Mixed-state evolution in the presence of gain and loss

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Over the past decade there have been considerable research interests, both theoretical and experimental, into the static and dynamic properties of classical and quantum systems for which gain and loss are present [1, 2]. This is in part motivated by the realisation that when a system is placed in a configuration in which its energy or amplitude is transferred into its environment through one channel, but at the same time is amplified by the same amount through another channel, the resulting dynamics can exhibit features that are similar to those seen in Hamiltonian dynamical systems. The time evolution of such a system can be described by a Hamiltonian that is symmetric under a space-time reflection, that is, invariant under the parity-time (PT) reversal.

Interest in the theoretical study of PT symmetry was triggered by the discovery that complex PT-symmetric Hamiltonians can possess entirely real eigenvalues [3]. One distinguishing feature of PT-symmetric quantum systems is the existence of phase transitions associated with the breakdown of the symmetry. That is, depending on the values of the matrix elements of the Hamiltonian, its eigenstates may or may not be symmetric under the parity-time reversal. In the ‘unbroken phase’ where the eigenstates respect PT symmetry, the eigenvalues are real and there exists a similarity transformation that maps a local PT-symmetric Hamiltonian into a typically nonlocal Hermitian Hamiltonian [1, 5]: whereas in the ‘broken phase’ the eigenvalues constitute complex conjugate pairs. The transition between these phases is similar to second-order phase transitions in statistical mechanics, accompanied by singularities in the covariance matrix of the estimators for the parameters in the Hamiltonian (this can be seen by using methods of information geometry [6]).

Experimental realisations of these phenomena are motivated in part by the observation that the presence of a loss, which traditionally has been viewed as an undesirable feature, can positively be manipulated so as to generate unexpected interesting effects (cf. [7]). In particular, PT phase transitions have been predicted or observed in laboratory experiments for a range of systems; most notably in optical waveguides [8–10], but also in laser physics [11–13], in electric circuits [14, 15], or in microwave cavity [16].

In the quantum context, theoretical investigations into the properties and predictions of the evolution equation where gain and loss are present have thus far been confined primarily to pure states. However, quantum systems are commonly described by mixed states, especially when they are subject to manipulations. Therefore, to describe or predict the behaviour of such quantum systems it is necessary to understand how a given mixed state might evolve. For this purpose we seek a complex extension of the von-Neumann equation that reduces to the Schrödinger equation when restricted to pure states.

To describe various forms of dissipation or noise, Lindblad-type equations [17, 18] are often considered. They can be related to pure state evolutions with complex Hamiltonians, but typically involve stochastic terms [19] that distinguish them from the complex Schrödinger equation. In particular, an initially pure state tends to evolve into a mixed state due to the influence of noise. Here we propose an alternative model that describes the evolution of a generic density matrix in the context of gain and loss such that it reduces to the complex Schrödinger equation for pure states. This model can be further extended to include additional dissipation or noise in the form of Lindblad terms or other effective descriptions, depending on the context. Our model is given by the dynamical equation

\[
\frac{d\rho}{dt} = -i[H, \rho] - ([\Gamma, \rho]_+ - 2\text{tr}(\rho \Gamma))\rho, \tag{1}
\]

where $H = H^\dagger$ is the Hermitian part of the Hamiltonian generating ambient unitary motion, $\Gamma = \Gamma^\dagger$ is the skew-Hermitian part of the Hamiltonian governing gain and loss, and $[\Gamma, \rho]_+ = \Gamma \rho + \rho \Gamma$ denotes the symmetric product. We refer to (1) as the covariance equation,
on account of the structure of the term involving $\Gamma$. In this Letter we shall motivate equation (1), investigate its properties in detail, identify the structure of stationary states, and show that a PT phase transition manifests itself by means of the time average of observables.

An experimental implementation of an evolution of a purely quantum system requires a careful balancing of loss and gain. It should be evident, however, that the realisation of such an evolution for a pure state is difficult, to say the least, since energetic manipulations of a quantum system inadvertently perturb the system. To account for the possible impact of uncontrollable ambient noise, we consider an extension of the model (1) that includes an additional term generated by uniform Gaussian perturbations. We shall study dynamical aspects of the extended model, identify the existence of equilibrium states by means of numerical studies, and show how PT phase transitions can be suppressed by noise.

Let us begin by motivating the introduction of the covariance equation (1). In the case of pure states, the norm-preserving evolution equation generated by a complex Hamiltonian $K = H - i\Gamma$ is given by

$$\frac{d\psi}{dt} = -i(H - \langle H \rangle)\psi - (\Gamma - \langle \Gamma \rangle)\psi. \quad (2)$$

Together with an additional equation for the overall probability $\dot{N} = -(\Gamma)N$, equation (2) is equivalent to the familiar complexified Schrödinger equation. The benefit of (2) is that it is defined on the projective Hilbert space.

Besides the covariance equation (1), there are many alternative evolution equations for mixed states that reduce to (2) when restricted to a pure state satisfying $\rho^2 = \rho$. An example is given by the double-bracket equation

$$\frac{d\rho}{dt} = -i[H, \rho] - [[\Gamma, \rho], \rho]. \quad (3)$$

For $\Gamma \propto H$, the norm-preserving equations (2) and (3) have been considered by Gisin [20] as candidate equations to describe dissipative quantum evolution. That (1) and (3) are identical for a pure state can be seen by observing that $\rho \Gamma \rho = \text{tr}(\rho \Gamma \rho)$ when $\rho^2 = \rho$. Among the possible dynamical equations, the covariance equation (1) is singled out on account of the fact that its formal solution, given an initial state $\rho_0$, can be expressed in the form

$$\rho_t = \frac{e^{-i(\langle H - \Gamma \rangle)t} \rho_0 e^{i(\langle H + \Gamma \rangle)t}}{\text{tr}(e^{-i(\langle H - \Gamma \rangle)t} \rho_0 e^{i(\langle H + \Gamma \rangle)t})}, \quad (4)$$

which provides a natural generalisation of its unitary counterpart when $\Gamma = 0$. Similarly, the dynamical equation satisfied by an observable $\langle F \rangle = \text{tr}(F \rho_t)$ reads

$$\frac{d\langle F \rangle}{dt} = i\langle [H, F] \rangle - \langle [\Gamma, F] \rangle_+ + 2 \langle \Gamma \rangle \langle F \rangle, \quad (5)$$

which agrees with the complex extension of the Heisenberg equation of motion obtained in Refs. [21, 22] for pure states. Note that the covariance-type structure in (1) has also appeared in the contexts of approach to thermal equilibrium [21], dissipative motion [20, 20], and constrained quantum dynamics [27].

Key properties of the evolution equation (1) can be summarised as follows: (i) It preserves the overall probability so that $\text{tr}(\rho_t) = 1$ for all $t \geq 0$. This can be checked by verifying the relation $\partial_t \text{tr}(\rho) = 0$. (ii) Unlike a unitary time evolution, it does not in general preserve the purity of the state. In particular, we have

$$\frac{d}{dt} \text{tr} \rho^2 = -4(\text{tr}(\Gamma \rho^2) - \text{tr}(\rho \Gamma \rho)) \rho^2, \quad (6)$$

and in general the right side of (6) is nonzero when $\rho^2 \neq \rho$. Thus, the purity of the initial state is not preserved by (1) when $\rho$ is not a fixed point of the dynamics, but an initially pure state will remain pure. When $H = 0$, we have the relation

$$\frac{d}{dt} \text{tr} \rho \Gamma = -2 \text{var}_\rho \Gamma \leq 0, \quad (7)$$

from which it follows that: (iii) The imaginary part $\Gamma$ of the Hamiltonian drives every state towards the ground state of $\Gamma$. (iv) The evolution equation (1) preserves the positivity of $\rho$, and is ‘autonomous’ in the sense that the dynamical trajectory in the space of density matrices is determined uniquely by the specification of the initial density matrix $\rho_0$, and is not dependent on the kind of probabilistic mixture the initial state might represent. (v) In the case of a unitary motion, the speed $v = \text{tr}(\partial_t \sqrt{\rho})^2$ of the evolution of the state is constant of motion and is given by the Wigner-Yanase skew information $v = 2\text{tr}(H^2 \rho) - 2\text{tr}(H \sqrt{\rho}H \sqrt{\rho})$ [28], which reduces to the Anandan-Aharonov relation $v = 2\Delta H^2$ for pure states $\sqrt{\rho} = \rho$. When the dynamics is governed by a complex Hamiltonian $H - i\Gamma$, the evolution speed is not a constant of motion and is given by the expression

$$v = 2 \left( \text{tr}(H^2 \rho) - \text{tr}(H \sqrt{\rho}H \sqrt{\rho}) \right) - 2i \text{tr}(\langle H, \Gamma \rangle \rho) + 2 \left( \text{tr}(\Gamma^2 \rho) + \text{tr}(\Gamma^\dagger \Gamma - \Gamma \Gamma^\dagger) - 2(\text{tr}(\Gamma \rho))^2 \right), \quad (8)$$

which reduces to $v = 2\Delta H^2 + 2\Delta \Gamma^2 - 2i\langle [\Gamma, H] \rangle$ for pure states.

Next we identify the fixed points of the dynamics. We begin by the following elementary observation concerning eigenstates of a generic complex Hamiltonian $K = H - i\Gamma$. Suppose that $|\phi\rangle$ is a normalised eigenstate of $K$:

$$K|\phi\rangle = \lambda|\phi\rangle. \quad (9)$$

Then, if $\lambda = E - i\gamma$, where $E, \gamma$ real, we have $\langle \phi|H|\phi\rangle = E$ and $\langle \phi|\Gamma|\phi\rangle = \gamma$. In particular, an eigenfunction $|\phi\rangle$ of a complex Hamiltonian $K$ has a real eigenvalue if and only if $\langle \phi|\Gamma|\phi\rangle = 0$. With this in mind, we establish the following results: (vi) Every eigenstate of the Hamiltonian $K$, irrespective of whether the eigenvalue is real, is a fixed point of the motion (1). They are the only stationary states that are pure. (vii) The mixed stationary
states of the dynamical equation (1) consist of convex combinations of the eigenstates of the Hamiltonian $K$ associated with real eigenvalues. Furthermore, the totality of mixed stationary states lies on the subspace of density matrices for which $\text{tr}(\Gamma \rho) = 0$.

The statement (vi) can be established as follows: From (4), if we set $\rho_0 = |\phi\rangle \langle \phi|$, where $|\phi\rangle$ is an eigenstate of $K$ with eigenvalue $E - i \gamma$, then we have

$$e^{-iKt} \rho_0 e^{iKt} = e^{-2\gamma t} |\phi\rangle \langle \phi|,$$

and hence $\text{tr}(e^{-iKt} \rho_0 e^{iKt}) = e^{-2\gamma t}$. Putting these together, it follows that $\rho_t = \rho_0$. To establish (vii) we set

$$\rho_0 = \sum_{j=1}^{m} p_j |\phi_j\rangle \langle \phi_j|,$$

where $\{p_j\}$ are nonnegative numbers adding up to unity, $\{|\phi_j\rangle\}$ are eigenstates of $K$ with real eigenvalues, and $m$ is the number of real eigenvalues. Substituting (11) in (4), a short calculation shows that $\rho_t = \rho_0$. To show that the stationarity breaks down if the convex combination contains eigenstates with complex eigenvalues, suppose that we add terms in (11) associated with complex eigenvalues. Then from (4) we obtain

$$\rho_t = \sum_{j,k} p_j e^{-2\gamma j t} |\phi_j\rangle \langle \phi_j| \sum_{j,k} p_k e^{-2\gamma k t},$$

where $\gamma_j = \langle \phi_j| \Gamma |\phi_j\rangle$. Since at least one of the $\gamma_j$ is nonzero by assumption, it follows that $\rho_t \neq \rho_0$. Finally, since all terms in (11) have the property that $\langle \phi_k| \Gamma |\phi_k\rangle = 0$, it follows that $\text{tr}(\Gamma \rho) = 0$ for all stationary states.

A corollary to (12) is that: (viii) If the initial state $\rho_0$ admits an eigenfunction expansion such that one or more terms are associated with complex eigenvalues, then

$$\lim_{t \to \infty} \rho_t = |\phi^*\rangle \langle \phi^*|,$$

where $|\phi^*\rangle$ is the member of the eigenfunctions $\{|\phi_j\rangle\}$ in the expansion for which the associated imaginary part $\gamma_j$ of the eigenvalue takes maximum value. Hence the flow structure in the space of density matrices, when there are imaginary eigenvalues, is rather complex and intricate in higher dimensions, where for each eigenstate $|\phi\rangle \langle \phi|$ associated with an imaginary eigenvalue there is a continuum of states for which $|\phi\rangle \langle \phi|$ is an asymptotic attractor. If, however, there is no real eigenvalue at all, then this segmentation disappears and the eigenstate with the largest $\gamma$ becomes the single attractor.

To investigate the behaviour in the PT-symmetric phase where all eigenvalues are real, let us put

$$\rho_0 = \sum_{j,k} \rho_{jk} |\phi_j\rangle \langle \phi_k|.$$  

Then the trace condition $\text{tr}(\rho_0) = 1$ implies that

$$\sum_{j=1}^{m} \rho_{jj} + \sum_{j \neq k} \rho_{jk} \langle \phi_k | \phi_j \rangle = 1,$$

since the eigenfunctions are not orthogonal when $\Gamma \neq 0$.

Substituting (14) in (4) we find

$$\rho_t = \frac{\sum_{j,k} \rho_{jk} e^{-i\omega_{jk} t} |\phi_j\rangle \langle \phi_k|}{\sum_{j,k} \rho_{jk} e^{-i\omega_{jk} t} |\phi_k\rangle \langle \phi_j|},$$

where $\omega_{jk} = E_j - E_k$. We thus deduce the following: (ix) When all eigenvalues of the Hamiltonian $K$ are real, every orbit is periodic if the energy eigenvalues are commensurable; otherwise, the evolution is typically ergodic on a small toroidal subspace of the space of density matrices containing $\rho_0$. Therefore, in the PT-symmetric phase, dynamical features of the system are analogous to those of a unitary system, albeit differences in detail such as the lack of constancy of the evolution speed. The similarity is due to the fact that the nonlinearity of (1) is merely to preserve $\text{tr}(\rho)$; hence the evolution equation cannot generate nontrivial fixed points such as saddle points.

In figure 1 we illustrate integral curves of (1) for a two-level example system with the Hamiltonian $K = \sigma_x - i \gamma \sigma_z$, where $\gamma$ is a real parameter. Note that the eigenvalues of $K$ are given by $\lambda_{\pm} = \pm \sqrt{1 - \gamma^2}$. Hence the symmetry is broken if $|\gamma| > 1$. Observe that in the unbroken phase the orbits are periodic, and hence the purity of mixed states oscillates, while in the broken phase every mixed state is asymptotically purified to the ground state. To visualise the effect of the phase transition it will be useful to introduce an 'order parameter' $m$ by the time average of $\sigma_z$:

$$m = \lim_{T \to \infty} \frac{1}{T} \int_0^T \text{tr}(\sigma_z \rho_t) dt.$$  

Note that $m$ is independent of the choice of the initial condition $\rho_0$. In figure 2(a) we plot $m$ as a function of $\gamma^{-1}$, showing the characteristic behaviour of the order parameter in a second-order phase transition.

Perhaps a surprising feature of the foregoing analysis is the observation that in the broken phase where eigenvalues are complex, convex combinations of energy eigenstates are not stationary. On account of the fact that the dynamical equation is autonomous, this implies, in
particular, that if an initial state $\rho_0$ is chosen randomly out of the eigenstates $|\phi_j\rangle\langle\phi_j|$, each one of which is stationary, and the system evolves under the presence of gain and loss such that PT symmetry is broken, then after a passage of time the statistics obtained from $\rho_t$ are different from those obtained from $\rho_0$. This feature has no analogue in the standard unitary theory, and can be used to test the applicability of the model $\mathbf{1}$ in laboratory experiments, provided that a coherent control of the system, in such a way that gain and loss can be balanced without perturbing the system, is possible.

If, on the other hand, a coherent implementation of gain and loss is not feasible, either because of fundamental quantum limits or current technological limits, then it is important to take into account additional effects arising from random perturbations. For this purpose, we shall assume that the model $\mathbf{1}$ remains valid, but in addition the system is perturbed at random. Specifically, we assume that the state is perturbed by Gaussian white noise in every orthogonal direction in the space of pure states, with strength $\sqrt{\kappa}$, where $\kappa \geq 0$. In Ref. $\mathbf{29}$ it was shown that such a perturbation, when averaged out, generates a flow in the space of density matrices given by $\kappa (\mathbb{1} - n\rho)$; this, in turn, leads to the extended model:

$$\frac{d\rho}{dt} = -i[H, \rho] - ([\Gamma, \rho]_+ - 2\text{tr}(\rho \Gamma)\rho) + \kappa (\mathbb{1} - n\rho),$$

where $\kappa \geq 0$ and $n$ is the Hilbert space dimensionality.

We proceed to analyse properties of $\mathbf{18}$. To begin, it should be evident that: (i) The evolution equation $\mathbf{18}$ preserves the overall probability so that $\text{tr}(\rho_t) = 1$ for all $t \geq 0$. On account of the presence of noise, however, an initially pure state ceases to remain pure. In particular, we have: (ii) The evolution of the purity is governed by the equation

$$\frac{d}{dt} \text{tr} \rho^2 = -4\left(\text{tr}(\Gamma \rho^2) - \text{tr}(\rho \Gamma)\text{tr}(\rho^2)\right) + 2\kappa \left(1 - n \text{tr}(\rho^2)\right).$$

Notice that when $\rho^2 = \rho$ the first term in the right side of $\mathbf{19}$ vanishes, whereas the second term is negative. Hence an initially pure state necessarily evolves into a mixed state due to noise. (iii) When $\Gamma = 0$, the solution to the dynamical equation $\mathbf{18}$ takes the form

$$\rho_t = \frac{1}{n} \left[\mathbb{1} + \left(\left.n e^{-iHt} \rho_0 e^{iHt} - \mathbb{1}\right)e^{-\kappa nt}\right]\right],$$

and has a single fixed point $\rho_{\infty} = n^{-1}\mathbb{1}$. This can be seen from the facts that the off diagonal elements of $\kappa (\mathbb{1} - n\rho)$ are negative, and that the diagonal elements are positive (reps. negative) if the diagonal element of $\rho$ is less than (reps. larger than) $n^{-1}$. The effect of the term $\kappa (\mathbb{1} - n\rho)$ therefore is to generate a gradient flow towards the uniformly mixed state $\rho_{\infty} = n^{-1}\mathbb{1}$. (iv) Like the model $\mathbf{1}$, the evolution equation $\mathbf{18}$ is positive and autonomous in the sense described above. (v) The dynamical equation satisfied by an observable $\langle F \rangle = \text{tr}(F\rho_t)$ is given by

$$\frac{d\langle F \rangle}{dt} = i\left[\langle H, F \rangle\right] - \langle [\Gamma, F]_+ \rangle + 2 \langle \Gamma \rangle \langle F \rangle + \kappa (\text{tr}(F) - n\langle F \rangle).$$

To gain insights into fixed-point structures of the extended model $\mathbf{18}$, we have performed numerical studies based on a two-level system with the Hamiltonian $K = \sigma_x - i\gamma \sigma_z$. Our analysis shows that once the noise strength $\kappa$ is turned on, irrespective of its magnitude, the phase transition is suppressed. This can be seen by the consideration of the order parameter $m$. As indicated above, in the noise-free case there is a clear indication of a second-order phase transition at the critical point $\gamma_c = 1$. Under a noisy environment, however, the symmetry is broken for all values of $\gamma \neq 0$; instead, for each value of $\gamma, \kappa$ an equilibrium state $\rho^*$ is established, to which every initial state converges. In figure $\mathbf{2(b)}$ we plot $m$ as a function of $\gamma^{-1}$ for a range of values for $\kappa > 0$, showing the removal of the phase transition, although for sufficiently small $\kappa$ the signature of the transition is visible. We have performed further numerical and analytical studies of the evolution equation $\mathbf{18}$, the results of which indicate that the emergence of a nontrivial equilibrium state is a generic feature of the model.

In summary, we have introduced a model for describing the evolution of a density matrix for a system having gain and loss, and investigated its properties in detail. In particular, we have identified the associated stationary states, and shown the existence of phase transitions in the generic mixed-state context (cf. figure $\mathbf{2(a)}$). We then extended the model to include a noise term, and showed evidences for the existence of equilibrium states that eliminate phase transitions (cf. figure $\mathbf{2(b)}$). The applicability of our models is expected to be verifiable in laboratory experiments.
EMG acknowledges support via the Imperial College JRF scheme. We thank H. F. Jones for comments.