Evolution of Damped Quantum Oscillators in Density Matrix Space

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Abstract. We examine the general form of the generators of time evolution on density matrices of damped oscillators and clarify the conditions that must be fulfilled by them. The generators must be adjoint-symmetric to preserve the hermiticity of density matrices and trace-preserving to conserve probability. The conditions lead to a set of basis generators where generic ones are formed by taking linear sums of the basis over real coefficients. The requirement on the positivity of density matrices then limit the range of the coefficients. In ordinary symmetry on state vectors (pure states) in the Hilbert space, symmetry operators are unitary and factorized. The symmetry on density matrices is more general in the sense that it is not limited to unitary and factorized transformation. The time evolution operators of quantum systems are examples of general transformation that form semigroups, but the generic general transformation is not limited to semigroup.

Keywords: General transformation, Open quantum systems, Damped oscillator, Positivity.

I. INTRODUCTION

In isolated quantum systems, physical states are described by state vectors $|\psi\rangle$ in the Hilbert space. Time evolution of the systems are reversible and initiated by unitary transformation. To describe the evolution of dissipative systems, which are also open quantum systems, in a way parallel to isolated systems, state vectors are no longer sufficient. The loss of quantum correlation in the initial states because of the interactions between system and external environment result in mixed states, which can only be described in terms of density matrices.

The density matrices of isolated systems $\rho_{\rm iso}$ are pure states $|\psi\rangle\langle\psi|$, which evolve reversibly in a factorized form:

$$u|\psi\rangle\langle\psi|u^\dagger , \tag{1}$$

where u is the time evolution operator. On the other hand, the density matrices of dissipative systems are in general mixed states $\sum_i c_i|\psi_i\rangle\langle\psi_i|$. A standard way to obtain the equation of

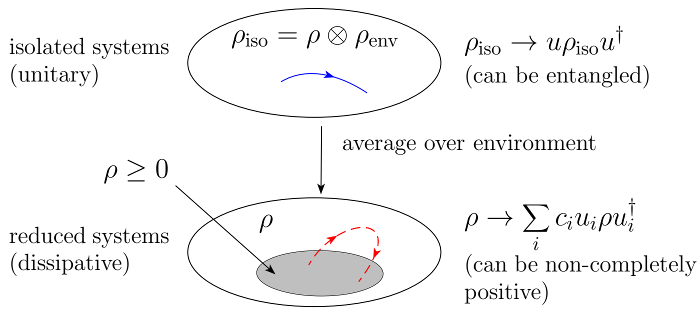

FIGURE 1. Time evolution in isolated and reduced systems. Dashed line shows that some generators occasionally evolve proper ρ into non-positive ρ.

motion of density matrices, ρ, for such systems is to add an auxiliary external environment that interacts with them, see Figure 1. Then with the total system evolves as an isolated system, we average over the influence of the external environment to obtain an effective equation of motion on the system of interest, or the so-called reduced system:

$$\frac{\partial}{\partial t}\rho = -K\rho \ , \tag{2}$$

which is governed by a generator of time evolution K. The equation has solutions that evolve in the positive time direction as a semigroup:

$$\rho(t) = \exp(-Kt)\rho(0) , \qquad t \geq 0 \tag{3}$$

which in general does not have the factorized form (1). Hence, the reduced systems could have general symmetry, in contrast to isolated systems with ordinary symmetry (1).

This process of reducing a full dynamics to a reduced dynamics on the system of interest can be carried out with different methods, usually coupled with some assumptions [1]. If we start with initial states of system and environment that are not correlated, we obtain completely positive maps on ρ where the evolution is guaranteed to be positive [2, 3]. The completely positive maps have the Kossakowski-Lindblad form.

However, if we start with initial states with constituents that are correlated, we obtain maps that are may not even be positive [4, 5]. As a result, proper ρ can evolve into a non-positive one. However, positive domain in which the evolutions of ρ remain positive can be identified [4, 5]. An example is provided by the Caldeira-Leggett (CL) equation [6] that describes the quantum Brownian motion of oscillator in a high temperature bath. Positivity in the density matrices can be violated when the temperature is lowered to a certain extent. Another way to circumvent the defect is through the slippage of initial conditions [7].

In this work, we approach the subject for the system of a quantum oscillator by constructing generators that fulfill conditions required by density matrices. The conditions are sufficient to give a generic form to the generators of time evolution. The stationary states of the solutions then help us to identify subspace of the generators that gives rise to positive evolution. The studies also reveal general transformations that are not limited to factorized unitary transformations. We will discuss this at the end of this work.

II. EXAMPLES OF GENERATORS

Density matrices in the position coordinate are denoted by $\langle\widetilde{x}|\rho|x\rangle$, where x is the usual dimensionless position coordinate in the $|x\rangle$ space, and $\widetilde{x}$ is its counterpart in the conjugate $\langle\widetilde{x}|$ space. To facilitate the upcoming discussions, we introduce the center and relative coordinates:

$$Q \equiv \frac{1}{2}(x+\widetilde{x}), \qquad r \equiv x-\widetilde{x}, \tag{4}$$

respectively, and denote density matrices by $\rho(Q,r)$. Probability density of the system lies along the diagonal components, $\rho(x,0)=\langle x|\rho|x\rangle$, with $r=0$, whereas quantum correlation is carried by the off-diagonal components $r\neq 0$.

We will consider a few examples of the generators governing the evolution of damped oscillators. The quantum Brownian motion of harmonic oscillators in a high temperature bath is described by the Caldeira-Leggett (CL) equation with the following generator [6]:

$$K_{\mathrm{CL}} = i\omega_0\left(-\frac{\partial^2}{\partial Q\partial r}+Qr\right)+\gamma r\frac{\partial}{\partial r}+\gamma\frac{kT}{\hbar\omega_0}r^2 \,. \tag{5}$$

In this equation, terms under the round bracket describe the oscillating motion of free harmonic oscillator with natural frequency ω_0. The third term with damping constant γ introduces friction to the oscillating motion when the oscillator oscillates in the bath.

It is typical in dissipative systems that the quantum correlation of the system deteriorates or decays away due to the influence of the environment. In the classic example of the Schrödinger's cat [8], whose state is initially in a superposition of $|\text{live}\rangle$ and $|\text{dead}\rangle$ states, the correlation components of $|\text{live}\rangle\langle\text{dead}|$ and its hermitian conjugate will eventually die off, leaving us with a superposition of the classical states, $|\text{live}\rangle\langle\text{live}|$ and $|\text{dead}\rangle\langle\text{dead}|$. We are then left with certain probabilities to find the cat alive or dead, but it cannot be alive and dead simultaneously.

The decay of the system's quantum correlation due to its interaction with external environment is called decoherence. This effect is brought by the last term in Eq. (5), where T denotes the temperature of the bath. An argument advanced in Ref. [8] nicely exhibits the decay in the quantum correlation of the density matrices. Consider large r such that the last term in K_{CL} dominates over the other terms. The solution to the equation of motion is then given by $\rho(t)\sim\exp(-r^2 t\cdot\gamma kT/\hbar\omega_0)\rho(0)$, which shows that the off-diagonal components of ρ decohere exponentially fast. We note that K_{CL} would violate the positivity of ρ if the temperature of the bath is too low.

The next example is the Hu-Paz-Zhang (HPZ) equation [9], whose generator has an extra "anomalous" diffusion term over K_{CL}:

$$K_{\mathrm{HPZ}} = i\omega_0\left(-\frac{\partial^2}{\partial Q\partial r}+Qr\right)+\gamma r\frac{\partial}{\partial r}+b\gamma r^2+idr\frac{\partial}{\partial Q}\,, \tag{6}$$

where b is a temperature related parameter:

$$b\equiv\frac{1}{2}\coth\frac{\hbar\omega_0}{2kT} \tag{7}$$

and d is a constant.

The last example is the Kossakowski-Lindblad (KL) equation which is often used in quantum optics to describe the relaxation of laser systems:

$$K_{\mathrm{KL}} = i\omega_0 \left(-\frac{\partial^2}{\partial Q \partial r} + Qr \right) + \frac{\gamma}{2} \left(r\frac{\partial}{\partial r} - Q\frac{\partial}{\partial Q} - 1 \right) + b\frac{\gamma}{2} \left(r^2 - \frac{\partial^2}{\partial Q^2} \right). \tag{8}$$

Eq. (8) has the Kossakowski-Lindblad form [2, 3]. Generators of this form is completely positive [2, 3], which implies that the generators preserve the positive semi-definiteness of ρ.

Notice that all the generators given above contain the damping term (γ-term) and the decoherence term (r^2-term). In Section 5 we find that they constitute three classes of generators that satisfy the conditions required by the properties of density matrices.

III. ADJOINT-SYMMETRIC AND TRACE-PRESERVING GENERATORS

Density matrices have three properties, they are (1) hermitian $\rho^\dagger = \rho$, (2) unit trace $\mathrm{tr}\rho = 1$, and (3) positive semi-definite $\rho \geq 0$. Consequently, generators of time evolution are required to preserve these properties.

Property (1) requires the generators to be adjoint-symmetric [10, 11]:

$$\widetilde{K}(Q,r) = K(Q,r), \qquad \text{(hermiticity condition)} \tag{9}$$

where $\sim$ is association defined by $\widetilde{K}(Q,r) = K^*(Q,-r)$.

Property (2) requires the generators to be trace-preserving. From Eq. (2) this implies that $\mathrm{tr}(K\rho) = 0$, or in the position coordinates:

$$\int_{-\infty}^{\infty} K(Q,r)\rho(Q,r;t)\big|_{r=0} dQ = 0, \qquad \text{(trace-preserving condition)} \tag{10}$$

where we require ρ to vanish fast enough at infinity. The Gaussian density matrices (11) fulfill this condition.

Although property (3) does not lead to a simple condition on the form of the generators, it can be imposed indirectly on density matrices. We consider density matrices for oscillators with the Gaussian form:

$$\rho(Q,r) = \sqrt{\frac{2\mu}{\pi}} \exp\left(-2\mu Q^2 - \kappa i Q r - \frac{1}{2}(\mu + \nu) r^2 \right), \tag{11}$$

where μ, κ and ν are real functions of time. The necessary and sufficient conditions for the positive semi-definiteness of Gaussian density matrices are [12]:

$$\mu > 0 \qquad \text{and} \qquad \nu \geq 0\,. \tag{12}$$

The conditions in Eq. (12) give rise to inequalities on the coefficients of the generators. Deriving these inequalities is one of the main result of this study, see Eqs. (17) and (19).

We find that there are seven generators bilinear in the position coordinates that satisfy the hermiticity and trace-preserving conditions simultaneously:

$$iL_0 \equiv \frac{i}{2}\left(-\frac{\partial^2}{\partial Q \partial r} + Qr\right), \quad iM_1 \equiv \frac{i}{2}\left(\frac{\partial^2}{\partial Q \partial r} + Qr\right), \quad iM_2 \equiv -\frac{1}{2}\left(Q\frac{\partial}{\partial Q} + r\frac{\partial}{\partial r} + 1\right), \tag{13a}$$

$$O_0 - \frac{1}{2} \equiv \frac{1}{2}\left(r\frac{\partial}{\partial r} - \frac{\partial}{\partial Q}Q\right), \qquad O_+ \equiv -\frac{1}{4}\left(r^2 - \frac{\partial^2}{\partial Q^2}\right), \tag{13b}$$

$$L_{1+} \equiv -\frac{1}{4}\left(\frac{\partial^2}{\partial Q^2} + r^2\right), \qquad L_{2+} \equiv -\frac{i}{2} r \frac{\partial}{\partial Q}. \tag{13c}$$

Together with three more generators that do not satisfy the trace-preserving condition for arbitrary ρ (not listed here, cf. [11]), they exhaust the list of bilinear generators that are adjoint-symmetric. Since they are also linearly independent, generic generators are obtained by taking linear sums of them over real coefficients [11]:

$$K_{\text{generic}} = \theta_0 iL_0 + \theta_1 iM_1 + \theta_2 iM_2 + \gamma(O_0 - 1/2) + \eta_0 O_+ + \eta_1 L_{1+} + \eta_2 L_{2+} \, . \tag{14}$$

This is the most general form of the generators of reduced dynamics that satisfies the hermiticity and trace-preserving conditions simultaneously. A similar form was also obtained by considering Gaussian Markov process [13].

IV. STATIONARY STATES

Equation of motion with the generic generator (14) can be solved analytically [14]. Here we only consider stationary states that satisfy the positive conditions. The conditions provide inequalities that let us determine the subspaces of the coefficients of K that guarantee positive evolution. The stationary states have the Gaussian form (11), where the coefficients have the following stationary values [14]:

$$\mu_{\text{st}} = \frac{1}{2(\Gamma_0 - \Gamma_1)}\, , \qquad \nu_{\text{st}} = \frac{-\vec{\Gamma}^2 - 1}{2(\Gamma_0 - \Gamma_1)}\, , \qquad \kappa_{\text{st}} = \frac{-\Gamma_2}{\Gamma_0 - \Gamma_1}\, , \tag{15}$$

in which $\vec{\Gamma} \equiv (\Gamma_0, \Gamma_1, \Gamma_2)$ is a three-component Minkowski vector with metric signature $(-1,1,1)$, i.e., $\vec{\Gamma}^2 = -\Gamma_0^2 + \Gamma_1^2 + \Gamma_2^2$. When the coefficients of the generators are combined into Minkowski vectors $\vec{\theta} = (\theta_0, \theta_1, \theta_2), \vec{\eta} = (\eta_0, \eta_1, \eta_2)$. $\vec{\Gamma}$ has the compact expression:

$$\vec{\Gamma} \equiv \frac{1}{\gamma(\gamma^2 - \vec{\theta}^2)}\left(-\gamma^2\vec{\eta} + (\vec{\theta}\cdot\vec{\eta})\vec{\theta} + \gamma\vec{\theta}\wedge\vec{\eta}\right) \, . \tag{16}$$

When we apply the necessary and sufficient conditions (12) to the stationary states, we obtain:

$$\Gamma_0 - \Gamma_1 > 0 \qquad \text{and} \qquad -\vec{\Gamma}^2 \geq 1. \qquad\qquad \text{(positive conditions)} \tag{17}$$

The positive conditions constrain the coefficients of K to a subspace in the seven-dimensional space spanned by $(\gamma, \vec{\theta}, \vec{\eta})$.

In Ref. [15], a positive condition (in our notations):

$$-\vec{\eta}^2 \geq \gamma^2, \tag{18}$$

was obtained by considering the uncertainty principle on the time evolution of density matrices. This condition is overly restrictive because the stationary states of CL and HPZ equation violate it. In contrast, the second positive condition of Eq. (17) looks

$$\frac{1}{\gamma^2}(\vec{\theta}\cdot\vec{\eta})^2 + \vec{\theta}^2 - \vec{\eta}^2 \geq \gamma^2 \,. \tag{19}$$

Because of the two extra terms on the left of Eq. (19) compared to Eq. (18), the stationary states of the CL and HPZ equations are now positive.

We notice that $\kappa_{\rm st} \propto \Gamma_2$ does not affect the positivity of $\rho_{\rm st}$. However, it gives rise to a useful factorized condition:

$$\Gamma_2 = 0\,. \qquad\qquad \text{(factorized condition)} \tag{20}$$

This condition results in density matrices that is factorized (or separable) in the Q and r coordinates, such as Eq. (22). By requiring the stationary states to satisfy the factorized condition in addition to the hermiticity and trace-preserving conditions, we are able to group the known generators into three classes, discussed in Section 5.

The canonical states in equilibrium with thermal bath are the Gibbs states:

$$\rho_{\rm Gibbs} \propto \sum_{n=0}^{\infty} e^{-n\hbar\omega_0/kT} |n\rangle\langle n| \,, \tag{21}$$

or in position coordinates:

$$\rho_{\rm Gibbs}(Q,r) = \frac{1}{\sqrt{2\pi b}} e^{-Q^2/2b - br^2/2} \,, \tag{22}$$

in which b is related to the bath's temperature through Eq. (7). The fact that Q and r coordinates are factorized means that the Gibbs states satisfy the factorized condition (20). Furthermore, we find that $\Gamma_1 = 0$, for Gibbs states.

V. CLASSES OF GENERATORS

An analysis on the coefficients of K that satisfy the factorized condition (20) enables us to group generators that satisfy the hermiticity and trace-preserving conditions into three classes [14], as listed in Table 1. In all the cases listed, γ, θ_1, and θ_2 satisfy:

$$0 < \gamma, \qquad -2\omega_0 \leq \theta_1 \leq 2\omega_0\,, \qquad -\gamma \leq \theta_2 \leq \gamma\,. \tag{23}$$

Class of Generators	Completely Positive
CL	no
Conjugate CL (no r^2-term)	no
Generalized CL	$\lvert\theta_2\rvert \leq \gamma\sqrt{1-(\hbar\omega_0/2kT)^2}$
HPZ	no
Conjugate HPZ (no r^2-term)	no
KL	yes
Generalized KL 1	yes
Generalized KL 2	yes

TABLE 1. Three classes of generators that satisfy the hermiticity (9) and trace-preserving (10) conditions, and with stationary states obeying the factorized condition (20).

There are two more members that live in the same class with K_{CL}. They are the conjugate and generalized CL generators, respectively given by:

$$K_{\mathrm{cCL}} = i\omega_0\left(-\frac{\partial^2}{\partial Q\partial r}+Qr\right)-\gamma\frac{\partial}{\partial Q}Q-\gamma\frac{kT}{\hbar\omega_0}\frac{\partial^2}{\partial Q^2} \tag{24a}$$

$$K_{\mathrm{gCL}} = i\omega_0\left(-\frac{\partial^2}{\partial Q\partial r}+Qr\right)+\frac{1}{2}(\gamma-\theta_2)\left(r\frac{\partial}{\partial r}+\frac{kT}{\hbar\omega_0}r^2\right)-\frac{1}{2}(\gamma+\theta_2)\left(\frac{\partial}{\partial Q}Q+\frac{kT}{\hbar\omega_0}\frac{\partial^2}{\partial Q^2}\right). \tag{24b}$$

The conjugate generators K_{cCL} and K_{cHPZ} (listed below) are related to K_{CL} and K_{HPZ}, respectively, by a unitary transformation [14]. The generalized generator K_{gCL} interpolates between the two extremes of K_{CL} and K_{cCL} as θ_2 increases from $-\gamma$ to γ.

The HPZ class consists of K_{HPZ} and its conjugate:

$$K_{\mathrm{cHPZ}} = i\omega_0\left(-\frac{\partial^2}{\partial Q\partial r}+Qr\right)-\gamma\frac{\partial}{\partial Q}Q-\gamma b\frac{\partial^2}{\partial Q^2}+idr\frac{\partial}{\partial Q}\,. \tag{25}$$

In the CL and HPZ class, we have dropped the term $\theta_1 iM_1$ for simplicity. This term renormalizes the natural frequency of the oscillator. The conjugate CL and HPZ generators may not be physical because they do not have the r^2-term that causes decoherence.

There are two more KL related generators that interpolate the different terms in K_{KL}:

$$K_{\mathrm{gKL1}} = i\omega_0\left(\theta_{1-}\frac{\partial^2}{\partial Q\partial r}-\theta_{1+}Qr\right)+\frac{\gamma}{2}\left(r\frac{\partial}{\partial r}-\frac{\partial}{\partial Q}Q\right)+b\frac{\gamma}{2}\left(\theta_{1+}r^2-\theta_{1-}\frac{\partial^2}{\partial Q^2}\right) \tag{26a}$$

$$K_{\mathrm{gKL2}} = i\omega_0\left(\theta_{1-}\frac{\partial^2}{\partial Q\partial r}-\theta_{1+}Qr\right)+\frac{\gamma}{2}\left(\theta_{1-}r\frac{\partial}{\partial r}-\theta_{1+}\frac{\partial}{\partial Q}Q\right)+b\frac{\gamma}{2}\left(r^2-\frac{\partial^2}{\partial Q^2}\right) \tag{26b}$$

where

$$\theta_{\pm} \equiv 1\pm\frac{\theta_1}{2\omega_0}\,,\qquad -2\omega_0\leq\theta_1\leq 2\omega_0\,. \tag{27}$$

We note that K_{gCL} and $K_{\mathrm{gKL1,2}}$ are not found in the literature, except in the special case $\theta_1 = 0$, when K_{gKL1} and K_{gKL2} reduce to K_{KL}.

Out of the three classes of generators, only the KL class is completely positive, whereas $K_{\rm gCL}$ is completely positive provided $|\theta_2| \leq \gamma\sqrt{1-(\hbar\omega_0/2kT)^2}$. Since $K_{\rm gCL}$ reduces to $K_{\rm CL}$ when θ_2 takes the value $-\gamma$, the inequality also implies that $K_{\rm CL}$ is not completely positive, because it cannot be fulfilled except in the limit $T \to \infty$.

VI. GENERAL TRANSFORMATION

In Section 2 we mentioned that the transformation on density matrices in dissipative systems, in general, cannot be put into the factorized form (1). If we examine the bilinear generators listed in Eqs. (13a)-(13c), we notice that those in Eq. (13a) can be cast into the form, $f(x) \pm f(\widetilde{x})$. As a result, when we exponentiate them to obtain transformation operators, they are separable into two transformations that act separately on the x and $\widetilde{x}$ coordinates, cf. Eq. (1). For example, $\exp(-2\omega_0\theta iL_0) = u(x)u^*(\widetilde{x})$, where:

$$u(x) = \exp\left[-i\omega_0\theta\left(-\frac{\partial^2}{\partial x^2} + x^2\right)\right], \tag{28}$$

is the time evolution operator of free harmonic oscillators if θ is the time parameter. Pure states remain pure under the actions of this sort of generators.

On the other hand, this is not the case for generators in Eqs. (13b) and (13c). They contain cross terms in x and $\widetilde{x}$, rendering them to be inseparable into the form $u(x)u^*(\widetilde{x})$. This kind of generators furnishes a larger symmetry on density matrices compared to the ordinary symmetry on state vectors in the Hilbert space, as discussed in Ref. [16]. For example, O_0 generates the thermal symmetry in the KL and CL equations [17], and relates the thermal oscillator states [18], where:

$$e^{\theta(O_0-1/2)} = e^{-\theta/2}\exp\left[-\theta\left(x\frac{\partial}{\partial\widetilde{x}} + \widetilde{x}\frac{\partial}{\partial x}\right)\right], \tag{29}$$

is not separable in the position coordinates. When it acts on the oscillator ground state $\langle\widetilde{x}|0\rangle\langle 0|x\rangle$, we obtain the Gibbs states [18]:

$$e^{\theta(O_0-1/2)}\langle\widetilde{x}|0\rangle\langle 0|x\rangle \propto \sum_{n=0}^{\infty} e^{-n\hbar\omega_0/kT}\langle\widetilde{x}|n\rangle\langle n|x\rangle , \tag{30}$$

which are mixed states, where $\tanh\theta = \exp(-\hbar\omega_0/kT)$. Mixed states like Eq. (30) can never be produced by acting ordinary transformation on pure states (1). The inverse of $e^{\theta(O_0-1/2)}$ is obtained by inverting the sign of θ, where $e^{-|\theta|(O_0-1/2)}$ may now transform mixed states into pure states. This shows that general transformation is not limited to semigroup. Consequently, larger classes of symmetry operations other than the ordinary factorized unitary transformations exist in the density matrix space.

VII. CONCLUSIONS

In this work, we review the main ideas behind our works in Refs. [11] and [14], and summarised the main results found in the works. We show that based on the hermitian and unit trace conditions of the density matrices, we obtain a set of basis generators that are adjoint-symmetric and trace-preserving, in contrast to the hermiticity requirement on the operators in the Hilbert space. Generic generators are formed by taking linear sums of the basis generators over real coefficients. Positive requirement on the density matrices then constrains the coefficients to a limited range. The generators yield transformations that describe symmetry beyond the ordinary one in the Hilbert space. The procedure that we apply to a single infinite-level system here can be used to study finite-level and multi-partite systems as well. We will consider these aspects in future works.

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