must be distinguished. From this perspective, the occurrence of exceptional points may create problems for defining the density matrix. On the other side, one can always use a Hermitian basis (which, for example, but not necessarily, arises from the Hermitian part of the full non-Hermitian operators) to represent non-Hermitian operators and the density matrix. From such a vantage point, the coalescence of the eigenvalues of the non-Hermitian Hamiltonian appears to be a foregoer of such major problems. It is worth mentioning that non-Hermitian Hamiltonians also appear in parity-time (PT) symmetric generalisations of quantum mechanics [11,12]. Such theories have recently found concrete applications in lossy optical waveguides [13,14] and photonic lattices [15,16].

However, we are interested here in open systems that can be effectively described by non-Hermitian Hamiltonians that are not necessarily PT-symmetric (and which, for such a reason, will be called general in the rest of this paper). For such Hamiltonians, it has been shown how to define a proper statistical mechanics [17] in order to study the behaviour of non equilibrium averages (e.g., the purity of quantum states [18]) and to provide the definition of correlation functions [19].

In order to try to build possible measures of quantum information [20–22] for systems with general non-Hermitian Hamiltonians, one can start by defining an entropy functional [23,24]. To this end, a non-Hermitian generalisation of the von Neumann entropy has been introduced in [25]. Nevertheless, entropies of the von Neumann form cannot be used when quantum theory is formulated by means of the Wigner function [26]. Since the (partial) Wigner representation is particularly useful in order to derive a mixed quantum-classical description of non-Hermitian systems [27], it becomes interesting to study the properties of the so-called linear entropy [26,28,29] and its generalisation to the case of open quantum systems described by general non-Hermitian Hamiltonians. To this end, we present in this paper, for the first time to our knowledge, a generalisation of the entropy for systems with non-Hermitian Hamiltonians that must be adopted when there is an embedding of the quantum subsystem in phase space. We associate the term "linear" to such an entropy as it arises from its first appearance in the literature [26,28,29].

This paper is organised as follows. In Section 2, we summarise the results of the density-matrix approach [17–19,25] to non-Hermitian dynamics that are useful for the study and generalisation of the linear entropy [26,28,29]. In particular, we introduce the equations of motion for the density matrices [17] and the von Neumann-like entropies studied in [25]. In Section 3, we study the linear entropy and its non-Hermitian generalisation, along the lines followed in [25]. Analytical solutions are given in the basic case of a constant decay operator. It is worth noting that even basic models with constant decay operators become interesting when one adds the additional level of complexity provided by the classical-like environment represented by means of the partially Wigner-transformed Hermitian part of the Hamiltonian. In order to fix the ideas, one can think of a light-emitting quantum dot coupled to an energy-absorbing optical guide in a classical environment, which introduces thermal fluctuations or some other type of noise. It is not even difficult to imagine how models like these one can be made more and more complex within our approach. In Section 4, we briefly recall how to formulate the dynamics of a non-Hermitian system that is embedded in a classical bath of degrees of freedom. In Section 5, we study the behaviour of the linear entropy and its non-Hermitian generalisation in a quantum-classical set-up. Once again, analytical solutions are provided for the case of a constant decay operator. Finally, our conclusions are presented in Section 6.

2. Quantum Dynamics with Non-Hermitian Hamiltonians

Let us consider a non-Hermitian Hamiltonian composed of two terms:

$$\hat{\mathcal{H}} = \hat{H} - i\hat{\Gamma} \ . \tag{1}$$

Both operators on the right-hand side, $\hat{H}$ and $\hat{\Gamma}$, are Hermitian; $\hat{\Gamma}$ is often called the decay rate operator. The quantum states $|\Psi\rangle$ and $\langle\Psi|$ evolve according to the Schrödinger equations

$$\partial_t|\Psi\rangle = -\frac{i}{\hbar}\hat{\mathcal{H}}|\Psi\rangle = -\frac{i}{\hbar}\hat{H}|\Psi\rangle - \frac{1}{\hbar}\hat{\Gamma}|\Psi\rangle \ , \tag{2}$$

$$\partial_t\langle\Psi| = \frac{i}{\hbar}\langle\Psi|\hat{\mathcal{H}}^\dagger = \frac{i}{\hbar}\langle\Psi|\hat{H} - \frac{1}{\hbar}\langle\Psi|\hat{\Gamma}. \tag{3}$$

On conceptual grounds, we can expect that the open quantum system dynamics produces statistical mixtures. Indeed, we have shown that the purity is not conserved [17,18]. Defining the non-normalised density matrix as

$$\hat{\Omega} = \sum_k \mathcal{P}_k|\Psi^k\rangle\langle\Psi^k| \ , \tag{4}$$

where $(|\Psi^k\rangle, \langle\Psi^k|)$ are the eigenstates of any good *Hermitian* operator that can cover the Hilbert space of the system and $\mathcal{P}_k$ is their probability of occurrence, the equation of motion can be written as

$$\partial_t\hat{\Omega} = -\frac{i}{\hbar}\left[\hat{H},\hat{\Omega}\right]_- - \frac{1}{\hbar}\left[\hat{\Gamma},\hat{\Omega}\right]_+ , \tag{5}$$

with $[\, , \,]_-$ and $[\, , \,]_+$ denoting the commutator and anticommutator, respectively. Equation (5) effectively describes the subsystem (with Hamiltonian $\hat{H}$) coupled to the environment (represented by $\hat{\Gamma}$). It is worth remarking again and explicitly that, in our approach [17,19,25,27], we use Hermitian basis sets to represent the equations of motion. This situation is commonly found when, for example, the non-Hermitian creation and destruction operators, $\hat{a}$ and $\hat{a^\dagger}$, respectively, are represented in the basis of the Hermitian number operator. It should be evident that, because of this, we do not need to worry about the left/right eigenvectors of the full non-Hermitian Hamiltonian [30,31].

Non-Hermitian dynamics do not conserve the probability. This can be easily seen by taking the trace of both sides of Equation (5):

$$\partial_t \mathrm{Tr}\,\hat{\Omega} = -\frac{2}{\hbar}\mathrm{Tr}\left(\hat{\Gamma}\,\hat{\Omega}\right) . \tag{6}$$

However, we can define a normalised density matrix [17] as

$$\hat{\rho} = \frac{\hat{\Omega}}{\mathrm{Tr}\,\hat{\Omega}} . \tag{7}$$

The density matrix in Equation (7) can be used in the calculation of statistical averages: $\langle\chi\rangle_t = \mathrm{Tr}\left(\hat{\chi}\hat{\rho}(t)\right)$, where $\hat{\chi}$ is an arbitrary operator. The normalised density matrix $\hat{\rho}$ obeys the equation [17]:

$$\partial_t\hat{\rho} = -\frac{i}{\hbar}\left[\hat{H},\hat{\rho}\right]_- - \frac{1}{\hbar}\left[\hat{\Gamma},\hat{\rho}\right]_+ + \frac{2}{\hbar}\hat{\rho}\,\mathrm{Tr}(\hat{\Gamma}\hat{\rho}) . \tag{8}$$

Similarly to Equation (5), Equation (8) effectively describes the evolution of the subsystem coupled to the environment; the role of the third term on the right-hand side is to conserve the probability during the dynamics. Equation (8) is nonlinear. This property was also noted when considering operator averages in [32]). Within the Feshbach–Fano projection formalism, the nonlinearity of the non-Hermitian approach has been suggested in [33] as well. While the density operator $\hat{\rho}$ is bounded and useful in the calculation of of the statistical averages, the gain or loss of probability of open systems are properly described by the non-normalised density operator $\hat{\Omega}$. Hence, it turns out that both $\hat{\Omega}$ and $\hat{\rho}$ are useful in the non-Hermitian formalism [19,25].

The normalised density matrix $\hat{\rho}$ allows us to define [25] the von Neumann entropy of a non-Hermitian system as

$$S_{\mathrm{vN}} \equiv -k_B\left\langle \ln\hat{\rho}\right\rangle = -k_B\mathrm{Tr}\left(\hat{\rho}\ln\hat{\rho}\right) . \tag{9}$$

The rate of the von Neumann entropy production is [25]:

$$\partial_t S_{\mathrm{vN}} = \frac{2k_B}{\hbar}\mathrm{Tr}\left(\hat{\Gamma}\hat{\rho}\ln\hat{\rho}\right) + \frac{2}{\hbar}\mathrm{Tr}\left(\hat{\Gamma}\hat{\rho}\right)S_{\mathrm{vN}}. \tag{10}$$

However, the gain or loss of information in a non-Hermitian system are more properly represented by introducing another entropy, given by the statistical average of the logarithm of the *non-normalised* density operator [25]:

$$S_{\mathrm{NH}} \equiv -k_B\langle\ln\hat{\Omega}\rangle = -k_B\mathrm{Tr}(\hat{\rho}\ln\hat{\Omega}) = -k_B\frac{\mathrm{Tr}(\hat{\Omega}\ln\hat{\Omega})}{\mathrm{Tr}\,\hat{\Omega}} . \tag{11}$$

The rate of change of S_{NH} is [25]

$$\partial_t S_{\mathrm{NH}} = \frac{2k_B}{\hbar}\mathrm{Tr}\left(\hat{\Gamma}\hat{\rho}\ln\hat{\Omega}\right) + \frac{2}{\hbar}\mathrm{Tr}\left(\hat{\Gamma}\rho\right)S_{\mathrm{NH}} + 2\frac{k_B}{\hbar}\mathrm{Tr}\left(\hat{\Gamma}\hat{\rho}\right) , \tag{12}$$

while the difference between the two entropies reads

$$S_{\rm vN} - S_{\rm NH} = k_{\rm B} \ln \left({\rm Tr}\, \hat{\Omega} \right) \ . \tag{13}$$

The fact that the $S_{\rm NH}$ entropy captures the expected physical behaviour of the flow of information out of an open system can be seen by considering the models where $\hat{H}$ is an arbitrary self-adjoint operator while $\hat{\Gamma}$ is proportional to the identity operator:

$$\hat{\Gamma} = \frac{1}{2} \hbar \gamma_0 \hat{I} \ , \tag{14}$$

where the parameter γ_0 is assumed to be real-valued. For such models, after imposing the initial conditions ${\rm Tr}\, \hat{\Omega}(0) = 1$, we obtain [25]:

$$\begin{aligned} {\rm Tr}\, \hat{\Omega}(t) &= \exp\left(-\gamma_0 t\right) , && (15) \\ S_{\rm vN}(t) &= S_{\rm vN}^{(0)} = {\rm const} \ , && (16) \\ S_{\rm NH}(t) &= S_{\rm vN}^{(0)} + k_{\rm B} \gamma_0 t \ . && (17) \end{aligned}$$

One can then see that, for positive values of γ_0, the $S_{\rm NH}$ entropy diverges at large times, as a good entropy functional of an open system is expected to do. On the contrary, the von Neumann entropy $S_{\rm vN}$ is always constant.

3. Non-Hermitian Dynamics and Quantum Linear Entropy

The quantum linear entropy is

$$S_{\rm lin} = 1 - {\rm Tr}\left[\hat{\rho}^2(t) \right] . \tag{18}$$

The entropy production is

$$\dot{S}_{\rm lin} = -2{\rm Tr}\left[\hat{\rho}(t) \frac{\partial \hat{\rho}(t)}{\partial t} \right] \ . \tag{19}$$

Substituting Equation (8) in Equation (19) and using the following identities

$$\begin{aligned} {\rm Tr}\left[\hat{\rho}\hat{H}\hat{\rho} - \hat{\rho}\hat{\rho}\hat{H} \right] &= {\rm Tr}\left[\hat{\rho}^2\hat{H} - \hat{\rho}^2\hat{H} \right] = 0 \ , && (20) \\ {\rm Tr}\left[\hat{\rho}\hat{\Gamma}\hat{\rho} + \hat{\rho}\hat{\rho}\hat{\Gamma} \right] &= 2{\rm Tr}\left[\hat{\Gamma}\hat{\rho}^2 \right] \ , && (21) \end{aligned}$$

we obtain

$$\dot{S}_{\rm lin} = \frac{4}{\hbar} {\rm Tr}\left[\hat{\Gamma}\hat{\rho}^2(t) \right] - \frac{4}{\hbar} {\rm Tr}\left[\hat{\Gamma}\hat{\rho}(t) \right] {\rm Tr}\left[\hat{\rho}^2(t) \right] \ . \tag{22}$$

Analogously with the entropy of Equation (11), we can also introduce a linear entropy involving the non-normalised density matrix as

$$S_{\rm lin}^{\rm NH} = 1 - {\rm Tr}\left[\hat{\rho}(t)\hat{\Omega}(t) \right] \ . \tag{23}$$

The rate of production of $S_{\rm lin}^{\rm NH}$ is

$$\dot{S}_{\rm lin}^{\rm NH} = -\frac{2}{{\rm Tr}\left[\hat{\Omega}(t) \right]} {\rm Tr}\left[\hat{\Omega}(t) \partial_t \hat{\Omega}(t) \right] - \frac{2{\rm Tr}\left(\hat{\Omega}^2(t) \right)}{\hbar \left[{\rm Tr}\left(\hat{\Omega}(t) \right) \right]^2} {\rm Tr}\left(\hat{\Gamma}\hat{\Omega}(t) \right) \ . \tag{24}$$

Using Equation (5), together with the identity

$${\rm Tr}\left[\hat{\Omega}[\hat{\Gamma}, \hat{\Omega}]_+ \right] = 2{\rm Tr}\left[\hat{\Gamma}\hat{\Omega}^2 \right] \ , \tag{25}$$

in Equation (24), we obtain

$$\dot{S}_{\text{lin}}^{\text{NH}} = \frac{4\text{Tr}\left[\hat{\Gamma}\hat{\Omega}^2(t)\right]}{\hbar\text{Tr}\left[\hat{\Omega}(t)\right]} - \frac{2\text{Tr}\left(\hat{\Omega}^2(t)\right)\text{Tr}\left(\hat{\Gamma}\hat{\Omega}(t)\right)}{\hbar\left[\text{Tr}\left(\hat{\Omega}(t)\right)\right]^2} . \tag{26}$$

Linear Entropy Production and Constant Decay Operator

Let us consider Equations (22) and (26) in the case of a decay operator defined by Equation (14). In such a case, the temporal dependence of $\text{Tr}(\hat{\Omega}(t))$ is given, when choosing $\text{Tr}\hat{\Omega}(0) = 1$, by Equation (15). Using Equation (5), we easily obtain

$$\partial_t \text{Tr}\hat{\Omega}^2(t) = -2\gamma_0 \text{Tr}\hat{\Omega}^2(t), \tag{27}$$

$$\text{Tr}\hat{\Omega}^2(t) = \text{Tr}\hat{\Omega}^2(0)\exp[-2\gamma_0 t] . \tag{28}$$

Hence, the calculation of

$$\partial_t \text{Tr}\hat{\rho}^2(t) = 2\text{Tr}\left[\hat{\rho}(t)\partial_t\hat{\rho}(t)\right] \tag{29}$$

can proceed upon considering the identities

$$-\frac{2}{\hbar}\text{Tr}\left\{\hat{\rho}(t)\left[\hat{\Gamma},\hat{\rho}(t)\right]_+\right\} = -2\gamma_0\text{Tr}\left[\hat{\rho}^2(t)\right] , \tag{30}$$

$$\frac{4}{\hbar}\text{Tr}\left\{\hat{\rho}^2(t)\text{Tr}\left[\hat{\Gamma}\hat{\rho}(t)\right]\right\} = 2\gamma_0\text{Tr}\left[\hat{\rho}^2(t)\right] . \tag{31}$$

Therefore, Equation (29) is found to give

$$\partial_t \text{Tr}\hat{\rho}^2(t) = -2\gamma_0\text{Tr}\left[\hat{\rho}^2(t)\right] + 2\gamma_0\text{Tr}\left[\hat{\rho}^2(t)\right] = 0 . \tag{32}$$

Given the above result, we can choose

$$\text{Tr}\hat{\rho}^2(t) = \text{const.} = \text{Tr}\hat{\rho}^2(0) . \tag{33}$$

Finally, Equation (22) becomes

$$\dot{S}_{\text{lin}} = 2\gamma_0\text{Tr}[\hat{\rho}^2(0)] - 2\gamma_0\text{Tr}[\hat{\rho}^2(t)] = 0 . \tag{34}$$

Equation (34) shows that S_{lin} is identically constant and is thus not suitable to describe the information flow or the evolution of the entanglement in systems with non-Hermitian Hamiltonians.

Let us now consider Equation (26): it becomes

$$\begin{aligned}\dot{S}_{\text{lin}}^{\text{NH}} &= 2\gamma_0\frac{\text{Tr}\hat{\Omega}^2(t)}{\text{Tr}\hat{\Omega}(t)} - \gamma_0\frac{\text{Tr}\hat{\Omega}^2(t)}{\text{Tr}\hat{\Omega}(t)} \\ &= \gamma_0\left[\text{Tr}\hat{\Omega}^2(0)\right]e^{-\gamma t} .\end{aligned} \tag{35}$$

Integrating between 0 and t, we obtain

$$S_{\text{lin}}^{\text{NH}} = \left[1 - e^{-\gamma_0 t}\right]\text{Tr}\hat{\Omega}^2(0) . \tag{36}$$

Equation (36) describes the increase of the linear entropy $S_{\text{lin}}^{\text{NH}}$ from the value of 0 at $t = 0$ to the plateau value of $\text{Tr}\hat{\Omega}^2(0)$ at $t = \infty$. Because of the choice of the initial condition $\text{Tr}\hat{\Omega}(0) = 1$, the quantity $\text{Tr}\hat{\Omega}^2(0)$ is the purity of the non-Hermitian system. Hence, Equation (36) monitors the loss of the initial purity of the system.

4. Non-Hermitian Dynamics in a Classical Environment

One particular class of open quantum systems is obtained when a quantum subsystem is embedded in a classical environment. In [27], an equation of motion for a quantum subsystem embedded in a classical bath, described in terms of its phase space coordinates, has been derived. To this end, we consider a total Hamiltonian

$$\hat{\mathcal{H}}(\hat{r},\hat{p},\hat{R},\hat{P}) = \hat{H}(\hat{r},\hat{p},\hat{R},\hat{P}) - i\hat{\Gamma}(\hat{r},\hat{p}) \;, \tag{37}$$

where $(\hat{r},\hat{p})$ are n light degrees of freedom with mass m, and $(\hat{R},\hat{P})$ are N heavy degrees of freedom of mass M. The small expansion parameter $\mu = \sqrt{m/M} << 1$ can be used to obtain the classical limit for the $(\hat{R},\hat{P})$ degrees of freedom, after taking a partial Wigner transform over the $2N$ heavy coordinates. Using a multidimensional notation and denoting the phase space point (R,P) with X, the partial Wigner transform of the density matrix is defined as

$$\hat{\Omega}_{\rm W}(X,t) = \frac{1}{(2\pi\hbar)^N}\int dZ e^{P\cdot Z/\hbar}\langle R - Z/2|\hat{\Omega}(t)|R+Z/2\rangle \;, \tag{38}$$

while the partial Wigner transform of an arbitrary operator $\hat{\chi}$ is defined as

$$\hat{\chi}_{\rm W}(X) = \int dZ e^{P\cdot Z/\hbar}\langle R - Z/2|\hat{\chi}|R+Z/2\rangle \;. \tag{39}$$

In [27], it was shown that, upon taking the partial Wigner transform of Equation (5), with the $\hat{H}$ and $\hat{\Gamma}$ of Equation (37), and performing a linear expansion in μ, one obtains the equation of motion

$$\begin{aligned}\frac{\partial}{\partial t}\hat{\Omega}_{\rm W}(X,t) &= -\frac{i}{\hbar}\left[\hat{H}_{\rm W},\hat{\Omega}_{\rm W}(X,t)\right]_{-} + \frac{1}{2}\mathcal{B}_{ab}\left(\partial_a\hat{H}_{\rm W}\right)\left(\partial_b\hat{\Omega}_{\rm W}(X,t)\right)\\ &- \frac{1}{2}\mathcal{B}_{ab}\left(\partial_a\hat{\Omega}_{\rm W}(X,t)\right)\left(\partial_b\hat{H}_{\rm W}\right) - \frac{1}{\hbar}\left[\hat{\Gamma},\hat{\Omega}_{\rm W}(X,t)\right]_{+} \;,\end{aligned} \tag{40}$$

where $\mathcal{B}_{ab} = -\mathcal{B}_{ba}^{\rm T}$ is the symplectic matrix [34] and $\partial_a = (\partial/\partial X_a)$ is the gradient operator in phase space. The Einstein convention of summing over repeated indices is used throughout this paper. One can note that $\mathcal{B}_{ab}(\partial_a\hat{H}_{\rm W})(\partial_b\hat{\Omega}_{\rm W})$ is the Poisson bracket between $\hat{H}_{\rm W}$ and $\hat{\Omega}_{\rm W}$.

Equation (40) describes the evolution of the non-normalised density matrix, $\hat{\Omega}_{\rm W}(X,t)$, when a quantum subsystem with probability sinks or sources (represented by the decay operator $\hat{\Gamma}$) is embedded in a classical environment (with phase space coordinates X). The classical bath produces both statistical noise and decoherence in addition to those eventually represented by the decay operator. As a consequence of Equation (40), the trace of $\hat{\Omega}_{\rm W}(X,t)$ is not a conserved quantity:

$$\begin{aligned}\frac{d}{dt}{\rm Tr}'\int dX\hat{\Omega}_{\rm W}(X,t) &= \frac{d}{dt}\tilde{\rm Tr}\left[\hat{\Omega}_{\rm W}(X,t)\right]\\ &= \tilde{\rm Tr}\left[\frac{\partial}{\partial t}\hat{\Omega}_{\rm W}(X,t)\right] \neq 0 \;,\end{aligned} \tag{41}$$

where we have denoted with the symbol ${\rm Tr}'$ a partial trace over the quantal degrees of freedom, with the symbol $\int dX$ the phase space integral, and with the symbol $\tilde{\rm Tr}$ both the partial trace and the phase space integral.

Using the cyclic invariance of the trace, we can easily see that

$$\tilde{\rm Tr}\left\{\left[\hat{H}_{\rm W},\hat{\Omega}_{\rm W}\right]_{-}\right\} = \tilde{\rm Tr}\left\{\hat{H}_{\rm W}\hat{\Omega}_{\rm W} - \hat{H}_{\rm W}\hat{\Omega}_{\rm W}\right\} = 0 \;, \tag{42}$$

$$\tilde{\rm Tr}\left\{\hat{H}_{\rm W}\overleftarrow{\nabla}_a\mathcal{B}_{ab}\overrightarrow{\nabla}_b\hat{\Omega}_{\rm W} - \hat{\Omega}_{\rm W}\overleftarrow{\nabla}_a\mathcal{B}_{ab}\overrightarrow{\nabla}_b\hat{H}_{\rm W}\right\} = 0 \;, \tag{43}$$

where, in the last identity, we have also performed an integration by parts and exploited the fact that $\mathcal{B}_{ab}$ are constants. If we also use the identity

$$\tilde{\mathrm{Tr}}\left\{\left[\hat{\Gamma},\hat{\Omega}_{\mathrm{W}}\right]_{+}\right\} = 2\mathrm{Tr}'\left[\hat{\Gamma}\hat{\Omega}_{\mathrm{S}}\right] , \quad (44)$$

where $\hat{\Omega}_{\mathrm{S}} = \int dX\hat{\Omega}_{\mathrm{W}}(X)$, we can then find

$$\frac{d}{dt}\tilde{\mathrm{Tr}}\left[\hat{\Omega}_{\mathrm{W}}(X,t)\right] = -\frac{2}{\hbar}\mathrm{Tr}'\left[\hat{\Gamma}\hat{\Omega}_{\mathrm{S}}(t)\right] . \quad (45)$$

Equation (45) is analogous to Equation (6) and shows that the probability is not conserved for the quantum-classical system because of the action of the decay operator. We can introduce a normalised density matrix as

$$\hat{\rho}_{\mathrm{W}}(X,t) = \frac{\hat{\Omega}_{\mathrm{W}}(X,t)}{\tilde{\mathrm{Tr}}\left[\hat{\Omega}_{\mathrm{W}}(X,t)\right]} , \quad (46)$$

and, using Equations (40) and (45), find its equation of motion:

$$\begin{aligned} \frac{\partial}{\partial t}\hat{\rho}_{\mathrm{W}}(X,t) = &-\frac{i}{\hbar}\left[\hat{H}_{\mathrm{W}},\hat{\rho}_{\mathrm{W}}(X,t)\right]_{-} + \frac{1}{2}\hat{H}_{\mathrm{W}}\overleftarrow{\nabla}\cdot\boldsymbol{\mathcal{B}}\cdot\overrightarrow{\nabla}\hat{\rho}_{\mathrm{W}}(X,t) \\ &-\frac{1}{2}\hat{\rho}_{\mathrm{W}}(X,t)\overleftarrow{\nabla}\cdot\boldsymbol{\mathcal{B}}\cdot\overrightarrow{\nabla}\hat{H}_{\mathrm{W}} \\ &-\frac{1}{\hbar}\left[\hat{\Gamma},\hat{\rho}_{\mathrm{W}}(X,t)\right]_{+} + \frac{2}{\hbar}\hat{\rho}_{\mathrm{W}}(X,t)\tilde{\mathrm{Tr}}\left[\hat{\Gamma}\hat{\rho}_{\mathrm{W}}(X,t)\right] . \end{aligned} \quad (47)$$

At variance with Equation (40), Equation (47) is nonlinear and allows one to define averages of the dynamical variables of the quantum-classical system with a non-Hermitian Hamiltonian that has a probabilistic meaning.

5. Entropy Production and Quantum-Classical Non-Hermitian Hamiltonians

As noted in [26], when considering the definition of the entropy for a quantum system in terms of the Wigner function, the typical choice in terms of the von Neumann definition, found in Equation (9) when the Wigner function $f_{\mathrm{W}}(x,X,t)$ replaces the density matrix $\hat{\rho}$, cannot work: $f_{\mathrm{W}}(x,X,t)$ can be negative in general. What one can do [26] is start from the linear entropy [28,29], $S_{\mathrm{lin}} = 1 - \mathrm{Tr}(\hat{\rho}^2)$, and perform the Wigner transform in order to obtain:

$$S_{\mathrm{lin}} = 1 - (2\pi\hbar)^{n+N}\int dxdX f_{\mathrm{W}}^2(x,X,t) , \quad (48)$$

where $f_{\mathrm{W}}(x,X,t)$ is the Wigner function, obtained by transforming $\hat{\rho}$ over all the coordinates.

In a mixed quantum-classical framework, the natural extension of Equation (48) is given by

$$S_{\mathrm{lin,W}} = 1 - (2\pi\hbar)^{N}\mathrm{Tr}'\int dX\hat{\rho}_{\mathrm{W}}^2(X,t) = 1 - (2\pi\hbar)^{N}\tilde{\mathrm{Tr}}\left[\hat{\rho}_{\mathrm{W}}^2(X,t)\right] . \quad (49)$$

When considering the non-Hermitian dynamics of the quantum subsystem embedded in the classical environment, given by Equation (47), we obtain the linear entropy production

$$\dot{S}_{\mathrm{lin,W}} = -2(2\pi\hbar)^{N}\tilde{\mathrm{Tr}}\left[\hat{\rho}_{\mathrm{W}}\frac{\partial\hat{\rho}_{\mathrm{W}}}{\partial t}\right] . \quad (50)$$

We have obtained Equation (50) by using the identities

$$\tilde{\mathrm{Tr}}\left\{\hat{\rho}_{\mathrm{W}}\left[\hat{H}_{\mathrm{W}},\hat{\rho}_{\mathrm{W}}\right]_{-}\right\} = 0 , \quad (51)$$

$$\tilde{\mathrm{Tr}}\left\{\hat{\rho}_{\mathrm{W}}\left[\mathcal{B}_{ab}(\nabla_a\hat{H}_{\mathrm{W}})(\nabla_b\hat{\rho}_{\mathrm{W}}) - \mathcal{B}_{ab}(\nabla_a\hat{\rho}_{\mathrm{W}})(\nabla_b\hat{H}_{\mathrm{W}})\right]\right\} = 0 , \quad (52)$$

together with $\mathcal{B}_{ab}(\nabla^2_{ab}\hat{\rho}_{\rm W})\hat{\rho}_{\rm W}\hat{H}_{\rm W}=0$ and $\mathcal{B}_{ab}\hat{\rho}_{\rm W}(\nabla^2_{ab}\hat{\rho}_{\rm W})\hat{H}_{\rm W}=0$, which follow from taking the trace of an antisymmetric matrix, $\mathcal{B}_{ab}$, and a symmetric one, $\nabla^2_{ab}\hat{\rho}_{\rm W}$. Noting that we also have

$$\tilde{\rm Tr}\left\{\hat{\rho}_{\rm W}\left[\hat{\Gamma},\hat{\rho}_{\rm W}\right]_+\right\} = 2\tilde{\rm Tr}\left\{\hat{\Gamma}\hat{\rho}^2_{\rm W}\right\}, \tag{53}$$

we finally obtain the entropy production

$$\dot{S}_{\rm lin,W} = \frac{4}{\hbar}(2\pi\hbar)^N\left\{{\rm Tr}'\left[\hat{\Gamma}\hat{\rho}^2_{\rm S}(t)\right]-{\rm Tr}'\left[\hat{\Gamma}\hat{\rho}_{\rm S}(t)\right]{\rm Tr}'\left[\hat{\rho}^2_{\rm S}(t)\right]\right\}. \tag{54}$$

Within the quantum-classical framework, we can also introduce a non-Hermitian linear entropy as

$$S^{\rm NH}_{{\rm lin},W} = 1-(2\pi\hbar)^N\tilde{\rm Tr}\left[\hat{\rho}_{\rm W}(X,t)\hat{\Omega}_{\rm W}(X,t)\right]. \tag{55}$$

The entropy production is given by

$$\dot{S}^{\rm NH}_{{\rm lin},W} = -2\frac{(2\pi\hbar)^N}{Z_{\rm W}}\tilde{\rm Tr}\left[\hat{\Omega}_{\rm W}\frac{\partial\hat{\Omega}_{\rm W}}{\partial t}\right]-\frac{2(2\pi\hbar)^N}{\hbar}\tilde{\rm Tr}\left[\hat{\Gamma}\hat{\Omega}_{\rm W}\right]\tilde{\rm Tr}\left[\hat{\rho}^2_{\rm W}\right], \tag{56}$$

where we have defined

$$Z_{\rm W} = \tilde{\rm Tr}\left[\hat{\Omega}_{\rm W}(X,t)\right]. \tag{57}$$

In the following, we will use

$$\dot{Z}_{\rm W} = -\frac{2}{\hbar}\tilde{\rm Tr}\left[\hat{\Gamma}\hat{\Omega}_{\rm W}(X,t)\right]. \tag{58}$$

In order to calculate $\tilde{\rm Tr}[\hat{\Omega}_{\rm W}\partial\hat{\Omega}_{\rm W}/\partial t]$, we are led to consider the following identities:

$$\tilde{\rm Tr}\left[\mathcal{B}_{ab}\hat{\Omega}_{\rm W}(\nabla_a\hat{H}_W)(\nabla_b\hat{\rho}_W)-\mathcal{B}_{ab}\hat{\Omega}_{\rm W}(\nabla_a\hat{\rho}_W)(\nabla_b\hat{H}_W)\right] = 0, \tag{59}$$

$$\tilde{\rm Tr}\left\{\hat{\Omega}_{\rm W}\left[\hat{\Gamma},\hat{\Omega}_{\rm W}\right]_+\right\} = 2\tilde{\rm Tr}'\left[\hat{\Gamma}\hat{\Omega}^2_{\rm S}\right]. \tag{60}$$

Finally, we obtain

$$\dot{S}^{\rm NH}_{\rm lin,W} = \frac{4(2\pi\hbar)^N}{\hbar}{\rm Tr}'\left[\hat{\Gamma}\hat{\rho}_{\rm S}\hat{\Omega}_{\rm S}\right]-\frac{2(2\pi\hbar)^N}{\hbar}{\rm Tr}'\left[\hat{\Gamma}\hat{\Omega}_{\rm S}\right]{\rm Tr}'\left[\hat{\rho}^2_{\rm S}\right]. \tag{61}$$

Quantum-Classical Linear Entropy Production and Constant Decay Operator

When the decay operator $\hat{\Gamma}$ is given by Equation (14), Equation (40) becomes

$$\begin{aligned}\frac{\partial}{\partial t}\hat{\Omega}_{\rm W}(X,t) = &- \frac{i}{\hbar}\left[\hat{H}_{\rm W},\hat{\Omega}_{\rm W}(X,t)\right]_- + \frac{1}{2}\hat{H}_{\rm W}\overleftarrow{\nabla}\cdot\boldsymbol{\mathcal{B}}\cdot\overrightarrow{\nabla}\hat{\Omega}_{\rm W}(X,t)\\ &- \frac{1}{2}\hat{\Omega}_{\rm W}(X,t)\overleftarrow{\nabla}\cdot\boldsymbol{\mathcal{B}}\cdot\overrightarrow{\nabla}\hat{H}_{\rm W}-\gamma_0\hat{\Omega}_{\rm W}(X,t),\end{aligned} \tag{62}$$

and Equation (45) becomes

$$\frac{d}{dt}\tilde{\rm Tr}\left[\hat{\Omega}_{\rm W}(X,t)\right] = -\gamma_0\tilde{\rm Tr}\left[\hat{\Omega}_{\rm W}(X,t)\right]. \tag{63}$$

Upon choosing the initial condition $\tilde{\rm Tr}\left[\hat{\Omega}_{\rm W}(X,0)\right]=1$, Equation (63) has the solution

$$\tilde{\rm Tr}\left[\hat{\Omega}_{\rm W}(X,t)\right] = \exp\left[-\gamma_0 t\right], \tag{64}$$

which is analogous to Equation (15). Equation (47) becomes

$$\frac{\partial}{\partial t}\hat{\rho}_{\rm W}(X,t) = -\frac{i}{\hbar}\left[\hat{H}_{\rm W},\hat{\rho}_{\rm W}(X,t)\right]_{-} + \frac{1}{2}\hat{H}_{\rm W}\overleftarrow{\nabla}\cdot\boldsymbol{\mathcal{B}}\cdot\overrightarrow{\nabla}\hat{\rho}_{\rm W}(X,t) - \frac{1}{2}\hat{\rho}_{\rm W}(X,t)\overleftarrow{\nabla}\cdot\boldsymbol{\mathcal{B}}\cdot\overrightarrow{\nabla}\hat{H}_{\rm W}\,. \quad (65)$$

Equation (65) shows that, in the case considered, the normalised density matrix $\hat{\rho}_{\rm W}(X,t)$ is not influenced by $\hat{\Gamma}$, so this evolves according to the unitary quantum-classical dynamics that were first derived in [35].

We also have that Equations (54) and (61) become

$$\dot{S}_{\rm lin,W} = 2\gamma_0(2\pi\hbar)^N\left\{\tilde{\rm Tr}'\left[\hat{\rho}^2_{\rm W}(X,t)\right] - \tilde{\rm Tr}\left[\hat{\rho}^2_{\rm W}(X,t)\right]\right\} = 0\,, \quad (66)$$

$$\begin{aligned}\dot{S}^{\rm NH}_{\rm lin,W} &= \frac{4(2\pi\hbar)^N}{\hbar}\tilde{\rm Tr}\left[\hat{\Gamma}\hat{\rho}_{\rm W}(X,t)\hat{\Omega}_{\rm W}(X,t)\right] - \frac{2(2\pi\hbar)^N}{\hbar}\tilde{\rm Tr}\left[\hat{\Gamma}\hat{\Omega}_{\rm W}(X,t)\right]\tilde{\rm Tr}\left[\hat{\rho}^2_{\rm W}(X,t)\right] \\ &= (2\pi\hbar)^N\gamma_0 e^{\gamma_0 t}\tilde{\rm Tr}\left[\hat{\Omega}^2_{\rm W}(X,t)\right]\,. \end{aligned} \quad (67)$$

In order to evaluate Equation (67), we need to calculate $\tilde{\rm Tr}[\hat{\Omega}^2_{\rm W}(X,t)]$. From Equation (62), we get

$$\frac{\partial}{\partial t}\tilde{\rm Tr}\left[\hat{\Omega}^2_{\rm W}(X,t)\right] = -2\gamma_0\tilde{\rm Tr}\left[\hat{\Omega}^2_{\rm W}(X,t)\right]\,, \quad (68)$$

$$\tilde{\rm Tr}\left[\hat{\Omega}^2_{\rm W}(X,t)\right] = \tilde{\rm Tr}\left[\hat{\Omega}^2_{\rm W}(X,0)\right]\exp\left[-2\gamma_0 t\right]\,. \quad (69)$$

Upon substituting Equation (69) into Equation (67) and integrating, we finally obtain

$$S^{\rm NH}_{\rm lin,W} = (2\pi\hbar)^N\tilde{\rm Tr}\left[\hat{\Omega}^2_{\rm W}(X,0)\right]\left(1-e^{-\gamma_0 t}\right)\,. \quad (70)$$

Analogously to the pure quantum case, the rate of production of the quantum-classical entropy in Equation (70) monitors the flow of information associated with the decay of the purity of the quantum-classical non-Hermitian system (for positive γ_0).

6. Conclusions

In this paper, we have shown that it is possible to define meaningful entropy functionals for open quantum systems described by non-Hermitian Hamiltonians. In particular, a non-Hermitian generalisation of the von Neumann entropy, which is able to signal the loss of information of the quantum subsystem, requires both the normalised and the non-normalised density matrix: this entropy can be defined as the normalised average of the logarithm of the non-normalised density matrix [25].

Motivated by the Wigner representation of quantum mechanics, we have also introduced the non-Hermitian generalisation of the linear entropy, defined as one minus the normalised average of the square of the non-normalised density matrix. Through the analytical solution of the basic case of a constant decay operator, we have shown that the non-Hermitian linear entropy is able to describe the loss of purity of the quantum subsystem. This is true both for pure non-Hermitian subsystems as well as for non-Hermitian subsystems embedded in a classical environment. It is worth repeating that even basic models with constant decay operators are interesting when one adds the additional level of complexity provided by the classical-like environment represented by means of the partially Wigner-transformed Hermitian part of the Hamiltonian, as in the case of a light-emitting quantum dot coupled to an energy-absorbing optical guide in a classical environment.

The results obtained so far [17–19,25] show that the correct description of the dynamics and of the information flow of systems described by non-Hermitian Hamiltonians needs the use of both the normalised and non-normalised density matrix. In this way, reasonable entropy functionals can be introduced. On conceptual grounds, one might have expected that the foundation of the non-Hermitian theory on the *normalised* density matrix alone would hide the interesting effects arising from the coupling to the probability sinks or sources. As a matter of fact, the density matrix $\hat{\rho}$ is constrained to be normalised in order to be able to define correctly (normalised) statistical averages. However, such a procedure inevitably masks the flow of information: it is as if one would like to study the motion of a body by choosing the frame of reference that moves together with the body itself. On the contrary, the flow of information in systems modelled with non-Hermitian Hamiltonians can be *solely* captured through the use of the *non-normalised* density matrix.

We hope that the results discussed in this paper may be a first step toward a rigorous analysis of the quantum information flow in systems with non-Hermitian Hamiltonians, after removing the constraints of PT-symmetry [36].

Acknowledgments: Our research has been self-funded through the salaries received from the University of Messina. We are very grateful to Ignazio Licata who encouraged and supported us through the waiver of the publications costs.

Author Contributions: Alessandro Sergi conceived the subject. Both authors contributed to the development and the writing of the paper and have read and approved the final manuscript.

Conflicts of Interest: The authors declare no conflict of interest.

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