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THE DENSITY MATRIX IN THE NON-HERMITIAN APPROACH TO OPEN QUANTUM SYSTEM DYNAMICS

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ABSTRACT. In this paper we review an approach to the dynamics of open quantum systems based of non-Hermitian Hamiltonians. Non-Hermitian Hamiltonians arise naturally when one wish to study a subsystem interacting with a continuum of states. Moreover, quantum subsystems with probability sinks or sources are naturally described by non-Hermitian Hamiltonians. Herein, we discuss a non-Hermitian formalism based on the density matrix. We show both how to derive the equations of motion of the density matrix and how to define statistical averages properly. It turns out that the laws of evolution of the normalized density matrix are intrinsically non-linear. We also show how to define correlation functions and a non-Hermitian entropy with a non zero production rate. The formalism has been generalized to the case of hybrid quantum-classical systems using a partial Wigner representation. The equations of motion and the statistical averages are defined analogously to the pure quantum case. However, the definition of the entropy requires to introduce a non-Hermitian linear entropy functional.

1. Introduction

Open quantum systems are ubiquitous in physics (Breuer and F. 2002; Rotter 2009; Rivas and Huelga 2012; Rotter and Bird 2015). They consists of a region of space, or subsystem, where quantum processes take place, that interacts with an environment, which is beyond the control of the experimenter (Rotter and Bird 2015). As a matter of fact, the very first step to identify a system is to select a region of space containing it. This can be more easily understood when one adopts the Eulerian point of view of field theory (Bender 2007; Assis 2010). The environment typically causes decoherence, dissipation, and non-linearity in the evolution of the subsystem (Breuer and F. 2002; Rotter 2009; Rivas and Huelga 2012; Rotter and Bird 2015). While their study constitutes the basis for the understanding and development of novel quantum devices (Wolf 2004; Binns 2008; Nouailhat 2008), open quantum systems are difficult to study theoretically. When the relevant quantum system is in contact with a probability sink (or source), the dynamical description naturally calls for a non-Hermitian Hamiltonian. This is typically the situation of a subsystem with a discrete number of energy levels interacting with a continuum of states; in this case, the Feshbach projection formalism (Feshbach 1958, 1962) leads naturally to a description of the subsystem in terms of a non-Hermitian Hamiltonian. Such a subsystem is classified as a non-Hermitian quantum system and the theory is called non-Hermitian quantum mechanics (Bender 2007; Moiseyev 2011). The dynamics arising from the non-Hermitian Hamiltonian is also referred to as non-Hermitian dynamics. A probability sink, for example, can be interpreted in terms of the irreversible disappearance of degrees of freedom from the system so that quantum probabilities are no longer conserved in time. The non-Hermitian Hamiltonian describes effectively the dynamics of the relevant subsystem, avoiding to keep explicitly into account the degrees of freedom of the environment (Wong 1967; Baskoutas *et al.* 1993; Hegerfeldt 1993; Angelopoulou *et al.* 1995; Geyer *et al.* 2008; Banerjee and Srikanth 2010; Reiter and Srensen 2012). Applications of non-Hermitian quantum mechanics are found, for example, when studying quantum scattering and transport (Muga *et al.* 2004; Varga and Pantelides 2007; Znojil 2009; Berggren *et al.* 2010; Wibking and Varga 2012), resonances (John *et al.* 1991; Nicolaides and Themelis 1992; Moiseyev 1998), decaying states (Sudarshan *et al.* 1978), multiphoton ionization (Chu and Reinhardt 1977; Baker 1983, 1984; Selst *et al.* 2011), and optical waveguides (Guo *et al.* 2009; Rter *et al.* 2010). Non-Hermitian Hamiltonians also appear in parity-time symmetric quantum mechanics (Bender and Boettcher 1998; Mostafazadeh 2010), an approach that has recently found applications in lossy optical waveguides (Guo *et al.* 2009; Rter *et al.* 2010) and photonic lattices (Regensburger *et al.* 2012; Wimmer *et al.* 2015). Non-Hermitian quantum mechanics is currently an area of intensive research: the field is rapidly developing in exciting ways, as a simple search of the keyword *non-Hermitian* in the published literature can demonstrate.

There are basically two different perspectives that can be taken with respect to non-Hermitian quantum mechanics. One assumes that parity-time symmetric non-Hermitian theory is alternative to Hermitian quantum mechanics (Bender and Boettcher 1998; Mostafazadeh 2010). Here, we do not pursue such a point of view. One of the reason is that Schrödinger's approach to quantum mechanics, which is most naturally connected with classical Hamilton-Jacobi theory (Holland 1977; Cook 2015), and which is abstracted into Dirac's canonical quantization (Dirac 1999), inevitably leads to Hermitian Hamiltonians. In turn hermiticity is inherently connected to a time-symmetric vision of quantum mechanics (Mead 2002; Kastner 2013, 2015; Cramer 2016): time-symmetry is a key feature of the fundamental theories of physics, *i.e.*, the standard model(Weinberg 1996a,b) and Einstein's gravitation (Weinberg 1996b), whether they are represented through the Hamiltonian formalism, by Lie algebras (Weinberg 1996a,b) or by the path integral approach (Feynman and Hibbs 1965; Feynman 2005). For the above reasons, notwithstanding the abstractness of hermiticity in comparison to parity-time symmetry, we do not see sufficient motivation in order to depart from it. An entirely different situation is found when non-Hermitian Hamiltonians are introduced as effective tools for describing the dynamics of discrete systems embedded into a continuum of scattering states (Feshbach 1958, 1962; Rotter 2009; Rotter and Bird 2015). As it will be more completely discussed in the following, in this case the possibility of an effective non-Hermitian quantum mechanics ultimately rests onto the theorem of Fock and Krylov (Krylov and Fock 1947). Hence, we take this second point of view.

Non-Hermitian quantum mechanics is usually formulated in terms of the Schrödinger equation (Faisal and Moloney 1981; Baker 1983, 1984; Dattoli *et al.* 1990) or derived methods (Thilagam 2012). A different approach was developed in (Graefe *et al.* 2010a;

Graefe and Schubert 2011), where the Wigner function of an initial Gaussian state was calculated considering correction terms up to quartic order in the Planck constant. Herein, we review an approach to non-Hermitian quantum mechanics that is based on the non-normalized density matrix (Sergi and Zloshchastiev 2013; Zloshchastiev and Sergi 2014; Sergi 2015; Sergi and Zloshchastiev 2015; Zloshchastiev 2015; Sergi and Giaquinta 2016; Sergi and Zloshchastiev 2016). Whenever there is an interest in setting up a statistical mechanical theory, it is natural to adopt the density matrix as the tool of choice. In non-Hermitian dynamics, the trace of the density matrix is not preserved, the equivalence between the Schrödinger and Heisenberg picture is broken, and the time-reversibility of the evolution is lost. However, the properly normalized density matrix allows one to define quantum averages with a definite probabilistic meaning, to introduce correlation functions, and to find expressions for entropies and rates of entropy production. The characteristics of open quantum system dynamics are explicated, among other things, by the fact that the equation of motion of the normalized density matrix of a non-Hermitian system is non-linear.

This paper is structured has follows. In Sec. **2** we introduce a density matrix approach to the dynamics of non-Hermitian systems. In Sec. **3** we show how to define the purity for a system with a non-Hermitian Hamiltonian. Non-Hermitian correlations functions in the Schrödinger picture are introduced in Sec. **4**. The non-Hermitian definition of the entropy functional with a non-zero production is given in Sec. **5**. In Sec. **6** we treat the case of a hybrid quantum-classical system and give equations of motion and a recipe for calculating statistical average, which are analogous to the pure quantum case. In Sec. **7** we discuss the linear entropy for the pure quantum case and we generalize it in the case of a hybrid quantum-classical system. The formulas of non-Hermitian entropy production are also given. Finally, our conclusions are given in Sec. **8**.

2. The density matrix in non-Hermitian Quantum Mechanics

The theorem of Fock and Krylov (Krylov and Fock 1947) states that the necessary and sufficient condition to have a decaying state is a continuum spectrum of the energy. Such a theorem leads to the possibility of describing systems having part of their spectrum in the continuum by means of decaying state. The finite lifetime of any decaying state implies in turn, by virtue of the Heisenberg uncertainty relation, that the associate energy has a finite width. As it is well known, finite energy widths can be represented in terms of imaginary terms added to the energy, resulting in overall complex energy eigenvalues. In turn, complex energy eigenvalues can be derived from non-Hermitian Hamiltonians. Such non-Hermitian Hamiltonians can be introduced as intuitive ansatz or derived for a discrete system embedded in a continuum of states by means of the Feschbach projection formalism (Feshbach 1958, 1962). Hence, a time evolution in terms of non-unitary operators can be introduced as in the standard Hermitian case (Dattoli *et al.* 1990). Alternatively, arguments based on dynamical maps can also be adopted in support of the Schrödinger's form of the law of motion (Grimaudo *et al.* 2018). In the following, we adopt a non-Hermitian time-dependent Schrödinger equation (Faisal and Moloney 1981; Baker 1983, 1984; Dattoli *et al.* 1990; Thilagam 2012) to derive a picture of non-Hermitian dynamics based on the density matrix (Sergi and Zloshchastiev 2013; Zloshchastiev and Sergi 2014; Sergi 2015;

Sergi and Zloshchastiev 2015; Zloshchastiev 2015; Sergi and Giaquinta 2016; Sergi and Zloshchastiev 2016).

Let us consider a quantum mechanical system with a discrete number of energy levels, described in terms of a non-Hermitian Hamiltonian $\hat{\mathscr{H}}$.

Such a non-Hermitian operator can always be written in terms of the sum of a Hermitian and an anti-Hermitian operator

$$\hat{\mathscr{H}} = \hat{H} + \hat{H}_- = \hat{H} - i\hat{\Gamma} , \tag{1}$$

where

$$\hat{H} = \hat{H}^\dagger = \frac{1}{2}(\hat{\mathscr{H}} + \hat{\mathscr{H}}^\dagger) \tag{2}$$

$$\hat{H}_- = -\hat{H}_-^\dagger = \frac{1}{2}(\hat{\mathscr{H}} - \hat{\mathscr{H}}^\dagger) = -i\hat{\Gamma} . \tag{3}$$

Both $\hat{H}$ and $\hat{\Gamma}$ are Hermitian; the operator $\hat{\Gamma} \equiv i\hat{H}_-$ is commonly known as the *decay rate operator*. The dynamics of the quantum states $|\Psi\rangle$ and $\langle\Psi|$ is given by the Schrödinger equations

$$|\dot{\Psi}(t)\rangle = -\frac{i}{\hbar}\hat{\mathscr{H}}|\Psi(t)\rangle = -\frac{i}{\hbar}\hat{H}|\Psi(t)\rangle - \frac{1}{\hbar}\hat{\Gamma}|\Psi(t)\rangle , \tag{4}$$

$$\langle\dot{\Psi}(t)| = \frac{i}{\hbar}\langle\Psi(t)|\hat{\mathscr{H}}^\dagger = \frac{i}{\hbar}\langle\Psi(t)|\hat{H} - \frac{1}{\hbar}\langle\Psi(t)|\hat{\Gamma} . \tag{5}$$

At the initial time, the non-normalized density matrix can be written in terms of the eigenstates $(|\Psi^k\rangle, \langle\Psi^k|)$ of any *Hermitian* operator, defined in the Hilbert space of the subsystem, and of their statistical weights w_k:

$$\hat{\Omega} = \sum_k w_k |\Psi^k\rangle\langle\Psi^k| , \tag{6}$$

where $\sum_k w_k = 1$.

The equation of motion of $\hat{\Omega}$ follows from Eqs. (4) and (5):

$$\frac{d}{dt}\hat{\Omega}(t) = -\frac{i}{\hbar}\left[\hat{H}, \hat{\Omega}(t)\right] - \frac{1}{\hbar}\left\{\hat{\Gamma}, \hat{\Omega}(t)\right\} , \tag{7}$$

with $[\cdot,\cdot]$ and $\{\cdot,\cdot\}$ denoting the commutator and anticommutator, respectively. The Hamiltonian operator $\hat{H}$ describes the subsystem while $\hat{\Gamma}$ describes the effect of the environment onto the subsystem. Equation (7) is also valid for mixed states.

If $\hat{H}_+$ is invertible and all the other operators are represented by full-rank matrices then, as shown in (Sergi 2011), Eq. (7) can be written in matrix form (Sergi 2005) as

$$\frac{d}{dt}\hat{\Omega}(t) = -\frac{i}{\hbar}\Omega^T_{\hat{H}_+}(t)\Lambda\Omega_{\hat{H}_+}(t) . \tag{8}$$

The matrix super-operator Λ is defined as

$$\Lambda = \left[\begin{array}{cc} 0 & 1 + \hat{H}_-(\hat{H}_+)^{-1} \\ -1 + (\hat{H}_+)^{-1}\hat{H}_- & 0 \end{array}\right] . \tag{9}$$

We have also introduced the the column vector

$$\Omega_{\hat{H}_+}(t) = \left[\begin{array}{c} \hat{\Omega}(t) \\ \hat{H}_+ \end{array} \right] , \tag{10}$$

together with the obvious definition for the corresponding row vector $\Omega^T_{\hat{H}_+}(t)$.

The probability is not conserved by Eq. (7). In fact, the trace of Eq. (7) gives

$$\frac{d}{dt}\mathrm{Tr}\,\hat{\Omega}(t) = -\frac{2}{\hbar}\mathrm{Tr}\left(\hat{\Gamma}\hat{\Omega}(t)\right) . \tag{11}$$

The non-conservation of probability for the subsystem is to be ascribed to its interaction with the environment. The statistical sense of the theory can be regained by defining a normalized density matrix (Sergi and Zloshchastiev 2013):

$$\hat{\rho}(t) = \frac{\hat{\Omega}(t)}{\mathrm{Tr}\,\hat{\Omega}(t)} . \tag{12}$$

Quantum statistical averages can be meaningfully calculated in terms of the normalized density matrix $\hat{\rho}(t)$:

$$\langle \chi \rangle_t = \mathrm{Tr}\left(\hat{\chi}\hat{\rho}(t)\right) , \tag{13}$$

where $\hat{\chi}$ is an arbitrary operator.

While $\hat{\Omega}(t)$ describes the irreversible subsystem, $\hat{\rho}(t)$ contains information on both the subsystem dynamics and the environment processes. Equation (13) allows one to preserve the probabilistic interpretation of quantum mechanics in the case of non-Hermitian dynamics.

Because of Eq. (11), the denominator of Eq. (12) may diverge or became zero at large times, in general (Moiseyev 2011). This represents either the continuous pumping or the disintegration, respectively, of degrees of freedom into the system, which is indeed one of the basic reason for introducing non-Hermitian quantum mechanics itself. In turn, as one can expect, such large time behavior will be reflected in the averages calculated through $\hat{\rho}(t)$. After all, the density matrix $\hat{\rho}(t)$ has been introduced in order to calculate averages in non Hermitian quantum mechanics and, while the average formula, $\langle \Psi(t)|\hat{\chi}|\Psi\rangle / \langle \Psi(t)|\Psi(t)\rangle$, given in Moiseyev (2011) is only valid at zero temperature, the formula in Eq. (13) is also valid when there is thermal (or other forms of) disorder. It will be shown by the direct study of a few relevant cases that the possible singular behavior of $\hat{\rho}(t)$ is not a problem for the calculation of averages. On the other hand, if problems should ever emerge, one could restrict the theory to time intervals where Eq. (13) is meaningful.

The equation of motion obeyed by $\hat{\rho}$ is (Sergi and Zloshchastiev 2013)

$$\frac{d}{dt}\hat{\rho}(t) = -\frac{i}{\hbar}\left[\hat{H}, \hat{\rho}(t)\right] - \frac{1}{\hbar}\left\{\hat{\Gamma}, \hat{\rho}(t)\right\} + \frac{2}{\hbar}\hat{\rho}(t)\mathrm{Tr}\left[\hat{\Gamma}\hat{\rho}(t)\right] . \tag{14}$$

It is derived (Sergi and Zloshchastiev 2013) by taking the time derivative of Eq. (12) and using Eqs. (7) and (11). The third term in the right hand side of Eq. (14) conserves the trace of $\hat{\rho}(t)$. Constant shifts of the Hamiltonian $\hat{\mathscr{H}}$, *e.g.* $\hat{\mathscr{H}} \to \hat{\mathscr{H}} + \alpha\hat{I}$, where $\hat{I}$ is the identity operator and α is an arbitrary complex c-number, are covariant transformations of Eq. (14). This property ensures that only energy differences are physically observable.

As noted in (Graefe *et al.* 2010b) for operator averages, Eq. (14) is non linear. There is an interesting resemblance between an equation introduced by Gisin in order to describe quantum dissipation (Bialynicki-Birula and Mycielski 1976; Yasue 1978; Gisin 1981, 1982, 1983) and Eq. (14). In general, the coupling of the subsystem to the environment can be represented by an effective non-linear quantum formalism (Bialynicki-Birula and Mycielski 1976; Yasue 1978; Gisin 1981, 1982; Sergi 2007; Sergi and Zloshchastiev 2013).

Moreover, as it can be inferred from Eq. (13), in non-Hermitian dynamics the equivalence between the Schrödinger and the Heisenberg dynamical picture is lost.

3. State Purity

The definition of state purity is generalized to non-Hermitian evolution by the following equation (Sergi and Zloshchastiev 2013; Zloshchastiev 2015)

$$\widetilde{\mathscr{P}}(\hat{\rho}(t)) \equiv \mathrm{Tr}\left(\hat{\rho}^2(t)\right) . \tag{15}$$

Equation (15) enforces the equality $\widetilde{\mathscr{P}}(\hat{\rho}(t)) = 1$, then $\hat{\Omega}(t)$ is a (generalized) projector. The rate of evolution of the purity is

$$\frac{d}{dt}\widetilde{\mathscr{P}}(\hat{\rho}(t)) = \frac{4}{\hbar}\left[\mathrm{Tr}\left(\hat{\rho}(t)\hat{\Gamma}\right)\mathrm{Tr}\left(\hat{\rho}^2(t)\right) - \mathrm{Tr}\left(\hat{\rho}^2(t)\hat{\Gamma}\right)\right] , \tag{16}$$

where we have used Eqs. (7) and (15). In general, non-Hermitian dynamics, as defined by Eq. (7), does not conserve the state purity.

In the case of a two-dimensional Hilbert space $\mathscr{H}_2$, the density matrix and the Hamiltonian are represented by 2×2 matrices. It can be proven (Sergi and Zloshchastiev 2013) that the right hand side of Eq. (16) reduces to

$$\frac{4}{\hbar}\frac{\det\left(\hat{\Omega}(0)\right)}{\mathrm{Tr}\left(\hat{\Omega}(t)\right)}\left[\mathrm{Tr}\left(\hat{\Gamma}\right) - 2\mathrm{Tr}\left(\hat{\rho}(t)\hat{\Gamma}\right)\right] e^{-\frac{2}{\hbar}t\mathrm{Tr}\left(\hat{\Gamma}\right)} , \tag{17}$$

Equation (17) shows that in the case of a two-dimensional space the non-Hermitian state purity, defined in Eq. (15), is conserved for quantum states whose initial density matrix has zero determinant.

4. Non-Hermitian correlation functions

Correlation functions are most commonly written in the Heisenberg picture. However, since non-Hermitian dynamics is most naturally expressed in the Schrödinger picture, and, as pointed out in the previous Section, the two pictures are not equivalent, we must define non-Hermitian correlation functions in the Schrödinger picture. In Appendix B we show how to do this in the case of Hermitian dynamics, obtaining Eq. (75). In the non-Hermitian case, a natural generalization of Eq. (75) is

$$\mathscr{C}_{\chi_2\chi_1}(t_1,t_2) \quad = \quad \mathrm{Tr}\left(\hat{\chi}_1\mathscr{U}(t_2,t_1)\hat{\chi}_2\mathscr{U}(t_1,t_0)\hat{\rho}(t_0)\right) , \tag{18}$$

where $\hat{\chi}_1$ and $\hat{\chi}_2$ are operators in the Schrödinger representation, and $\mathscr{U}$ is a generalized propagator defined as follows: When $\mathscr{U}(t_b,t_a)$ acts on its right, it realizes the propagation from time t_a to time t_b in terms of the non linear equation (14).

Accordingly, $\mathscr{U}$ propagates $\hat{\rho}$ from time t_0 to time t_1 in agreement with equation (14), it also propagates the product of operators $\hat{\chi}_2\hat{\rho}(t_1)$ from t_1 to t_2. Equation (18) reduces to the definition of the Hermitian correlation function when $\hat{\Gamma} = 0$ and to the normalized average of $\hat{\chi}_1$ when $\hat{\chi}_2$ is the identity operator.

Non-Hermitian correlation functions can alternatively be defined in terms of the linear equation (7) as

$$\mathscr{C}^{(L)}_{\chi_2\chi_1}(t_1,t_2) \quad = \quad \frac{\mathrm{Tr}\left\{\hat{\chi}_1\mathscr{U}_L(t_2,t_1)\hat{\chi}_2\mathscr{U}_L(t_1,t_0)\hat{\Omega}(t_0)\right\}}{\mathrm{Tr}\left(\hat{\Omega}(t_2)\right)}\ , \tag{19}$$

where $\mathscr{U}_L$ is a generalized propagator defined as follows. When $\mathscr{U}_L(t_b,t_a)$ acts on its right, it propagates the non-normalized density matrix from t_a up to time t_b according to Eq. (7). In Equation (19) $\mathscr{U}_L$ first evolves the non-normalized density matrix $\hat{\Omega}$ from time t_0 to time t_1 under Eq. (7), then propagates the product $\hat{\chi}_2\hat{\Omega}(t_1)$ from time t_1 to time t_2. The denominator of Eq. (19) takes into account the final normalization. Equation (19) also reduces to the definition of the correlation function of Hermitian quantum mechanics when $\hat{\Gamma} = 0$ and to the normalized average of $\hat{\chi}_1$ when $\hat{\chi}_2$ is the identity operator.

The generalization of the definitions of correlation functions in (18) and (19) to the multi-time case is straightforward (Sergi and Zloshchastiev 2015).

The description of non-Hermitian dynamics needs the use of both the normalized and non-normalized density matrices. The normalization of ρ allows one to define statistical averages but somehow masks the flow of information. It is a similar situation to that of studying the motion of a system in a frame of reference moving with the system itself. Instead, the non-normalized density matrix $\hat{\Omega}(t)$ can be expected to capture more naturally the flow of information in systems with non-Hermitian Hamiltonians. Equations (18) and (19) are a consequence of the possibility of characterizing the statistical state of a non-Hermitian system through either $\hat{\Omega}(t)$ or$\hat{\rho}(t)$.The different correlation functions given in Eqs. (18) and (19) have been compared for specific model systems in Ref. (Sergi and Zloshchastiev 2015). What follows (and the discussion in Ref. (Sergi and Giaquinta 2016)) will eventually clarify the different role of $\hat{\Omega}(t)$ and $\hat{\rho}(t)$ in the theory.

5. Non-Hermitian Quantum Entropy

In Appendix C we briefly show how the entropy and its rate production are defined in Hermitian quantum mechanics. In non-Hermitian quantum mechanics, the straightforward generalization of Eq. (78) is (Sergi and Zloshchastiev 2016):

$$S_{\mathrm{vN}}(t) = -k_B \mathrm{Tr}\left[\hat{\rho}(t)\ln\left(\hat{\rho}(t)\right)\right]\ . \tag{20}$$

Equation (20) clearly becomes identical to Eq. (78) when $\hat{\Gamma} \to 0$.

Using Eqs. (20) and (14), the rate of entropy production

$$\dot{S}_{\mathrm{vN}}(t) = \frac{2k_B}{\hbar}\mathrm{Tr}\left[\hat{\Gamma}\hat{\rho}(t)\ln\left(\hat{\rho}(t)\right)\right] + \frac{2}{\hbar}\mathrm{Tr}\left(\hat{\Gamma}\hat{\rho}(t)\right)S_{\mathrm{vN}} \tag{21}$$

can be obtained. Equation (21) shows that in general non-Hermitian dynamics gives rise to a non-zero entropy production.

However, the entropy can also be defined in terms of the non-normalized density matrix:

$$S_{\mathrm{nH}} \equiv -k_B \mathrm{Tr}(\hat{\rho}\ln\hat{\Omega})\ . \tag{22}$$

The von Neumann entropy S_{vN} is not able to describe the gain or loss of probability of the subsystem (Sergi and Zloshchastiev 2016) because it depends only on $\hat{\rho}(t)$. Instead, the operator $\ln\hat{\Omega}$ monitors well the probability evolution of the subsystem and leads to the correct entropy production (Sergi and Zloshchastiev 2016). The rate of change of the non-Hermitian entropy S_{nH} is

$$\dot{S}_{\mathrm{nH}} = \frac{2k_{\mathrm{B}}}{\hbar}\mathrm{Tr}\left(\hat{\Gamma}\hat{\rho}(t)\ln\hat{\Omega}(t)\right) + \left(\frac{2}{\hbar}S_{\mathrm{nH}} + 2\frac{k_B}{\hbar}\right)\mathrm{Tr}\left(\hat{\Gamma}\hat{\rho}(t)\right) \ . \tag{23}$$

The von Neumann (20) and non-Hermitian (22) entropies are related by the formula

$$S_{\mathrm{nH}}(t) = S_{\mathrm{vN}}(t) - k_{\mathrm{B}}\ln\left[\mathrm{Tr}\left(\hat{\Omega}(t)\right)\right] \ . \tag{24}$$

The difference between S_{nH} and S_{vN} measures how much $\mathrm{Tr}\left(\hat{\Omega}(t)\right)$ differs from one.

At variance with the von Neumann entropy (20), the non-Hermitian entropy S_{nH} is not invariant under constant shifts of the Hamiltonian that preserve the form of Eq. (14) for the normalized density matrix, see App. A. If a constant shift is applied to the decay operator $\hat{\Gamma}$, $\hat{\Gamma} \to \hat{\Gamma} + (1/2)\hbar\alpha\hat{I}$, where I is the identity operator, both the normalized density matrix $\hat{\rho}(t)$, $\hat{\rho}(t) \to \hat{\rho}(t)$, and the von Neumann entropy (20), $S_{\mathrm{vN}} \to S_{\mathrm{vN}}$, are left invariant. However, the non-Hermitian entropy S_{nH} is modified according to:

$$S_{\mathrm{nH}} \to S_{\mathrm{nH}} + k_B\alpha t \ , \tag{25}$$

where α is a real constant.

5.1. Constant decay operator $\hat{\Gamma}$. Let us consider a non-Hermitian Hamiltonian $\mathscr{H}$ in Eq (1) defined by an arbitrary Hermitian $\hat{H}$ and a decay operator $\hat{\Gamma}$ proportional to the identity operator:

$$\hat{\Gamma} = \frac{1}{2}\hbar\gamma_0\hat{I}, \tag{26}$$

where the parameter γ_0 is assumed to be real-valued.

The value of the parameter γ_0 does not influence the dynamics of the normalized density matrix, defined by Eq. (14).

However, the decay operator (26) has an important role in the evolution of both $\hat{\Omega}$ and S_{nH}.

Considering the initial conditions $\mathrm{Tr}\hat{\Omega}(0) = 1$ and $S_{\mathrm{vN}}(0) = S_{\mathrm{vN}}^{(0)} = \mathrm{const}$, and using the Eq. (24), one obtains (Sergi and Zloshchastiev 2016)

$$S_{\mathrm{vN}}(t) = S_{\mathrm{vN}}^{(0)} = \mathrm{const}\ , \tag{27}$$

$$S_{\mathrm{nH}}(t) = S_{\mathrm{vN}}^{(0)} + k_{\mathrm{B}}\gamma_0 t\ . \tag{28}$$

While the von Neumann entropy remains constant, the entropy S_{nH} changes. For positive values of γ_0, S_{nH} grows linearly with time as the thermodynamic entropy is expected to do.

6. Non-Hermitian Hybrid Quantum-Classical Systems

Consider a composite system with quantum coordinates $(\hat{r},\hat{p},\hat{R},\hat{P}) = (\hat{x},\hat{X})$. With $\hat{x}$ we denote the quantum position and momentum operators of the degrees of freedom in the subsystem, while $\hat{X}$ stands for the quantum position and momentum operators of the degrees of freedom of the bath. A multidimensional notation will be adopted, *e.g.*, $\hat{R}$

denotes $(\hat{R}_1, \hat{R}_2, ..., \hat{R}_N)$, where N is the number of degrees of freedom of the bath. The non-Hermitian Hamiltonian is given by Eq. (1). We assume that, while $\hat{\Gamma}$ is arbitrary, the Hamiltonian operator $\hat{H}$ of the subsystem has the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{\hat{P}^2}{2M} + V(\hat{r}, \hat{R}) , \tag{29}$$

where m and M are the masses of the of the particles of the subsystem and of the bath, respectively. The symbol $V(\hat{r}, \hat{R})$ denotes the interaction potential among all the degrees of freedom. We also assume that $M >> m$ so that $\mu = (m/M)^{1/2} << 1$. The non-normalized density matrix $\hat{\Omega}(t)$ of the composite system with non-Hermitian Hamiltonian $\mathscr{H}$ obeys Eq. (7).

In order to take a classical limit on the bath degrees of freedom and to obtain a hybrid quantum-classical system, we use the partial Wigner transform of $\hat{\Omega}$ (Kapral 1999)

$$\hat{\Omega}_{\mathrm{W}}(X,t) = \frac{1}{(2\pi\hbar)^N} \int dZ e^{iP\cdot Z/\hbar} \langle R - Z/2 | \hat{\Omega}(t) | R + Z/2 \rangle . \tag{30}$$

We notice that $\hat{\Omega}_{\mathrm{W}}(X,t)$ is an operator in terms of the quantum $\hat{x}$ variables and a function in terms of the X variables. Analogously, an arbitrary quantum operator $\hat{\chi}$ of the composite system is partially transformed in Wigner phase space as

$$\hat{\chi}_{\mathrm{W}}(X) = \int dZ e^{iP\cdot Z/\hbar} \langle R - Z/2 | \hat{\chi} | R + Z/2 \rangle . \tag{31}$$

The partial Wigner transform of a product of arbitrary operators $\hat{\chi}$ and $\hat{\xi}$ is given by (Imre *et al.* 1967; Hillery *et al.* 1984)

$$\left(\hat{\chi}\hat{\xi}\right)_{\mathrm{W}}(X) \equiv \hat{\chi}_{\mathrm{W}}(X) e^{\frac{i\hbar}{2}[\cdot,\cdot]_{\mathrm{P}}} \hat{\xi}_{\mathrm{W}}(X) , \tag{32}$$

where $[\cdot,\cdot]_{\mathrm{P}}$ is the Poisson bracket operator.

$$\begin{aligned} \frac{\partial}{\partial t}\hat{\Omega}_{\mathrm{W}}(X,t) = & - \frac{i}{\hbar}\left[\hat{H}_{\mathrm{W}}(X), \hat{\Omega}_{\mathrm{W}}(X,t)\right] - \frac{1}{\hbar}\left\{\hat{\Gamma}_{\mathrm{W}}(X), \hat{\Omega}_{\mathrm{W}}(X,t)\right]_{\mathrm{P}} \\ & + \frac{1}{2}\left(\left[\hat{H}_{\mathrm{W}}(X), \hat{\Omega}_{\mathrm{W}}(X,t)\right]_{\mathrm{P}} - \left[\hat{\Omega}_{\mathrm{W}}(X,t), \hat{H}_{\mathrm{W}}(X)\right]_{\mathrm{P}}\right) \\ & - \frac{i}{2}\left(\left[\hat{\Gamma}_{\mathrm{W}}(X), \hat{\Omega}_{\mathrm{W}}(X,t)\right]_{\mathrm{P}} + \left[\hat{\Omega}_{\mathrm{W}}(X,t), \hat{\Gamma}_{\mathrm{W}}(X)\right]_{\mathrm{P}}\right) . \end{aligned} \tag{33}$$

Equation (33) provides an equation of motion for the density matrix of a hybrid quantum-classical system. It is a valid approximation of the true and complete quantum dynamics when the degrees of freedom of the composite system have two different De Broglie wavelengths, one short and one much longer long. Equation (33) is exact when the decay operator $\hat{\Gamma}_{\mathrm{W}}(X)$ is linear in X, $\hat{H}_{\mathrm{W}}(X)$ is at most quadratic in the X coordinates and is linearly coupled through the Xs with the quantum subsystem. Equation (33) defines non-Hermitian dynamics for a hybrid quantum-classical system when the decay operator $\hat{\Gamma}_{\mathrm{W}}(X)$ couples the subsystem with the bath.

6.1. Pure quantum decay operator. An important special case arises when the decay operator $\hat{\Gamma}$ does not depend on the bath coordinates. Hence, Equation (33) reduces to

$$\begin{aligned}\frac{\partial}{\partial t}\hat{\Omega}_{\rm W}(X,t) = & - \frac{i}{\hbar}\left[\hat{H}_{\rm W}(X),\hat{\Omega}_{\rm W}(X,t)\right] - \frac{1}{\hbar}\left\{\hat{\Gamma},\hat{\Omega}_{\rm W}(X,t)\right\} \\ & + \frac{1}{2}\left(\left[\hat{H}_{\rm W}(X),\hat{\Omega}_{\rm W}(X,t)\right]_{\rm P} - \left[\hat{\Omega}_{\rm W}(X,t),\hat{H}_{\rm W}(X)\right]_{\rm P}\right) . \end{aligned} \quad (34)$$

Equation (34) describes two effects: probability leakage (or pumping) of a quantum subsystem and fluctuations arising from the coupling to a classical bath. Because of Eq. (34), the trace of $\hat{\Omega}_{\rm W}(X,t)$ is not conserved:

$$\frac{d}{dt}{\rm Tr}'\int dX\hat{\Omega}_{\rm W}(X,t) = \frac{d}{dt}\widetilde{\rm Tr}\left[\hat{\Omega}_{\rm W}({\rm X,t})\right] \neq 0\,, \quad (35)$$

where we have denoted with the symbol ${\rm Tr}'$ a partial trace over the quantal degrees of freedom, with $\int dX$ the phase space integral, and with the symbol $\widetilde{\rm Tr}$ both of them. The evolution in time of the trace is given by

$$\frac{d}{dt}\widetilde{\rm Tr}\left(\hat{\Omega}_{\rm W}(X,t)\right) = -\frac{2}{\hbar}{\rm Tr}'\left(\hat{\Gamma}\hat{\Omega}_{\rm S}(t)\right) . \quad (36)$$

where $\hat{\Omega}_{\rm S} = \int dX\hat{\Omega}_{\rm W}(X)$.

Equation (36) is derived using the identities

$$\begin{aligned} \widetilde{\rm Tr}\left(\left[\hat{H}_{\rm W},\hat{\Omega}_{\rm W}\right]\right) &= 0\,, & (37)\\ \widetilde{\rm Tr}\left(\left[\hat{H}_{\rm W},\hat{\Omega}_{\rm W}\right]_{\rm P} - \left[\hat{\Omega}_{\rm W},\hat{H}_{\rm W}\right]_{\rm P}\right) &= 0\,, & (38)\\ \widetilde{\rm Tr}\left(\left[\hat{\Gamma},\hat{\Omega}_{\rm W}\right]\right) &= 2{\rm Tr}'\left(\hat{\Gamma}\hat{\Omega}_{\rm S}\right) . & (39)\end{aligned}$$

Equation (36) is analogous to Eq. (11) and implies the non-conservation of the probability of the hybrid quantum-classical system. A normalized density matrix is introduced as

$$\hat{\rho}_{\rm W}(X,t) = \frac{\hat{\Omega}_{\rm W}(X,t)}{\widetilde{\rm Tr}\left(\hat{\Omega}_{\rm W}(X,t)\right)} . \quad (40)$$

The definition of $\rho_{\rm W}(X,t)$ in Eq. (40) can be used to calculate averages of the dynamical variables of the hybrid quantum classical system with a probabilistic meaning. Using Eqs. (34) and (36), we obtain the equation of motion of $\hat{\rho}_{\rm W}(X,t)$:

$$\begin{aligned}\frac{\partial}{\partial t}\hat{\rho}_{\rm W}(X,t) = & -\frac{i}{\hbar}\left[\hat{H}_{\rm W},\hat{\rho}_{\rm W}(X,t)\right] + \frac{1}{2}\left[\hat{H}_{\rm W},\hat{\rho}_{\rm W}(X,t)\right]_{\rm P} - \frac{1}{2}\left[\hat{\rho}_{\rm W}(X,t),\hat{H}_{\rm W}\right]_{\rm P} \\ & - \frac{1}{\hbar}\left\{\hat{\Gamma},\hat{\rho}_{\rm W}(X,t)\right\} + \frac{2}{\hbar}\hat{\rho}_{\rm W}(X,t)\widetilde{\rm Tr}\left(\hat{\Gamma}\hat{\rho}_{\rm W}(X,t)\right) . \end{aligned} \quad (41)$$

Equation (41) is non-linear.

7. Non-Hermitian linear entropy for hybrid quantum-classical systems

In order to try to build possible measures of quantum information (Gemmer *et al.* 2005; Nielsen and Chuang 2010; Mahler 2015) for systems with general non-Hermitian Hamiltonians, one can start by defining an entropy functional (Von Neumann 1955; Ohya and Petz 2004). To this end, a non-Hermitian generalization of the von Neumann entropy has been introduced in Sergi and Zloshchastiev (2016). Nevertheless, entropies of the von Neumann form cannot be used when quantum theory is formulated by means of the Wigner function (Manfredi and Feix 2000). Since the (partial) Wigner representation is particularly useful in order to derive a mixed quantum-classical description of non-Hermitian systems (Sergi 2015), it becomes interesting to study the properties of the so-called linear entropy (Zurek *et al.* 1993; Pattanayak 1999; Manfredi and Feix 2000) and its generalization to the case of open quantum systems described by general non-Hermitian Hamiltonians. To this end, we present a generalization 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 (Zurek *et al.* 1993; Pattanayak 1999; Manfredi and Feix 2000).

The quantum linear entropy is

$$S_{\rm lin} = 1 - {\rm Tr}\left(\hat{\rho}^2(t)\right) \tag{42}$$

The entropy production is (Sergi and Giaquinta 2016)

$$\dot{S}_{\rm lin} = \frac{4}{\hbar}{\rm Tr}\left[\hat{\Gamma}\hat{\rho}^2(t)\right] - \frac{4}{\hbar}{\rm Tr}\left[\hat{\Gamma}\hat{\rho}(t)\right]{\rm Tr}\left[\hat{\rho}^2(t)\right] \ . \tag{43}$$

We can also introduce a linear entropy (Sergi and Giaquinta 2016) involving the non-normalized density matrix as

$$S_{\rm lin}^{\rm nH} = 1 - {\rm Tr}\left(\hat{\rho}(t)\hat{\Omega}(t)\right) \ . \tag{44}$$

The rate of production of $S_{\rm lin}^{\rm nH}$ is (Sergi and Giaquinta 2016)

$$\dot{S}_{\rm lin}^{\rm nH} = \frac{4}{\hbar}{\rm Tr}\left[\hat{\Gamma}\hat{\rho}(t)\hat{\Omega}(t)\right] - \frac{2}{\hbar}{\rm Tr}\left(\hat{\rho}^2(t)\right){\rm Tr}\left(\hat{\Gamma}\hat{\Omega}(t)\right) \ . \tag{45}$$

7.1. Linear Entropy Production and Constant Decay Operator. We can consider Eqs. (43) and (45) in the case of a decay operator defined by Eq.(26). In such a case, choosing the initial condition ${\rm Tr}\left(\hat{\Omega}(0)\right) = 1$, the evolution of ${\rm Tr}(\hat{\Omega}(t))$ is given by Eq. (35). Using the identities

$$\frac{d}{dt}{\rm Tr}\left(\hat{\Omega}^2(t)\right) = -2\gamma_0{\rm Tr}\left(\hat{\Omega}^2(t)\right) \ , \tag{46}$$

$${\rm Tr}\left(\hat{\Omega}^2(t)\right) = {\rm Tr}\left(\hat{\Omega}^2(0)\right)e^{-2\gamma_0 t} \ , \tag{47}$$

$$-\frac{2}{\hbar}{\rm Tr}\left(\hat{\rho}(t)\left\{\hat{\Gamma},\hat{\rho}(t)\right\}\right) = -2\gamma_0{\rm Tr}\left(\hat{\rho}^2(t)\right) \ , \tag{48}$$

$$\frac{4}{\hbar}{\rm Tr}\left\{\hat{\rho}^2(t){\rm Tr}\left[\hat{\Gamma}\hat{\rho}(t)\right]\right\} = 2\gamma_0{\rm Tr}\left[\hat{\rho}^2(t)\right] \ , \tag{49}$$

we can calculate

$$\partial_t{\rm Tr}\hat{\rho}^2(t) = 2{\rm Tr}\left[\hat{\rho}(t)\partial_t\hat{\rho}(t)\right] \ , \tag{50}$$

obtaining

$$\partial_t{\rm Tr}\hat{\rho}^2(t) = -2\gamma_0{\rm Tr}\left[\hat{\rho}^2(t)\right] + 2\gamma_0{\rm Tr}\left[\hat{\rho}^2(t)\right] = 0 \ . \tag{51}$$

Upon choosing $\mathrm{Tr}\left(\hat{\rho}^2(t)\right) = \mathrm{Tr}\left(\hat{\rho}^2(0)\right) = \mathrm{const}$, Eq. (43) finally becomes

$$\dot{S}_{\mathrm{lin}} = 2\gamma_0 \mathrm{Tr}\left(\hat{\rho}^2(0)\right) - 2\gamma_0 \mathrm{Tr}\left(\hat{\rho}^2(t)\right) = 0 \,. \tag{52}$$

According to Eq. (52), S_{lin} is not suitable for describing the information flow in non-Hermitian systems.

Equation (45) becomes

$$\dot{S}^{\mathrm{nH}}_{\mathrm{lin}} = \gamma_0 \left[\mathrm{Tr}\hat{\Omega}^2(0)\right] e^{-\gamma t} \,. \tag{53}$$

Integrating Eq. (53) between 0 and t we obtain

$$S^{\mathrm{nH}}_{\mathrm{lin}} = \left(1 - e^{-\gamma_0 t}\right) \mathrm{Tr}\left(\hat{\Omega}^2(0)\right) \,. \tag{54}$$

According to Eq. (54), the linear entropy $S^{\mathrm{nH}}_{\mathrm{lin}}$ increases from the value of 0 at $t = 0$ to the plateau value of $\mathrm{Tr}\left(\hat{\Omega}^2(0)\right)$ at $t = \infty$.

Given the chosen initial condition, *e.g.*, $\mathrm{Tr}\left(\hat{\Omega}(0)\right) = 1$, $\mathrm{Tr}\left(\hat{\Omega}^2(0)\right)$ describes the purity of the non-Hermitian system. Hence, Eq. (54) monitors the loss of the initial purity of the system.

7.2. Non-Hermitian Entropy Production in Hybrid Quantum-Classical Systems. When defining the quantum entropy in terms of the Wigner function (Manfredi and Feix 2000), since the Wigner function $f_{\mathrm{W}}(x, X, t)$ can be negative, we cannot adopt the von Neumann definition, *e.g.*, Eq. (20). However, we can use the linear entropy (Zurek *et al.* 1993; Pattanayak 1999; Manfredi and Feix 2000), $S_{\mathrm{lin}} = 1 - \mathrm{Tr}(\hat{\rho}^2)$, and apply the Wigner transform:

$$S_{\mathrm{lin}} = 1 - (2\pi\hbar)^{n+N} \int dx dX f^2_{\mathrm{W}}(x, X, t) \,. \tag{55}$$

For a hybrid quantum-classical system, the generalization of Eq. (55) is given by

$$S_{\mathrm{lin,W}} = 1 - (2\pi\hbar)^N \mathrm{Tr}' \int dX \hat{\rho}^2_{\mathrm{W}}(X, t) = 1 - (2\pi\hbar)^N \widetilde{\mathrm{Tr}}\left[\hat{\rho}^2_{\mathrm{W}}(X, t)\right] \,. \tag{56}$$

The non-Hermitian evolution in the classical environment, defined by Eq. (41), implies the linear entropy production (Sergi and Giaquinta 2016)

$$\dot{S}_{\mathrm{lin,W}} = \frac{4}{\hbar}(2\pi\hbar)^N \left[\widetilde{\mathrm{Tr}}\left(\hat{\Gamma}\hat{\rho}^2_{\mathrm{W}}(t)\right) - \widetilde{\mathrm{Tr}}\left(\hat{\Gamma}\hat{\rho}_{\mathrm{W}}(t)\right)\widetilde{\mathrm{Tr}}\left(\hat{\rho}^2_{\mathrm{W}}(t)\right)\right] \,. \tag{57}$$

We can also introduce a non-Hermitian linear entropy (Sergi and Giaquinta 2016) as

$$S^{\mathrm{nH}}_{\mathrm{lin},W} = 1 - (2\pi\hbar)^N \widetilde{\mathrm{Tr}}\left[\hat{\rho}_{\mathrm{W}}(X, t)\hat{\Omega}_{\mathrm{W}}(X, t)\right] \,. \tag{58}$$

The entropy production is given by (Sergi and Giaquinta 2016)

$$\dot{S}^{\mathrm{nH}}_{\mathrm{lin,W}} = \frac{4(2\pi\hbar)^N}{\hbar}\widetilde{\mathrm{Tr}}\left(\hat{\Gamma}\hat{\rho}_{\mathrm{W}}(X)\hat{\Omega}_{\mathrm{W}}(X)\right) - \frac{2(2\pi\hbar)^N}{\hbar}\widetilde{\mathrm{Tr}}'\left(\hat{\Gamma}\hat{\Omega}_{\mathrm{W}}\right)\widetilde{\mathrm{Tr}}\left(\hat{\rho}^2_{\mathrm{W}}\right) \,. \tag{59}$$

7.2.1. *Linear Entropy Production and Constant Decay Operator.* If $\hat{\Gamma}$ is given by Eq. (26), Eq. (34) simplifies to

$$\begin{aligned}\frac{\partial}{\partial t}\hat{\Omega}_{\mathrm{W}}(X,t) &= -\frac{i}{\hbar}\left[\hat{H}_{\mathrm{W}},\hat{\Omega}_{\mathrm{W}}(X,t)\right]+\frac{1}{2}\left[\hat{H}_{\mathrm{W}},\hat{\Omega}_{\mathrm{W}}(X,t)\right]_{\mathrm{P}}\\ &- \frac{1}{2}\left[\hat{\Omega}_{\mathrm{W}}(X,t),\hat{H}_{\mathrm{W}}\right]_{\mathrm{P}}-\gamma_0\hat{\Omega}_{\mathrm{W}}(X,t)\,, \qquad (60)\end{aligned}$$

and Eq. (36) becomes

$$\frac{d}{dt}\widetilde{\mathrm{Tr}}\left(\hat{\Omega}_{\mathrm{W}}(X,t)\right)=-\gamma_0\widetilde{\mathrm{Tr}}\left(\hat{\Omega}_{\mathrm{W}}(X,t)\right)\,. \qquad (61)$$

Requiring that $\widetilde{\mathrm{Tr}}\left(\hat{\Omega}_{\mathrm{W}}(X,0)\right)=1$, Eq. (61) can be integrated giving

$$\widetilde{\mathrm{Tr}}\left(\hat{\Omega}_{\mathrm{W}}(X,t)\right)=e^{-\gamma_0 t}\,. \qquad (62)$$

Equation (41) becomes

$$\frac{\partial}{\partial t}\hat{\rho}_{\mathrm{W}}(X,t) = -\frac{i}{\hbar}\left[\hat{H}_{\mathrm{W}},\hat{\rho}_{\mathrm{W}}(X,t)\right]+\frac{1}{2}\left[\hat{H}_{\mathrm{W}},\hat{\rho}_{\mathrm{W}}(X,t)\right]_{\mathrm{P}}-\frac{1}{2}\left[\hat{\rho}_{\mathrm{W}}(X,t),\hat{H}_{\mathrm{W}}\right]_{\mathrm{P}} \qquad (63)$$

Equations. (57) and (59) can be written as

$$\begin{aligned}\dot{S}_{\mathrm{lin,W}} &= 0\,, \qquad (64)\\ \dot{S}^{\mathrm{nH}}_{\mathrm{lin,W}} &= (2\pi\hbar)^N\gamma_0 e^{\gamma_0 t}\widetilde{\mathrm{Tr}}\left(\hat{\Omega}^2_{\mathrm{W}}(X,t)\right)\,. \qquad (65)\end{aligned}$$

We can derive

$$\widetilde{\mathrm{Tr}}\left(\hat{\Omega}^2_{\mathrm{W}}(X,t)\right)=\widetilde{\mathrm{Tr}}\left(\hat{\Omega}^2_{\mathrm{W}}(X,0)\right)e^{-2\gamma_0 t} \qquad (66)$$

and substitute it into Eq. (65) and integrating we obtain

$$S^{\mathrm{nH}}_{\mathrm{lin,W}}=(2\pi\hbar)^N\widetilde{\mathrm{Tr}}\left(\hat{\Omega}^2_{\mathrm{W}}(X,0)\right)\left(1-e^{-\gamma_0 t}\right)\,. \qquad (67)$$

The rate of production of the quantum-classical entropy in Eq. (67) monitors the flow of information associated to the decay of the purity (for positive γ_0) of the non-Hermitian system hybrid quantum-classical.

8. Conclusions

The dynamics of open quantum systems may be studied by means of non-Hermitian Hamiltonians and non-Hermitian dynamics. In particular, such an approach naturally arises in the case of a subsystem interacting with a continuum of states because of the Fock and Krylov theorem. More in general, quantum subsystems with probability sinks/sources are naturally described by non-Hermitian Hamiltonians.

In this paper, we have reviewed an approach to non-Hermitian dynamics in terms of the density matrix. We have shown both how to derive the equations of motion of the density matrix and how to define properly statistical averages. It turns out that the laws of evolution of the normalized density matrix are intrinsically non-linear. We have shown how to define correlation functions and a non-Hermitian entropy with a non-zero production.

The formalism has been generalized to the case of hybrid quantum-classical systems using a partial Wigner representation. The equations of motion and the statistical averages are defined analogously to the pure quantum case. However, the definition of the entropy requires to introduce a non-Hermitian linear entropy functional. The definition of correlation functions and entropy functionals supports the idea that the statistical states of systems described by non-Hermitian Hamiltonians require both the non-normalized and normalized density matrix to be properly characterized.

Open areas of research over which we will focus in the near future are both the development of efficient algorithms for integrating non-Hermitian dynamics and the study of the interplay between sinks/source and noise determined by the classical bath.

Appendix A. Hamiltonian shift transformations and entropy

Following the discussions presented in Sergi and Zloshchastiev (2013) and Zloshchastiev and Sergi (2014), let us consider the following transformation of the $\hat{\Gamma}$ operator

$$\hat{\Gamma} = \hat{\Gamma}' + \frac{1}{2}\hbar\alpha\hat{I}, \tag{68}$$

where α is an arbitrary real constant and $\hat{I}$ is the unity operator. This transformation is a subset of the transformation

$$\hat{\mathscr{H}} = \hat{\mathscr{H}}' + c_0\hat{I}, \tag{69}$$

c_0 being an arbitrary complex number, which is the non-Hermitian generalization of the energy shift in Hermitian quantum mechanics.

In Sergi and Zloshchastiev (2013) it was shown that the non-unitary evolution of the normalized density matrix, defined by Eq. (14), is invariant under the transformation (68). Consequently, one finds

$$\hat{\rho} = \hat{\rho}',\ S_{\mathrm{vN}} = S'_{\mathrm{vN}}\ r., \tag{70}$$

One can conclude obviously that the von Neumann entropy is not affected by the transformation (68).

Instead, Equation (11) is not invariant under the shift (68). If $\hat{\mathscr{H}}$ is time-independent, the application of the shift (68) to Eq. x (11) makes the non-normalized density matrix acquire an exponential factor:

$$\hat{\Omega} = \hat{\Omega}' e^{-\alpha t}\ . \tag{71}$$

Hence, using relation (24), one obtains

$$S_{\mathrm{nH}} = S'_{\mathrm{vN}} - k_B \ln \mathrm{Tr}\,\hat{\Omega} = S'_{\mathrm{nH}} + k_B\alpha t, \tag{72}$$

indicating that the nH entropy is affected by the shift (68).

Appendix B. Time correlation functions in Hermitian Quantum Mechanics

Given two arbitrary operators $\hat{\chi}_1$ and $\hat{\chi}_2$, it is known that their time-dependent correlation function in the Heisenberg picture of Hermitian quantum mechanics is defined as

$$C_{\chi_1\chi_2}(t_2,t_1) \equiv \langle\hat{\chi}_1(t_2)\hat{\chi}_2(t_1)\rangle \equiv \mathrm{Tr}\left(\hat{\chi}_1(t_2)\hat{\chi}_2(t_1)\hat{\rho}(0)\right). \tag{73}$$

Now, assuming that the evolution takes place under the Hermitian operator $\hat{H}_+$, upon using the definition of the time-dependent Heisenberg operator

$$\hat{\chi}_1(t) \equiv \exp\left[\frac{it}{\hbar}\hat{H}_+\right]\hat{\chi}_1 \exp\left[\frac{-it}{\hbar}\hat{H}_+\right]\ , \tag{74}$$

and the properties of the trace, the Hermitian correlation function (73) can be rewritten as

$$C_{\chi_1\chi_2}(t_2,t_1) = \mathrm{Tr}\left\{\hat{\chi}_1 \exp\left[\frac{-i(t_2-t_1)}{\hbar}\hat{H}_+\right]\hat{\chi}_2\hat{\rho}_{\hat{H}_+}(t_1)\exp\left[\frac{i(t_2-t_1)}{\hbar}\hat{H}_+\right]\right\}, \quad (75)$$

where

$$\hat{\rho}_{\hat{H}_+}(t_1) \equiv \exp\left[\frac{-it_1}{\hbar}\hat{H}_+\right]\hat{\rho}\exp\left[\frac{it_1}{\hbar}\hat{H}_+\right]. \quad (76)$$

The definition given in Eq. (75) represents the correlation function written in the Schrödinger picture, where the time dependence has been transferred from the operators to the density matrix. We take the Schrödinger form of the correlation function as the basis for the generalization to the non-Hermitian case, which is treated in Sec. **4**.

Appendix C. Von Neumann Entropy

Let us consider Hermitian quantum mechanics and introduce a normalized density matrix $\hat{\Xi}(t)$ obeying the quantum Liouville equation:

$$\frac{d}{dt}\hat{\Xi}(t) = -\frac{i}{\hbar}\left[\hat{H},\hat{\Xi}(t)\right] . \quad (77)$$

The von Neumann entropy is defined as

$$S_{\mathrm{vN}}(t) = -k_B \mathrm{Tr}\left\{\hat{\Xi}(t)\ln[\hat{\Xi}(t)]\right\} , \quad (78)$$

where k_B is Boltzmann's constant. The rate of entropy production is

$$\dot{S}_{\mathrm{vN}}(t) = -k_B \mathrm{Tr}\left\{\frac{d}{dt}\hat{\Xi}(t)\ln[\hat{\Xi}(t)]\right\} = 0 . \quad (79)$$

Von Neumann entropy in Eq. (78) describes well processes in equilibrium quantum systems. However, non-equilibrium situations are not well described since Eq. (79) implies that there can be no entropy increase. In order to agree with the second law of thermodynamics, one must either coarse-grain the entropy, *e.g.*, see Oerter (2011), or adopt so-called relevant entropies (Balian 1999). For such reasons, non-Hamiltonian structures have been invoked (Nosé 1984; Andrey 1985; Hoover 1985; Andrey 1986; Sergi and Ferrario 2001; Sergi 2003; Sergi and Giaquinta 2007; Sergi and Giaquinta 2016) to find an agreement between microscopic dynamics and the second law of thermodynamics.

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