

Positivity violations of the density operator in the Caldeira-Leggett master equation

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Abstract. The Caldeira-Leggett master equation as an example of Markovian master equation without Lindblad form is investigated for mathematical consistency. We explore situations both analytically and numerically where the positivity violations of the density operator occur. We reinforce some known knowledge about this problem but also find new surprising cases. Our analytical results are based on the full solution of the Caldeira-Leggett master equation obtained via the method of characteristics. The preservation of positivity is mainly investigated with the help of the density operator's purity and we give also some numerical results about the violation of the Robertson-Schrödinger uncertainty relation.

1 Introduction

States of a quantum mechanical system are given by density operators with spectra consisting only positive eigenvalues and they sum up to one [1]. A master equation, governing the time evolution of density operators, has to map density operators to density operators in order to keep the physical interpretation. It has been shown by references [2,3] that a dynamical evolution given by a semigroup of completely positive maps provides us a Markovian master equation with a generator in Lindblad form. The Markovian master equation obtained within the Caldeira-Leggett model does not belong to the Lindblad class [4,5] and thus the generated semigroup is not completely positive. Despite that a stronger condition than positivity fails the dynamical evolution may still map density operators to density operators, a point of view discussed by references [6–8]. However, due to the use of a system plus reservoir model with unitary dynamics and an uncorrelated initial product state the reduced dynamics of the system is always completely positive [9,10]. Thus, the completely positive property of the map generated by the Caldeira-Leggett master equation is lost due to the assumptions made in the derivation and proposals to correct this issue have been made since [11–18]. Without these corrections the Caldeira-Leggett master

equation can in principle violate the positivity of the density operator.

Therefore the circumstances under which the mathematical consistency breaks down are worth investigating. Every now and then, the necessity of clarifying the status of master equations without Lindblad form have initiated investigations in the subject, see for example reference [19] and the references therein. In fact, the task is to investigate those conditions which forbid the positivity violation of density operator and finally compare them with the approximations used in the derivation of the master equation. Here, we undertake this task with the explicit focus on the Caldeira-Leggett master equation where the central system is a harmonic oscillator.

In this paper, we solve exactly the Caldeira-Leggett master equation by using the method of characteristic curves. The idea is based on [20], where the differential equation of the density operator in position representation is solved but with an algebraic mistake. It has to be mentioned that in the case of Wigner phase space representations of density operators the method of characteristic curves has been applied to a more general set of master equations involving also the Caldeira-Leggett master equation [21]. The detailed analysis presented in the latter one does not involve short time evolutions and furthermore only initial Gaussian states are considered. Here, we try to identify general conditions for which the Caldeira-Leggett master equation exhibits mathematically inconsistent behavior. Therefore, we have to

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keep track of the whole time evolution from the initial conditions to the steady state. Essentially, we correct and extend the method of reference [20], which is more adaptable in our investigations, due to the technically inconvenient double Fourier transform which connects the Wigner phase space representation with the position representation of the density operator.

The Caldeira-Leggett master equations without the Lindblad form preserves the self-adjointness of the initial density operator. Hence, we require methods which separate self-adjoint trace-class operators from density operators. Our first choice is the purity of the density operators, which has to be smaller or equal to one (a necessary but not sufficient condition for a self-adjoint trace-class operator with trace one to be a density operator). A violation of it implies that some of the eigenvalues are not in the interval $[0, 1]$, a mathematical inconsistency in the physical interpretation of these eigenvalues. The other choice is the Robertson-Schrödinger uncertainty relation [22,23], whose derivation is based on the positivity properties of density operators. Thus, deviations from positivity may lead to the violation of the uncertainty relation. The logical implication of these two methods being used to test the positivity of the density operator is very intricate and apart from some comments made in this work we are not going to determine it. Thus, we conduct a study on the purity and the Robertson-Schrödinger uncertainty relation and identify some necessary conditions for the master equation, which guarantee the mathematical consistency.

The paper is organized as follows. In Section 2 we discuss some general facts about the purity and the Robertson-Schrödinger uncertainty relation. We present the exact solution of the Caldeira-Leggett master equation in Section 3. In Section 4 we investigate the conditions for the parameters of the master equation based on steady state solutions. In the next step, the time evolution of the purity and the restrictions to initial conditions are discussed in Section 5. Numerical simulations of both the purity and the Robertson-Schrödinger uncertainty relation are collected in Section 6. Technical details, supporting the main text, are given in Appendices A and B.

2 Positivity violation in Markovian master equations

A general quantum state is mathematically represented by a self-adjoint positive trace-class operator with unit trace $\hat{\rho} : \mathcal{H} \rightarrow \mathcal{H}$, where \mathcal{H} denotes the complex Hilbert space. A Markovian master equation describing the time evolution of a $\hat{\rho}(t)$ density operator is of the form

$$\frac{d\hat{\rho}}{dt} = \mathcal{L}\hat{\rho} \quad \text{with} \quad \Phi_t = e^{\mathcal{L}t}, \quad (1)$$

and we denote by $\mathcal{D}(\mathcal{H})$ the set of density operators being in the domain of the not necessarily bounded generator \mathcal{L} . Mark the set of self-adjoint trace class operators with unit trace $\mathcal{D}_1^H(\mathcal{H})$, being also in the domain of \mathcal{L} , and thus implying automatically $\mathcal{D}(\mathcal{H}) \subset \mathcal{D}_1^H(\mathcal{H})$. An operator is

positive if and only if all of its eigenvalues are greater than or equal to zero, which implies that the eigenvalues of any density operator must satisfy this property. In addition, because the trace of a density operator is one and the trace is just the sum of the eigenvalues, we have that if λ_n is an eigenvalue of a density operator, then $0 \leq \lambda_n \leq 1$. If

$$\exists |\Psi\rangle : \quad \langle \Psi | \hat{O} | \Psi \rangle < 0 \quad |\Psi\rangle \in \mathcal{H},$$

then this is equivalent to the existence of at least one negative eigenvalue of an operator $\hat{O} \in \mathcal{D}_1^H(\mathcal{H})$.

If we want to determine the set $\mathcal{D}_1^H(\mathcal{H}) \setminus \mathcal{D}(\mathcal{H})$, then the exact knowledge on the spectrum of all operators in $\mathcal{D}_1^H(\mathcal{H})$ is necessary. However, a well-defined subset of $\mathcal{D}_1^H(\mathcal{H}) \setminus \mathcal{D}(\mathcal{H})$ can be filtered out without the complete knowledge of the spectrum by using a simple trick. The next result guarantees the existence of at least one negative eigenvalue.

Let $\hat{\rho}$ be a self-adjoint trace-class operator with $\text{Tr}\hat{\rho} = 1$. If $\text{Tr}(\hat{\rho}^2) > 1$ then $\hat{\rho}$ has at least one negative eigenvalue. The proof of this statement reads as follows. Assume that

$$\sum_{j=1}^{\infty} \lambda_j = 1 \quad \text{and} \quad \sum_{j=1}^{\infty} \lambda_j^2 > 1, \quad (2)$$

where $\lambda_1, \lambda_2, \dots \in \mathbb{R}$ denote the eigenvalues of $\hat{\rho}$. Then

$$0 < \sum_{j=1}^{\infty} (\lambda_j^2 - \lambda_j), \quad (3)$$

so there must be a j_0 such that $\lambda_{j_0} \notin [0, 1]$; if $\lambda_{j_0} > 1$, then there must be a j_1 with $\lambda_{j_1} < 0$ since $\text{Tr}\hat{\rho} = 1$. In the context of the Markovian master equation in (1) we are looking for the class of operators for which the purity $\text{Tr}(\hat{\rho}^2)$ is larger than one. In this case we say that $\hat{\rho} \in \mathcal{D}_1^H(\mathcal{H}) \setminus \mathcal{D}(\mathcal{H})$, because $\text{Tr}(\hat{\rho}^2) \leq 1$ is a necessary but not sufficient condition for $\hat{\rho}$ to be an element in $\mathcal{D}(\mathcal{H})$. In typical physical models $\hat{\rho}$ represents a quantum-mechanical system which interacts with an external quantum system and therefore the evolution in (1) is physically consistent if $\hat{\rho}(t) \in \mathcal{D}(\mathcal{H})$ for all $t \geq 0$ or being more accurate Φ_t is a dynamical semigroup with generator \mathcal{L} [24]. If $\exists t'$ such that $\hat{\rho}(t') \in \mathcal{D}_1^H(\mathcal{H}) \setminus \mathcal{D}(\mathcal{H})$ with initial state $\hat{\rho}_{\text{in}} \in \mathcal{D}(\mathcal{H})$, then the time evolution of the density operator is mathematically inconsistent. If a Markovian master equation generates a uniformly continuous completely positive dynamical semigroup (quantum dynamical semigroup), i.e., \mathcal{L} is bounded and $\mathcal{D}(\mathcal{H})$ is the convex set of all density operators on \mathcal{H} , then it is in Lindblad form [2,3,25]

$$\frac{d\hat{\rho}}{dt} = \mathcal{L}\hat{\rho}(t) = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \sum_{\alpha} \left[\hat{L}_{\alpha} \hat{\rho} \hat{L}_{\alpha}^{\dagger} - \frac{1}{2} \left\{ \hat{L}_{\alpha}^{\dagger} \hat{L}_{\alpha}, \hat{\rho} \right\} \right],$$

where \hat{H} is the Hamilton operator and \hat{L}_{α} are the corresponding Lindblad operators.

There is another possibility to study deviations from the set $\mathcal{D}(\mathcal{H})$. The Robertson-Schrödinger uncertainty

relation with A and B essentially self-adjoint operators defined on a dense subset of \mathcal{H} has the following form [22,23,26]

$$\sigma_{RS} \geq \frac{1}{4} \left| \langle \hat{A}\hat{B} - \hat{B}\hat{A} \rangle \right|^2, \tag{4}$$

with

$$\sigma_{RS} = \Delta \hat{A}^2 \Delta \hat{B}^2 - \left(\langle \hat{A}\hat{B} + \hat{B}\hat{A} \rangle / 2 - \langle \hat{A} \rangle \langle \hat{B} \rangle \right)^2,$$

where $\Delta \hat{O}^2 = \langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2$ with $\langle \hat{O} \rangle = \text{Tr}\{\hat{O}\hat{\rho}\}$. Since we are going to study the Caldeira-Leggett master equation, we will set $\hat{A} = \hat{x}$, the position operator, and $\hat{B} = \hat{p}$, the momentum operator, which is going to guarantee that the set $\mathcal{D}(\mathcal{H})$ of this specific problem is in the domain of these operators and the right hand side of (4) is simply $\hbar^2/4$ [23]. The inequality in (4) is based on the positivity of $\hat{\rho}$, which is going to be violated whenever $\hat{\rho} \in \mathcal{D}_1^I(\mathcal{H}) \subset \mathcal{D}_1^H(\mathcal{H}) \setminus \mathcal{D}(\mathcal{H})$. The relation between the sets $\mathcal{D}_1^P(\mathcal{H})$ and $\mathcal{D}_1^I(\mathcal{H})$ is not trivial, however we are going to investigate it briefly with the help of numerical simulations. After solving equation (1) one can determine those time intervals when the solution is in the set $\mathcal{D}_1^H(\mathcal{H}) \setminus \mathcal{D}(\mathcal{H})$ with the help of the purity and/or the violation of the Robertson-Schrödinger uncertainty relation, and of course, if there exists at least one such interval, then the time evolution of the solution is mathematically inconsistent.

3 Solution to the Caldeira-Leggett master equation

In this section we consider the Caldeira-Leggett master equation [5] for a quantum harmonic oscillator with frequency ω ($\hbar = m = k_B = 1$)

$$i \frac{\partial \hat{\rho}}{\partial t} = \left[\frac{\hat{p}^2}{2} + \frac{\omega^2 \hat{x}^2}{2}, \hat{\rho} \right] - i D_{pp} [\hat{x}, [\hat{x}, \hat{\rho}]] + \gamma [\hat{x}, \{\hat{p}, \hat{\rho}\}] - 2i D_{px} [\hat{x}, [\hat{p}, \hat{\rho}]], \tag{5}$$

where $[\cdot, \cdot]$ stands for commutators while $\{\cdot, \cdot\}$ for anti-commutators, and γ is the relaxation constant. D_{pp} is the momentum diffusion coefficient and finally D_{px} is the cross diffusion coefficient. This master equation is derived from the Caldeira-Leggett model [5], where an environment of harmonic oscillators in thermal equilibrium with temperature T is considered with Ohmic spectral density and a high frequency cut-off Ω . The central system, a harmonic oscillator in our case, is taken to be slow compared to the bath correlation time $\Omega, T \gg \omega$ and the Born-Markov approximation $\Omega, T \gg \gamma$ is also employed during the derivation. The master equation in (5) is not in Lindblad form and therefore, according to the introductory notions in Section 2 there may be time intervals where $\hat{\rho}(t) \in \mathcal{D}_1^H(\mathcal{H}) \setminus \mathcal{D}(\mathcal{H})$. In order to examine closely these situations we are going to determine the exact solution of this master equation.

As a first step we rewrite equation (5) in the position representation

$$i \frac{\partial}{\partial t} \rho(x, y, t) = \left[\frac{1}{2} \left(\frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial x^2} \right) + \frac{\omega^2}{2} (x^2 - y^2) - i D_{pp} (x - y)^2 - i \gamma (x - y) \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) - 2 D_{px} (x - y) \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) \right] \rho(x, y, t).$$

We introduce the center of mass and relative coordinates $R = (x + y)/2$, $r = x - y$, and the master equation becomes

$$\frac{\partial \rho(R, r, t)}{\partial t} = \left[i \frac{\partial^2}{\partial r \partial R} - 2\gamma r \frac{\partial}{\partial r} - D_{pp} r^2 + 2i D_{px} r \frac{\partial}{\partial R} + \frac{\omega^2 r R}{i} \right] \rho(R, r, t).$$

Fourier transforming the equation in the variable R reduces it to a first order partial differential equation

$$\left[(2\gamma r - K) \frac{\partial}{\partial r} + \omega^2 r \frac{\partial}{\partial K} + D_{pp} r^2 - 2 D_{px} r K \right] \rho(K, r, t) = - \frac{\partial \rho(K, r, t)}{\partial t},$$

where we used the following identity

$$\rho(R, r, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dK \exp(iKR) \rho(K, r, t).$$

This equation was written by Roy and Venugopalan in [20] for the case of $D_{px} = 0$, but we found that their solution did not satisfy the master equation for every instance of time due to an algebraic mistake. They used the method of characteristics to find the solution of this equation, and we applied the same technique for the extended case of $D_{px} \neq 0$.

The method of characteristics (see [27]) is a very useful technique for solving first order partial differential equations by reducing partial differential equations to a family of ordinary differential equations along which the solution can be integrated from some initial data given on a suitable hypersurface. In our case the method of characteristics leads to the following system of ordinary differential equations:

$$\begin{aligned} \frac{\partial}{\partial t} r(t) &= 2\gamma r(t) - K(t) \\ \frac{\partial}{\partial t} K(t) &= \omega^2 r(t) \\ \frac{\partial}{\partial t} \rho(t) &= (2D_{px} r(t) K(t) - D_{pp} r^2(t)) \rho(t) \end{aligned}$$

with initial conditions $r(0) = r_0, K(0) = K_0, \rho(K_0, r_0, 0) = \rho_0$. In order to obtain simple formulas we introduce

the following notations

$$Y := \omega^2 r_0 - K_0 \lambda_1, \quad \Gamma := r_0 \lambda_2 - K_0, \quad \lambda_{1,2} := \gamma \pm \sqrt{X}, \\ X := \gamma^2 - \omega^2$$

and with these markings, the solution of the ordinary differential equation system is as follows

$$K(t) := \frac{Y e^{\lambda_1 t} - e^{\lambda_2 t} (Y - 2K_0 \sqrt{X})}{2\sqrt{X}},$$

and

$$r(t) := \frac{\Gamma e^{\lambda_1 t} - e^{\lambda_2 t} (\Gamma - 2r_0 \sqrt{X})}{2\sqrt{X}}.$$

A compact form of the final results reads

$$\rho(t) = \rho_0 \exp \left[-\frac{A e^{-2t(2\sqrt{X}+\gamma)} D_{pp} + B e^{-2t(2\sqrt{X}+\gamma)} D_{px}}{8X^{3/2}\gamma\omega^2} \right],$$

where the notations A and B can be found in Appendix A. After substituting $K(t) \rightarrow K, r(t) \rightarrow r$, and $\rho(t) \rightarrow \rho(K, r, t)$, we get

$$K_0 = \frac{[(\sqrt{X} + \gamma) K - \omega^2 r] e^{2\sqrt{X}t} + (\sqrt{X} - \gamma) K + \omega^2 r}{2\sqrt{X} e^{\lambda_1 t}}, \\ r_0 = \frac{[(\sqrt{X} - \gamma) r + K] e^{2\sqrt{X}t} + (\sqrt{X} + \gamma) r - K}{2\sqrt{X} e^{\lambda_1 t}}.$$

Thus,

$$\rho_0 = \rho(K, r, t) e^{\frac{A e^{-2t(2\sqrt{X}+\gamma)} D_{pp} + B e^{-2t(2\sqrt{X}+\gamma)} D_{px}}{8X^{3/2}\gamma\omega^2}},$$

and finally the exact solution at an arbitrary time is

$$\rho(K, r, t) = \rho_0 e^{-\frac{A e^{-2t(2\sqrt{X}+\gamma)} D_{pp} + B e^{-2t(2\sqrt{X}+\gamma)} D_{px}}{8X^{3/2}\gamma\omega^2}}. \quad (6)$$

4 Some requirements for the parameters of the master equation

In this section, we analyze some relations between the parameters of the master equations. We reintroduce for the physically important relations the dimensions of all parameters ($\hbar, m, k_B \neq 1$) and for the pure mathematical observations we avoid them again in order to obtain simple formulas. Let us consider the steady state of the master

Table 1. Diffusion's coefficients in literature.

Case	D_{pp}	D_{px}
I [5]	$2\gamma m k_B T / \hbar^2$	0
II [10]	$2\gamma m k_B T / \hbar^2$	$-\gamma k_B T / (\hbar^2 \Omega)$
III [12]	$2\gamma m k_B T / \hbar^2$	$\Omega \gamma / (6\pi k_B T)$
IV [13]	$\gamma m \omega^2 / (2\hbar \sqrt{\omega^2 - \gamma^2})$	$\gamma^2 / (\hbar \sqrt{\omega^2 - \gamma^2})$

equation (5) in position representation with reintroduced physical dimensions

$$\rho(x, y, \infty) = \frac{\sqrt{\gamma} m \omega}{\hbar \sqrt{\pi} \sqrt{D_{pp} - 4\gamma m D_{px}}} \\ \times \exp \left\{ -\frac{\gamma [m\omega(x+y)]^2}{4\hbar^2 (D_{pp} - 4\gamma m D_{px})} - \frac{D_{pp}(x-y)^2}{4\gamma} \right\},$$

which agrees with the steady state known in the literature for $D_{px} = 0$, see for example [10]. The eigenproblem of the steady state reads [28]

$$\int_{-\infty}^{+\infty} \rho(x, y, \infty) \phi_n(y) dy = \epsilon_n \phi_n(x)$$

and is solved by

$$\phi_n(x) = H_n \left(x, \frac{1}{4\sqrt{AC}} \right) \exp \left\{ -2\sqrt{AC}x^2 \right\}, \\ \epsilon_n = \epsilon_0 \epsilon^n, \quad \epsilon_0 = \frac{2\sqrt{C}}{\sqrt{A} + \sqrt{C}}, \quad \epsilon = \frac{\sqrt{A} - \sqrt{C}}{\sqrt{A} + \sqrt{C}}, \\ A = \frac{D_{pp}}{4\gamma}, \quad C = \frac{\gamma(m\omega)^2}{4\hbar^2 (D_{pp} - 4\gamma m D_{px})}, \quad (7)$$

where $H_n(x, a)$ is a generalized Hermite polynomial with $a > 0$. Therefore, the model is not physical if the following inequality does not hold: $A \geq C$ or

$$\hbar^2 \frac{D_{pp}^2 - 4\gamma m D_{pp} D_{px}}{\gamma^2 m^2 \omega^2} \geq 1. \quad (8)$$

If this inequality is not satisfied then the stationary density operator has negative eigenvalues for every odd $n \in \mathbb{N}$.

The coefficients D_{pp} and D_{px} of the Caldeira-Leggett master equation in (5) are determined in the high temperature limit $k_B T \geq \hbar \Omega \gg \hbar \omega$. First, we consider the master equation of reference [5], see case I in Table 1. Substituting into equation (8) we obtain

$$T_{\min}^I \geq \frac{1}{2} \frac{\hbar \omega}{k_B}, \quad (9)$$

a minimum temperature for the environment, which guarantees that the steady state has no negative eigenvalues. This condition is in accordance with the high temperature limit $k_B T \gg \hbar \omega$ employed in the derivation of the master equation, thus is always fulfilled. Secondly, one may consider the Markovian limit of the more general

non-Markovian master equation of the Caldeira-Leggett model also in the high temperature limit, see case II in Table 1 [10,29–31]. Now, equation (8) yields

$$T_{\min}^{\text{II}} \geq \frac{1}{2} \frac{\hbar\omega}{k_B \sqrt{1 + 2\gamma/\Omega}}, \quad (10)$$

which is always fulfilled due to the Born-Markov approximation $\Omega \gg \gamma$ and the high temperature limit $k_B T \gg \hbar\omega$.

In the following, we consider two Markovian master equations which are in Lindblad form [12,13], but neglecting the position diffusion term $-D_{xx}[\hat{\rho}, [\hat{\rho}, \hat{\rho}]]$, we arrive at the same evolution as in equation (5). This brief study is motivated by the fact that in experiments the position diffusion has not been detected yet. Therefore, it is worth to ask what conditions do the parameters of the truncated master equations have to fulfill. In the case of [12], where medium temperatures are considered $\hbar\Omega \geq k_B T \gg \hbar\omega$, equation (8) yields

$$T_{\min}^{\text{III}} \geq \frac{1}{2} \frac{\hbar\omega}{k_B} \sqrt{1 + \frac{2}{3\pi} \frac{\Omega\gamma}{\omega^2}}, \quad (11)$$

see the coefficients D_{pp} and D_{px} in the case III of Table 1. This condition is true only when the cutoff energy $\hbar\Omega$ is not too large compared with $k_B T$. The second truncated Markovian master equation of reference [13] is obtained via a phenomenological phase space quantization of an underdamped $\omega > \gamma$ harmonic oscillator. Thus no model for the environment is required, i.e., $T = \Omega = 0$, yielding the coefficients D_{pp} and D_{px} in case IV of Table 1. Hence, for (8) we have

$$0 \geq 3\omega^2 + 4\gamma^2,$$

which is true only if $\omega = \gamma = 0$. Therefore, the master equation of [13] cannot be truncated at will.

In the subsequent discussion, we focus only on the first three cases of Table 1 and investigate the behavior of $\text{Tr}\hat{\rho}^2$ as a function of temperature T . As it will be a purely mathematical discussion we return to the convention $\hbar = k_B = m = 1$. Applying the Plancherel theorem [32] we can get the purity in the following form:

$$\text{Tr}(\hat{\rho}^2) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho(K, r, t) \rho^*(K, r, t) dK dr.$$

Taking into account (6) the purity becomes

$$\begin{aligned} \text{Tr}(\hat{\rho}^2) &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\rho(K_0, r_0, 0)|^2 \\ &\times \left| e^{-\frac{Ae^{-2t(2\sqrt{X}+\gamma)} D_{pp} + Be^{-2t(2\sqrt{X}+\gamma)} D_{px}}{8X^{3/2}\gamma\omega^2}} \right|^2 dK dr, \end{aligned} \quad (12)$$

where the details about A and B can be found in Appendix A and $X = \gamma^2 - \omega^2$. Furthermore, both D_{pp}

and D_{px} are functions of T . In the following we will show that the derivative of the purity with respect to temperature $\partial\text{Tr}(\hat{\rho}^2)/\partial T$, regardless of the initial conditions and other parameters,

$$\begin{aligned} \frac{\partial\text{Tr}(\hat{\rho}^2)}{\partial T} &= 2\Re \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\rho(K_0, r_0, 0)|^2 \\ &\times e^{2\Re \left[-\frac{Ae^{-2t(2\sqrt{X}+\gamma)} D_{pp} + Be^{-2t(2\sqrt{X}+\gamma)} D_{px}}{8X^{3/2}\gamma\omega^2} \right]} \\ &\times \frac{\partial}{\partial T} \left(-\frac{Ae^{-2t(2\sqrt{X}+\gamma)} D_{pp} + Be^{-2t(2\sqrt{X}+\gamma)} D_{px}}{8X^{3/2}\gamma\omega^2} \right) dK dr \end{aligned}$$

is always non-positive. \Re denotes the real part of a complex number.

Since case I is just a simplified version of case II in Table 1 with $D_{px} = 0$, we are going to consider case II in the subsequent discussion. Let us introduce function $H(K, r, t)$ as follows

$$\begin{aligned} H(K, r, t) &:= G(K, r, t) + c \\ &= 2\Re \frac{\partial}{\partial T} \left(-\frac{Ae^{-2t(2\sqrt{X}+\gamma)} D_{pp} + Be^{-2t(2\sqrt{X}+\gamma)} D_{px}}{8X^{3/2}\gamma\omega^2} \right), \end{aligned}$$

where $G(K, r, t)$ is given in Appendix A and

$$c = -\frac{1}{2} \frac{(-2K^2\gamma + \Omega(\omega^2 r^2 + K^2))T}{\Omega\omega^2} \leq 0.$$

The maximum of $H(K, r, t)$ is at $t = 0$, because it is exponentially decreasing with time, hence it is enough to investigate the derivative of the purity with respect to temperature at $t = 0$. After a brief calculation we get:

$$H(K, r, 0) = 0,$$

and consequently

$$\begin{aligned} \frac{\partial\text{Tr}(\hat{\rho}^2)}{\partial T} &= \int_{-\infty}^{\infty} dK \int_{-\infty}^{\infty} dr |\rho(K_0, r_0, 0)|^2 \\ &\times e^{2\Re \left[-\frac{Ae^{-2t(2\sqrt{X}+\gamma)} D_{pp} + Be^{-2t(2\sqrt{X}+\gamma)} D_{px}}{8X^{3/2}\gamma\omega^2} \right]} H(K, r, t) \\ &\leq \int_{-\infty}^{\infty} dK \int_{-\infty}^{\infty} dr |\rho(K_0, r_0, 0)|^2 \\ &\times e^{2\Re \left[-\frac{Ae^{-2t(2\sqrt{X}+\gamma)} D_{pp} + Be^{-2t(2\sqrt{X}+\gamma)} D_{px}}{8X^{3/2}\gamma\omega^2} \right]} H(K, r, 0) \\ &= 0 \end{aligned}$$

for all t and all possible parameter values and initial conditions.

Taking case III from Table 1 $H(K, r, t)$ reads now as follows

$$\begin{aligned} H(K, r, t) &:= F(K, r, t) + k(K, r) \\ &= 2\Re \frac{\partial}{\partial T} \left(-\frac{Ae^{-2t(2\sqrt{X}+\gamma)} D_{pp} + Be^{-2t(2\sqrt{X}+\gamma)} D_{px}}{8X^{3/2}\gamma\omega^2} \right), \end{aligned}$$

where

$$k(K, r) = -\frac{3T^2 (\omega^2 r^2 + K^2) \pi + K^2 \Omega \gamma}{3\pi T^2 \omega^2}$$

and details about $F(K, r, t)$ are shown in Appendix A. Starting from this point the course of the proof is the same as in case II and ultimately the derivative of the purity with respect to temperature $\partial \text{Tr}(\hat{\rho}^2)/\partial T$, regardless of the initial conditions and other parameters is always non-positive in this case as well. Thus, whenever $\hat{\rho} \in \mathcal{D}_1^{\hat{P}}(\mathcal{H})$ or $\text{Tr}(\hat{\rho}^2) > 1$, by the increase of the temperature the purity is decreased and the positivity violation of the density operator might be corrected for a given temperature provided that the condition $\text{Tr}(\hat{\rho}^2) \leq 1$ is not fulfilled in a pathological way. Here, we remind the reader about the condition $\text{Tr}(\hat{\rho}^2) \leq 1$, which is necessary but not sufficient for $\hat{\rho}$ to be a density operator.

In summary, we made a brief analysis on the steady state of (5) and we found in regard to three Markovian master equations (cases I, II, III in Tab. 1) known in the literature that the steady state does not violate the positivity for the parameter ranges used in the approximations of the derivations. In the case IV of reference [13] the master equation cannot be truncated to obtain (5), because the steady state will be no longer a density operator. Furthermore, the purities of the density operators in cases I, II, III are monotonically decreasing with temperature, which means that the study of purity for the positivity violation becomes obsolete for very high temperatures. Therefore, we turn our attention to the temporal behavior of $\text{Tr}\hat{\rho}^2$ and keeping the temperature within the range of approximations of the master equations, but not too high.

5 Temporal behavior of the purity and physical conditions for pure initial states

In this section, we investigate the temporal behavior of the purity for all cases in Table 1. The main issue is in fact the situation when the purity is one at a particular time and its derivative with respect to time is positive, thus the purity will increase above one for later times. A special case of this situation is when we have a pure initial state.

The time evolution of the purity is governed by the following differential equation

$$\begin{aligned} \frac{1}{2} \frac{\partial \text{Tr}\hat{\rho}^2}{\partial t} &= \gamma \text{Tr}\hat{\rho}^2 + 2D_{pp} \text{Tr} \left[(\hat{x}\hat{\rho})^2 - \hat{x}^2 \hat{\rho}^2 \right] + 4D_{px} \\ &\times \text{Tr} \left[(\hat{x}\hat{\rho}) (\hat{p}\hat{\rho}) - \left(\frac{1}{2} \hat{I} + \hat{p}\hat{x} \right) \hat{\rho}^2 \right] \\ &= (\gamma - 2D_{px}) \text{Tr}\hat{\rho}^2 + 4D_{px} F_1(t) + \frac{1}{2} F_2(t), \end{aligned}$$

where we have used equation (5) and introduced the notations:

$$\begin{aligned} F_1(t) &= \text{Tr} \left[(\hat{x}\hat{\rho}) (\hat{p}\hat{\rho}) - \hat{p}\hat{x}\hat{\rho}^2 \right] \\ F_2(t) &= 4D_{pp} \text{Tr} \left[(\hat{x}\hat{\rho})^2 - \hat{x}^2 \hat{\rho}^2 \right]. \end{aligned}$$

For the sake of simplicity let us introduce $P(t) = \text{Tr}\hat{\rho}^2$, which yields

$$\frac{\partial}{\partial t} P(t) = (2\gamma - 4D_{px}) P(t) + 8D_{px} F_1(t) + F_2(t)$$

and the solution to this differential equation with initial condition $P(0)$ is

$$\begin{aligned} P(t) &= P(0) e^{(\gamma - 2D_{px})t} \\ &+ \int_0^t e^{(-\gamma + 2D_{px})(t'-t)} [8D_{px} F_1(t') + F_2(t')] dt'. \end{aligned}$$

It is interesting to note the case when $\hat{x}\hat{\rho}$ is a Hilbert-Schmidt operator [32]. As the Hilbert-Schmidt operators form a Hilbert space, the Cauchy-Schwartz-Bunyakovsky inequality of the inner product for $\hat{x}\hat{\rho}$ yields

$$\begin{aligned} \text{Tr} [(\hat{\rho}\hat{x})^\dagger (\hat{x}\hat{\rho})] &\leq \sqrt{\text{Tr} [(\hat{\rho}\hat{x})(\hat{\rho}\hat{x})^\dagger]} \sqrt{\text{Tr} [(\hat{x}\hat{\rho})(\hat{x}\hat{\rho})^\dagger]} \\ &= \sqrt{\text{Tr} [(\hat{\rho}^2 \hat{x}^2)]} \sqrt{\text{Tr} [\hat{x}^2 \hat{\rho}^2]} = \text{Tr} [\hat{\rho}^2 \hat{x}^2], \end{aligned}$$

which results $F_2(t) \leq 0$.

The purity $P(t)$ is monotonically decreasing or constant at a time t if

$$(2\gamma - 4D_{px}) P(t) + 8D_{px} F_1(t) + F_2(t) \leq 0.$$

This inequality must be fulfilled at any time t when the purity $P(t) = 1$, i.e., $\hat{\rho}$ is a pure state. Hence, we have

$$\begin{aligned} 1 - 2F_1(t) &= \langle \hat{x}\hat{p} + \hat{p}\hat{x} \rangle - 2\langle \hat{x} \rangle \langle \hat{p} \rangle = \sigma_{px}^2, \\ F_2(t) &= 4D_{pp} (\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2) = 4D_{pp} \sigma_{xx}^2, \end{aligned}$$

and

$$\gamma - 2(D_{pp} \sigma_{xx}^2 + 2D_{px} \sigma_{px}^2) \leq 0. \quad (13)$$

In general, the above condition applies to all situations when the state is pure. However, the most convenient way of application is for initial pure states. Therefore, we consider an initial pure state and all parameters have dimensions $(\hbar, m, k_B \neq 1)$. Case I from Table 1 results in

$$\frac{1}{2} \frac{\hbar}{\sqrt{mk_B T}} \leq \sigma_{xx},$$

which means that σ_{xx} – the width of the initial wave packet – has to be approximately five times larger than the thermal wavelength. A condition, which is not satisfied by many initial states, but for example all the eigenstates of the quantum harmonic oscillator are subject to (13) due to the high temperature limit $k_B T \gg \hbar \omega$ approximation employed in derivation of the master equation of case I.

In case II we have

$$\frac{1}{2} \sqrt{\frac{\hbar^2}{mk_B T} + \frac{2\sigma_{px}^2}{m\Omega}} \leq \sigma_{xx},$$

which is a very similar condition to case I and it is satisfied also by all the eigenstates of the quantum harmonic oscillator.

Considering the truncated master equations of references [12,13], we are able to obtain conditions for the initial states. Case III from Table 1 yields

$$\sqrt{\frac{\hbar^2}{4mk_B T} - \frac{\hbar^2 \Omega}{12\pi m (k_B T)^2} \sigma_{px}^2} \leq \sigma_{xx},$$

and the self-consistency condition

$$\sqrt{\frac{3\pi k_B T}{\Omega}} \geq \sigma_{px}.$$

Surprisingly, we get the same conclusion obtained in the investigation of the steady state (see Sect. 4), namely the cutoff energy $\hbar\Omega$ cannot be too large compared with $k_B T$. Otherwise the self-consistency condition reads: σ_{px} is smaller or equal to a very small number, which most of the pure states do not satisfy.

Finally, case IV from Table 1 results in

$$\sqrt{\frac{\hbar\sqrt{\omega^2 - \gamma^2}}{m\omega^2} - \frac{2\gamma}{m\omega^2} \sigma_{px}^2} \leq \sigma_{xx},$$

and the self-consistency condition

$$\sqrt{\frac{\hbar\sqrt{\omega^2 - \gamma^2}}{2\gamma}} \geq \sigma_{px}.$$

These conditions can be subject to many initial pure states, but we already know from Section 4 that the truncated master equations of case IV violates positivity of the steady state. Thus, the truncated master equation of reference [13] may be applied for short time evolutions but definitely not for longer times.

In this section we obtained conditions for initial pure states by studying the time evolution of the purity. Thus, those initial pure states, which fulfill these conditions, guarantee a short time evolution where the value of the purity does not exceed one. The Caldeira-Leggett master equation, which is covered by cases I and II, shows that the eigenstates of the quantum harmonic oscillator are subject to these conditions. One may think with these initial pure states the purity never exceeds one. In contrary this can happen and we will present our numerical experiences in the next section.

6 Numerical results

In this section, we present the time evolution of the purity $P(t)$ by using the solution to the master equation in Section 3 and equation (12). In parallel we are going to carry out a numerical investigation on the Robertson–Schrödinger uncertainty (4) with the position operator \hat{x} and the momentum operator \hat{p} . This time we focus only on the two non-Lindblad master equations, cases I and II

in Table 1, for a few interesting parameter constellations. The other two cases, where a Lindblad master equations is truncated to form of equation (5), are neglected due to our findings in Sections 4 and 5.

In Section 5 we have found that the eigenstates of the quantum harmonic oscillator are subject to condition (13) and therefore the purity will decrease from its initial value of one. Our purpose is to investigate whether the purity will exceed one at a later time with these particular pure initial states and when the Robertson–Schrödinger uncertainty is violated, i.e. $4\sigma_{RS} < \hbar^2$. We involve this extra task due to some previous investigations, where the positivity violation is investigated through the uncertainty principle, see for example [21]. We consider for our numerical investigations the first three eigenstates of the quantum harmonic oscillator ($n = 0, 1, 2$) and in the representation used in Section 3 they read

$$\rho(R, r, 0) = \frac{H_n\left(\beta R + \frac{\beta r}{2}\right) H_n\left(\beta R - \frac{\beta r}{2}\right)}{2^n n!} \times e^{-\frac{1}{2}\beta^2(2R^2 + \frac{1}{2}r^2)} \sqrt{\frac{\beta^2}{\pi}}, \quad (14)$$

where we have used the center of mass and relative coordinates $R = (x + y)/2$, $r = x - y$. $H_n(x)$ are the Hermite polynomials. The parameter β is the inverse width $x_0 = \sqrt{\hbar/(m\omega)}$ of the quantum harmonic oscillator’s ground state. Furthermore, we introduce the following dimensionless parameters:

$$D'_{pp} = \frac{D_{pp} x_0^2}{\omega}, \quad D'_{px} = D_{px} m x_0^2, \quad \gamma' = \frac{\gamma}{\omega},$$

$$\Omega' = \frac{\Omega}{\omega}, \quad \beta' = \beta x_0, \quad \tau = \omega t, \quad T' = \frac{k_B T}{\hbar\omega}. \quad (15)$$

It is apparent from Figure 1 that the eigenstates of the quantum harmonic oscillator subject to condition (13) prescribe a short initial time evolution, where purity does not exceed one and the Robertson–Schrödinger uncertainty relation is also not violated.

We argued in Section 2 about the relation between the purity and the inequality of Robertson–Schrödinger uncertainty principle. In Figure 2 we see that for high enough temperatures there is a striking analogous behavior in both cases, namely the slopes of the plotted curves are almost identical. Motivated by this fact we have carried out a brief calculation in Appendix B, which shows that whenever the derivative of the purity with respect to time is zero it corresponds in most of the cases to situations where the time derivative of $4\sigma_{RS}$ is also zero. However, there are some cases when this is not true and they belong to situations where violations with respect to purity or the Robertson–Schrödinger uncertainty relation occur.

According to condition (2), we have considered not too high temperatures due to the small width of the initial wave packet, but they are still way above T'_{\min} which has been determined in Section 4 in the context of the steady state. In numbers, the first temperature choice is $T_1 = 10 \times T'_{\min}$ or $k_B T_1 = 20\hbar\omega$ and the second one

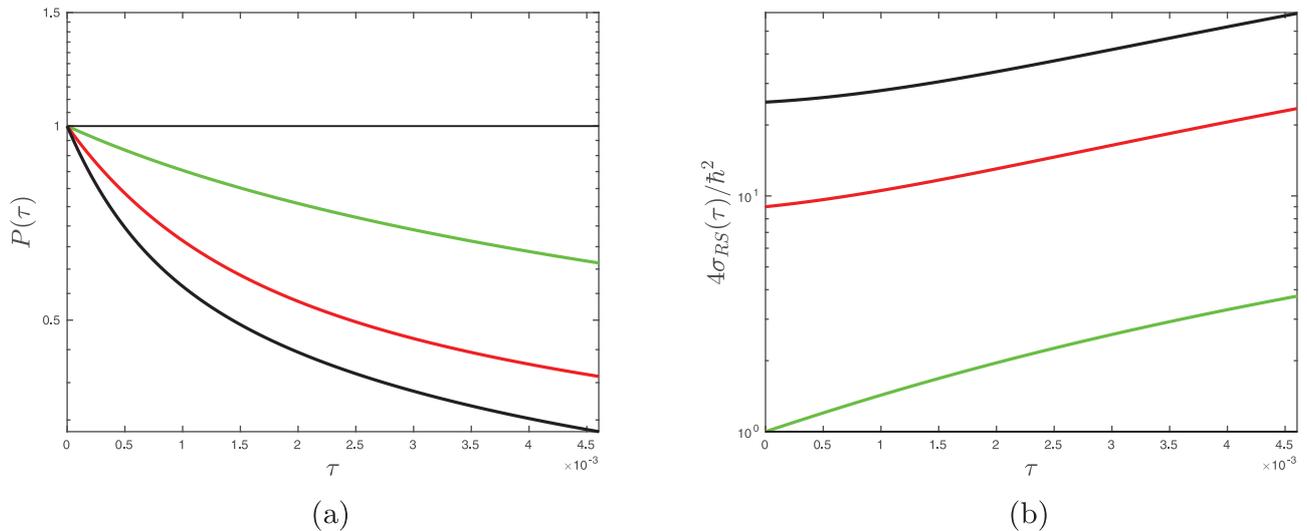


Fig. 1. Left panel: Semilogarithmic plot of purity $P(\tau)$ as a function of dimensionless time $\tau = \omega t$. Right panel: Left hand-side of the Robertson–Schrödinger uncertainty relation in (4), used in dimensionless form $4\sigma_{RS}(\tau)/\hbar^2$, as a function of τ . The three different curves are plotted for the following initial states of equation (14): $n = 0$ (green); $n = 1$ (red); and $n = 2$ (black). We set $D_{px} = 0$, $\gamma' = 0.35$, $T' = T'_{\min}$ (see Eq. (9)), and $\beta' = 0.6$ according to equation (15). The solid black lines mark both the allowed upper bound for the purity in the left panel and the right hand-side of the Robertson–Schrödinger uncertainty relation in the right panel. In the short time evolution, the purity does not exceed one and the Robertson–Schrödinger uncertainty relation is not violated.

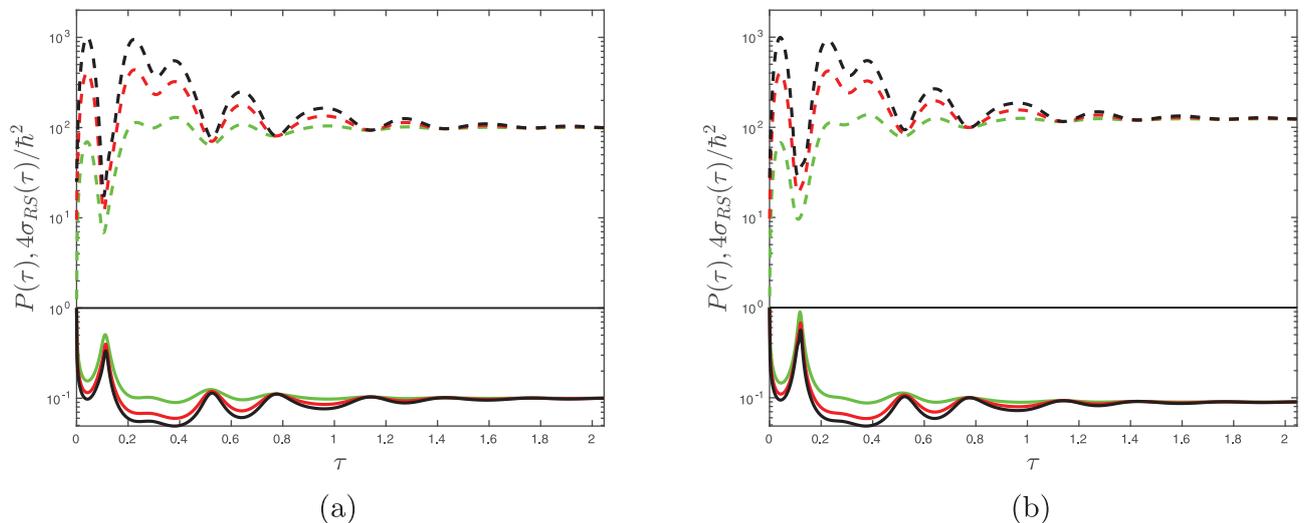


Fig. 2. Semilogarithmic plot of purity $P(\tau)$ (solid) and $4\sigma_{RS}(\tau)/\hbar^2$ (dashed) in equation (4) as a function of dimensionless time τ . The parameters are $\gamma' = 0.15$, $T' = 10 \times T'_{\min}$ (see Eq. (9)), and $\beta' = 0.6$ according to equation (15). Left panel: $D_{px} = 0$ or case I in Table 1. Right panel: case II in Table 1 with $\Omega' = 1.25$ defined in equation (15). The solid black lines mark both the allowed upper bound for the purity and the right hand-side of the Robertson–Schrödinger uncertainty relation. Both figures show that purity does not exceed one and the Robertson–Schrödinger uncertainty relation is not violated. Here, we have a high enough temperature, which is always understood in the context of the inverse of the width of the initial wave packet β' . Furthermore, curves on both sides of the line at value one show some similar behavior in their slopes.

$T_2 = 10^3 \times T'_{\min}$ or $k_B T_2 = 2000\hbar\omega$, thus both temperatures fulfill the high temperature approximation $k_B T_{1,2} \gg \hbar\omega$ employed in the derivation of the master equation. Figures 3 and 4 show that initial states which are subject to the condition (2) may lead to the violation of the positivity of the density operator. As the temperature is increased

these issues are resolved, a demonstration of our analytical results on the derivative of the purity with respect to the temperature in Section 4. We can also see violations which do not occur in the same time in purity $P(\tau)$ and $4\sigma_{RS}(\tau)/\hbar^2$, the left hand-side of the Robertson–Schrödinger uncertainty relation in (4), thus Appendix B

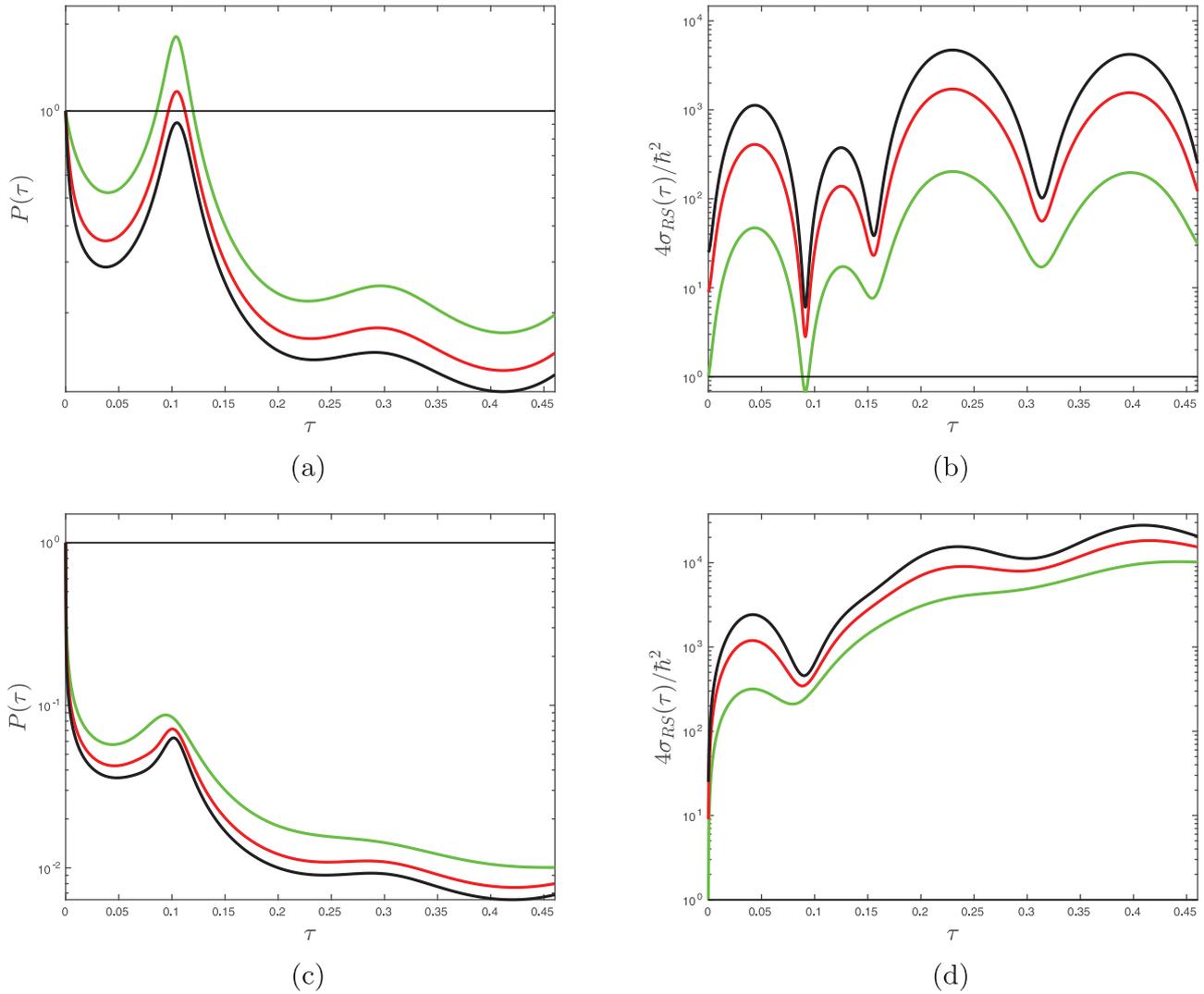


Fig. 3. Left panel: Semilogarithmic plot of purity $P(\tau)$ as a function of dimensionless time τ . Right panel: Semilogarithmic plot of $4\sigma_{RS}(\tau)/\hbar^2$ in equation (4) as a function of τ . The parameters are considered for case I in Table 1, i.e., $D_{px} = 0$, $\gamma' = 10^{-2}$, and $\beta' = 0.6$ according to equation (15). (a) and (b) Plotted for the same temperature $T' = 10 \times T'_{\min}$ (see Eq. (9)). (c) and (d) The temperature is set to $T' = 10^3 \times T'_{\min}$. (a) and (b) Violations with respect to the purity and $4\sigma_{RS}(\tau)/\hbar^2$ occur. Increasing the temperature these issues are resolved in (c) and (d). The solid black lines mark both the allowed upper bound for the purity and the right hand-side of the Robertson–Schrödinger uncertainty relation.

cannot cover these cases analytically. In other words, the sets $\mathcal{D}_1^P(\mathcal{H})$ and $\mathcal{D}_1^I(\mathcal{H})$, introduced in Section 2, do not overlap at all times. Furthermore, the numerical results show that somehow the purity is more sensitive than the Robertson–Schrödinger uncertainty relation to the positivity violation of the density operator. In summary, we have been able to demonstrate numerically that initial states fulfilling condition (2) still might lead to the positivity violation of the density operator in the later time of evolution.

7 Discussion and conclusions

We have solved analytically the Caldeira–Leggett master equation of a quantum harmonic oscillator with the

method of characteristics curves. Our choice on the method of characteristics is motivated by our focus on positivity violations of the density operator. The out most goal would be to find all initial states for which there are times during the time evolution such that there exists at least one negative eigenvalue of the master equation’s solution. In general this is not a simple mathematical task, definitely not for the infinite dimensional Hilbert space of the quantum harmonic oscillator. Therefore, we have taken the purity of the states, but we have to remind the reader about the fact that the purity being between the values one and zero is a necessary but not sufficient condition that there is no positivity violation during the time evolution.

As a first task, we have investigated the steady state solution and we have considered four cases for the

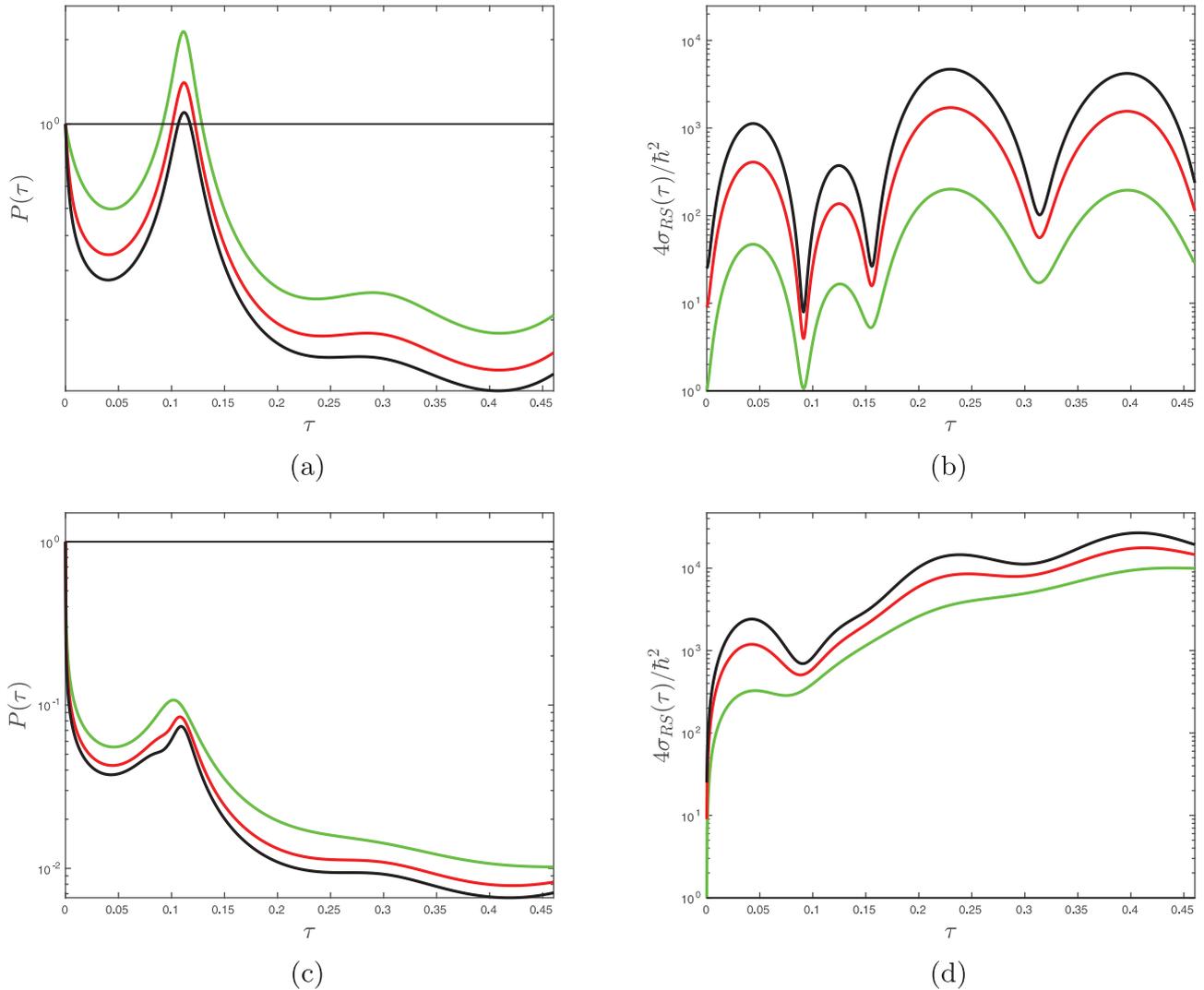


Fig. 4. Left panel: Semilogarithmic plot of purity $P(\tau)$ as a function of dimensionless time τ . Right panel: Semilogarithmic plot of $4\sigma_{RS}(\tau)/\hbar^2$ in equation (4) as a function of τ . The parameters are considered for case II of Table 1: $\Omega' = 2$, $\gamma' = 10^{-2}$ and $\beta' = 0.6$ according to equation (15). The temperatures are set for (a), (b), (c) and (d) to the same value as in Figure 3. Small width of the initial wave packets result in violations with respect to the purity and $4\sigma_{RS}(\tau)/\hbar^2$. Increasing the temperature resolves again these issues. The solid black lines mark both the allowed upper bound for the purity and the right hand-side of the Robertson–Schrödinger uncertainty relation.

values of the diffusion coefficients D_{pp} and D_{px} . These cases consist of: the pioneering work of Caldeira and Leggett [5]; an extended derivation of their result in [10]; another extension [12], where the derivation drops the high temperature limit and focuses on medium temperatures; and finally the master equation obtained via a phenomenological phase space quantization of an under-damped harmonic oscillator [13]. The last two cases deal with Lindblad master equations, where positivity violations cannot occur due to the form of mathematical map on the density operators. However, we have truncated these master equations in order to obtain a Caldeira-Leggett master equation. In the first three cases the investigation on the steady states led to some conditions upon the temperature which are in accordance

with the approximations used for the derivation of the master equations. In the last case, it turned out that the master equation of Dekker [13] derived for zero temperature cannot be truncated at will. We have also shown the derivative of the purity with respect to the temperature is always smaller than zero. Hence, situations where the purity exceeds one can be resolved by increasing the temperature. Thus, we have concluded: any kind of positivity violations of the density operator have to be searched for short and intermediate evolution times.

Therefore, in the next task we have focused on cases where the purity is one at a certain time. We have found the requirements on the width of the wave packet such that the time derivative of the purity is not positive, i.e., the purity decreases from the value one. In fact, the

$$\begin{aligned}
A &:= 2 X^{3/2} (\omega^2 r^2 + K^2) e^{2t(2\sqrt{X}+\gamma)} + \left((-\gamma\omega^2 r^2 + 2K\omega^2 r - K^2\gamma) \sqrt{X} + X (-\omega^2 r^2 + K^2) \right) \gamma e^{2t\sqrt{X}} \\
&\quad + 2 e^{4t\sqrt{X}} \omega^2 \sqrt{X} (\omega^2 r^2 - 2K\gamma r + K^2) - e^{6t\sqrt{X}} \times \left((\gamma\omega^2 r^2 - 2K\omega^2 r + K^2\gamma) \sqrt{X} + X (-\omega^2 r^2 + K^2) \right) \gamma, \\
B &:= -8 X^{3/2} \gamma K^2 e^{2t(2\sqrt{X}+\gamma)} + \left(\left((4\gamma^2 - 2\omega^2) K^2 - 4\omega^2 r \gamma K + 2\omega^4 r^2 \right) \sqrt{X} + X (4K\omega^2 r - 4K^2\gamma) \right) \gamma e^{2t\sqrt{X}} \\
&\quad - 4 e^{4t\sqrt{X}} \omega^2 \sqrt{X} (\omega^2 r^2 - 2K\gamma r + K^2) \gamma - e^{6t\sqrt{X}} \\
&\quad \times \left(\left[(-4\gamma^2 + 2\omega^2) K^2 + 4\omega^2 r \gamma K - 2\omega^4 r^2 \right] \sqrt{X} + X (4K\omega^2 r - 4K^2\gamma) \right) \gamma.
\end{aligned}$$

most natural way to apply this result is for initial pure states. In the case of the parameters given in the work of Caldeira and Leggett the initial width of the wave packet has to be larger than five times the thermal wavelength, which does not apply to many pure states. This statement suggests that one may find short time evolutions of the Caldeira-Leggett master equation for certain initial states to be mathematically inconsistent. Due to the steady state positivity, these initial problems disappear and in fact they can be ignored. This argument is more or less known in the community, however based on our full analytical knowledge on the evolving state and the exact details on the width of the wave packet, we have considered the first three eigenstates of the quantum harmonic oscillator as initial states. While they fulfill the condition on their wave packet width, at later times of the evolution the positivity violation of the density operator can be found. To show it, we have carried out numerical simulations and indeed we have been able to show that the purity exceeds one for later times. In the numerical investigations we have also compared the behavior of the purity and the Robertson-Schrödinger uncertainty relation, where the latter one is mostly preferred as a test for the positivity violation [21]. We have found a remarkable agreement between the slopes of their curves. However, when the positivity violation occurs, the purity seems to be a more sensitive indicator for the existence of any negative eigenvalue. As this observation is made with the help of numerical investigations the analytical proof is still missing and is subject of ongoing investigations.

Finally let us make some comments on our results. Both the analytical and numerical results clearly indicate inconsistencies in the Caldeira-Leggett master equation. We have reobtained some known facts, but also some new ones like the situations with initial eigenstates of the quantum harmonic oscillator. One fact is clear, if this Markovian master equation with high enough temperature is applied for long times of evolution, then effective and desirable descriptions of certain physical systems can be obtained. For example, in optomechanics, where quantum effects at low temperatures are important the use of the Caldeira-Leggett master equation may lead to inconsistencies, a fact which has initiated

extended studies on quantum dissipative models for harmonic oscillators [18,33]. However, the requirement for mathematical consistency is still looming over the master equation and there might be other surprising situations than those presented in this work, where the positivity of the density operator is violated not only for short time evolutions.

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Author contribution statement

J.Z.B. and G.H. conceived of the presented idea. G.H. and J.Z.B. developed the theory. G.H. and L.L. performed the computations. All authors verified the analytical methods, discussed the results and contributed to the final manuscript.

Appendix A: Detailed expressions of the introduced notations

In this Appendix, we present the full expressions of several notations introduced in the main text. First, the notations supporting equation (6) read

See equation above.

Secondly, the specific functions of Section 4 read

See equation next page

where \Re stands for the real part of a complex number.

$$\begin{aligned}
G(K, r, t) = & -\Re \left[\frac{T}{X^{\frac{3}{2}} \Omega \omega^2} \left[-\frac{1}{2} \gamma \left((-2K^2 \gamma^2 + ((\Omega r^2 + 2Kr) \omega^2 + K^2 \Omega) \gamma + (-\omega^2 r^2 + K(-2\Omega r + K)) \omega^2) \sqrt{X} \right. \right. \right. \\
& + (-2K^2 \gamma + (-\Omega r^2 + 2Kr) \omega^2 + K^2 \Omega) X \left. \left. \left. e^{4t\sqrt{X}} + \omega^2 \sqrt{X} (\omega^2 r^2 - 2\gamma Kr + K^2) (\Omega - \gamma) e^{2t\sqrt{X}} \right. \right. \right. \\
& + \frac{1}{2} \left((2K^2 \gamma^2 + ((-\Omega r^2 - 2Kr) \omega^2 - K^2 \Omega) \gamma - (-\omega^2 r^2 + K(-2\Omega r + K)) \omega^2) \sqrt{X} \right. \\
& \left. \left. \left. + (-2K^2 \gamma + (-\Omega r^2 + 2Kr) \omega^2 + K^2 \Omega) X \right) \gamma \right] e^{-2tX} \right]
\end{aligned}$$

$$\begin{aligned}
F(K, r, t) = & \Re \left[\frac{1}{2 \left(X^{\frac{3}{2}} T^2 \omega^2 \pi \right)} \left[\gamma \left(\left(\frac{1}{3} K^2 \Omega \gamma^2 + \left(\left(\pi T^2 r^2 - \frac{1}{3} Kr \Omega \right) \omega^2 + \pi T^2 K^2 \right) \gamma \pi T^2 K^2 \right) X \right) \right. \right. \\
& \times e^{2t\sqrt{X}} + \left(\left(\frac{1}{3} K^2 \Omega \gamma^2 + \left(\left(\pi T^2 r^2 - \frac{1}{3} Kr \Omega \right) \omega^2 + K(12\pi T^2 r + K\Omega) \right) \right) \sqrt{X} \right. \\
& + \left(\frac{1}{3} K^2 \Omega \gamma + \left(-\pi T^2 r^2 - \frac{1}{3} Kr \Omega \right) \omega^2 + \pi T^2 K^2 \right) X \left. \left. \gamma e^{6t\sqrt{X}} - 2\sqrt{X} \omega^2 \right. \right. \\
& \left. \left. \left. \times (\omega^2 r^2 - 2K\gamma r + K^2) e^{4t\sqrt{X}} \left(\pi T^2 + \frac{1}{6} \gamma \Omega \right) \right] e^{-2t(2\sqrt{X} + \gamma)} X^{\frac{3}{2}} T^2 \omega^2 \pi \right]
\end{aligned}$$

Appendix B: Existence proof about common extrema in the time evolution of $\sigma_{RS}(t)$ and $P(t)$

First we calculate the expression for the derivative of the Robertson–Schrödinger formula with respect to time in a Fourier transformed representation. The suitable moments of position and momentum operators in this representation are

$$\begin{aligned}
\langle \hat{x} \rangle &= \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{iKR} \frac{\partial \rho(K, 0, t)}{\partial K} dK dR, \\
\langle \hat{x}^2 \rangle &= -\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{iKR} \frac{\partial^2 \rho(K, 0, t)}{\partial K^2} dK dR,
\end{aligned}$$

$$\begin{aligned}
\langle \hat{p} \rangle &= -\frac{i}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{iKR} \\
&\quad \times \left[\frac{i}{2} K + \frac{\partial}{\partial r} \right] \rho(K, r, t) \Big|_{r=0} dK dR,
\end{aligned}$$

$$\begin{aligned}
\langle \hat{p}^2 \rangle &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{iKR} \\
&\quad \times \left\{ \left[\frac{1}{4} K^2 + iK \frac{\partial}{\partial r} - \frac{\partial^2}{\partial r^2} \right] \rho(K, r, t) \right\} \Big|_{r=0} dK dR,
\end{aligned}$$

$$\begin{aligned}
\frac{1}{2} \langle \hat{x} \hat{p} + \hat{p} \hat{x} \rangle &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{iKR} \\
&\quad \times \left\{ \left[-\frac{1}{2} K \frac{\partial}{\partial K} + \frac{Kr}{4} + \frac{\partial^2}{\partial r \partial K} + \frac{r}{2} \frac{\partial}{\partial r} \right] \rho(K, r, t) \right\} \Big|_{r=0} \\
&\quad \times dK dR,
\end{aligned}$$

and we finally get

$$\begin{aligned}
\frac{d\sigma_{RS}(t)}{dt} = & \left[\frac{d}{dt} \langle \hat{x}^2 \rangle - 2 \langle \hat{x} \rangle \frac{d}{dt} \langle \hat{x} \rangle \right] \cdot \left[\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2 \right] \\
& + \left[\frac{d}{dt} \langle \hat{p}^2 \rangle - 2 \langle \hat{p} \rangle \frac{d}{dt} \langle \hat{p} \rangle \right] \cdot \left[\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2 \right] \\
& - 2 \left[\frac{1}{2} \langle \hat{x} \hat{p} + \hat{p} \hat{x} \rangle - \langle \hat{x} \rangle \langle \hat{p} \rangle \right] \\
& \times \left(\frac{1}{2} \frac{d}{dt} \langle \hat{x} \hat{p} + \hat{p} \hat{x} \rangle - \langle \hat{p} \rangle \frac{d}{dt} \langle \hat{x} \rangle - \langle \hat{x} \rangle \frac{d}{dt} \langle \hat{p} \rangle \right).
\end{aligned}$$

The purity in the Fourier transformed representation reads

$$\begin{aligned}
\frac{d}{dt} P(t) = & \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho(K, r, t) \frac{\partial}{\partial t} \rho^*(K, r, t) dK dr \\
& + \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho^*(K, r, t) \frac{\partial}{\partial t} \rho(K, r, t) dK dr.
\end{aligned}$$

Let us suppose that there are times t^* , when

$$\frac{\partial \rho(K, r, t)}{\partial t} \Big|_{t=t^*} = 0 \rightarrow \frac{\partial \rho^*(K, r, t)}{\partial t} \Big|_{t=t^*} = 0,$$

because the real and imaginary parts of derivative of the density function with respect to time must disappear in the same time. If the necessary mathematical conditions are satisfied, the derivation and the integration can be exchanged, then the following mathematical identity is

fulfilled:

$$\begin{aligned} & \frac{d}{dt} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathcal{O}(K, r) \rho(K, r, t) dK dr \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathcal{O}(K, r) \frac{\partial}{\partial t} \rho(K, r, t) dK dr, \end{aligned}$$

where $\mathcal{O}(K, r)$ is the corresponding representation of an operator $\hat{\mathcal{O}}$.

Hence, there are times t^* when the time derivative of both functions $\sigma_{RS}(t)$ and $P(t)$ disappear, since in this case the constant zero function is integrated in both cases.

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