We investigate a non-Markovian master equation of the Caldeira-Leggett model obtained in the weak coupling limit up to the second order expansion. The evolution of the non-Markovian master equation is unphysical when the stationary solution is unphysical, and we prove that the solution always remains physical for small times. Moreover, we are able to find even stronger anomalous behavior, when the trace of the solution is diverging. We also provide results for the Markovian master equation and show that positivity violations occur for various types of initial conditions even when the stationary solution is physical. In our study we use Gaussian initial states to simplify the problem and employ a sufficient and necessary condition to detect unphysical behavior. Based on our numerical experiments we conclude that the non-Markovian master equation is superior to the Markovian one.

I. INTRODUCTION

The density operator completely describes the state of a quantum mechanical system and it is defined as a positive trace class operator of trace one [1]. The quantum system in study can be subject to interactions with its environment, which is colloquially referred to as an open quantum system. It is expected that the whole system evolves unitarily and by tracing out the environment’s degrees of freedom one obtains a positive trace preserving map acting on the states of the open system [2]. If one further assumes an initially uncorrelated joint state, then a stronger kind of positivity, called complete positivity, is obtained [3]. Some particular aspects of this assumption have been discussed in Refs. [4–8]. In physical applications these maps are subject to further approximations, which either leads to Markovian or non-Markovian master equations [9]. However, the positivity of the approximation-free map may be violated implying that complete positivity fails as well. A known case is the Caldeira-Leggett model [10] of the quantum Brownian motion [11, 12], where different approaches may result in a master equation, which may not preserve the positivity of the density operator for short times [13–16]. In the model of Unruh and Zurek [17] (where the environment is modeled differently from the Caldeira-Leggett model) issues with respect to rapid decoherence for short time evolutions have been found.

Recently, the Markovian master equation of the Caldeira-Leggett model was investigated with the help of the purity of the density operator for arbitrary initial states [18]. The authors exploited the fact that the purity indicates positivity violation when it takes values bigger than one. They have been able to identify circumstances where intermediate-time positivity violations occur. The non-Markovian master equation obtained from the Caldeira-Leggett model [14] is believed to be a more precise description than the Markovian one. Both the Markovian and the non-Markovian master equation can be formally solved [18–20] for all possible initial conditions. However, the obtained solutions in the phase space representation cannot determine in general the positivity of the associated Weyl operator [21, 22], because one has to verify either a non-countable or a countable set of inequalities. In a special case, the eigenvalue spectrum of Gaussian density operators can be analytically determined [23, 24], and the special form of the spectrum implies that the Gaussian state is positive if and
only if the purity is between zero and one. In particular, results in [19] implies that an initially Gaussian state remains Gaussian for all times. Therefore, using a Gaussian ansatz the solution of master equation can be reduced to a system of ordinary differential equations for the unknown coefficients in the exponent.

The main parameters of the Caldeira-Leggett model are the temperature of thermal bath and the spectral density of the environment. In the phenomenological modeling one expects that the spectral density goes to zero for very high frequencies. A special case is when the spectral density is proportional to the frequency for small values of frequency i.e., the Ohmic spectral density, which gives rise to frequency-independent damping rate. Other spectral densities are also subject to investigations, see e.g., [14, 19, 25]. In this paper, we choose the Ohmic spectral density with a Lorentz-Drude cut-off function and assume that the coupling between the system and the reservoir is weak, therefore the whole system can be treated in second order [9]. Furthermore, we consider the open quantum system to be a quantum harmonic oscillator.

The paper is organized as follows. In Sec. II we introduce the model and derive the system of linear differential equations for coefficients of the density operator with a Gaussian form which is the starting point for our analysis. In Sec. III we study the positivity of the stationary state. In parameter space we identify regions where positivity violations can occur. Concrete examples of these violations are given Sec. IV Here, we concentrate on the differences of the Markovian and non-Markovian time evolutions of a Gaussian density operators. Sec. V summarizes our main results. Technical details are provided in the Appendices.

II. NON-MARKOVIAN MASTER EQUATION WITH GAUSSIAN INITIAL CONDITIONS

In this section we discuss basic features of the non-Markovian master equation [14, 20, 26] by focusing on terms up to the second order expansion in the weak coupling strength [27]. The non-Markovian master equation for a quantum harmonic oscillator with physically observable frequency \( \omega_p \) and mass \( m \) reads

\[
\begin{align*}
\frac{i\hbar}{\partial t} & \hat{\rho} = \left[ \frac{\hat{p}^2}{2m} + \frac{m\omega_p^2(t)x^2}{2}, \hat{\rho} \right] - iD_{pp}(t)[\hat{x}, [\hat{x}, \hat{p}]] \\
& + \lambda(t)[\hat{x}, \{\hat{p}, \hat{\rho}\}] + 2iD_{px}(t)[\hat{x}, [\hat{p}, \hat{\rho}]],
\end{align*}
\]

(1)

where \([,]\) stands for commutators while \{,\} for anti-commutators. In the weak coupling limit the coefficients in the second order expansion entering the master equation read

\[
\begin{align*}
\omega_p^2(t) &= \omega_0^2 - \frac{2}{m} \int_0^t dsD(s) \cos(\omega_0 s), \\
\lambda(t) &= \frac{1}{m\omega_0} \int_0^t dsD(s) \sin(\omega_0 s), \\
D_{px}(t) &= \frac{1}{2m\omega_0} \int_0^t dsD_1(s) \sin(\omega_0 s), \\
D_{pp}(t) &= \int_0^t dsD_1(s) \cos(\omega_0 s),
\end{align*}
\]

(2)

where \( \omega_0 \) contains the environment-induced frequency shift of the original oscillator frequency \( \omega_0 \). We warn the reader that we use different conventions for the coefficients from that of [27]. We have introduced the following correlation functions:

\[
\begin{align*}
D(s) &= \int_0^\infty d\omega J(\omega) \sin(\omega s) \\
D_1(s) &= \int_0^\infty d\omega J(\omega) \coth(\frac{\hbar\omega}{2k_B T}) \cos(\omega s).
\end{align*}
\]

(3)

Making use of an Ohmic spectral density with a Lorentz-Drude type function and a high-frequency cutoff \( \Omega \),

\[
J(\omega) = \frac{2m\gamma \Omega^2}{\pi} \frac{\omega}{\Omega^2 + \omega^2},
\]

where \( \gamma \) is the frequency-independent damping constant. Then the bath correlation \( D(s) \) can be determined analytically as

\[
D(s) = 2m\gamma \Omega^2 \exp(-\Omega s), \quad s \geq 0.
\]

(5)

For the other correlation function \( D_1(s) \) see Eq. (A1) in Appendix A Furthermore, for \( t \) > 0

\[
\omega_p^2(t) = \omega_0^2 - 2\gamma \Omega - \frac{2}{m} \int_0^t dsD(s) \cos(\omega_0 s) = \omega_0^2 + 2\gamma \Omega - \frac{2\gamma \Omega^2}{\Omega^2 + \omega_0^2} e^{-\Omega t} \left[ \Omega e^{\Omega t} - \Omega \cos(\omega_0 t) + \omega_0 \sin(\omega_0 t) \right],
\]

where for \( t \gg 1 \), \( \omega_p(t) \) is approximately equal to \( \omega_0 \), and

\[
\lambda(t) = \frac{\gamma \Omega^2}{\omega_0^2} \frac{\Omega^2 e^{-\Omega t}}{\Omega^2 + \omega_0^2} e^{-\Omega t} \left[ \omega_0 e^{\Omega t} - \omega_0 \cos(\omega_0 t) - \Omega \sin(\omega_0 t) \right].
\]

Closed formulas for \( D_{px}(t) \) and \( D_{pp}(t) \) are given in Appendix A

Now, we rewrite equation (11) in the position representation

\[
\begin{align*}
\int \frac{\partial}{\partial t} \rho(x, y, t) = & \left[ \frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial x^2} \right) + \frac{m\omega_p^2(t)}{2} (x^2 - y^2) \\
- iD_{pp}(t)(x - y)^2 - i\lambda(t)(x - y) \left( \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) \\
+ 2iD_{px}(t)(x - y) \left( \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) \right] \rho(x, y, t).
\end{align*}
\]

(6)
Naively, the non-Markovian master equation starts at $t = 0$ as a von Neumann equation. This would imply that positivity violations never occur around $t = 0$. We prove this fact rigorously in Appendix [C] for small temperatures. For longer times it is not guaranteed that positivity will not be violated.

Another property of (8) is that Gaussian initial state remains Gaussian during the whole evolution. In [19], the time evolution of a Wigner function (namely, in eq. (78) of their paper) starting from an arbitrary initial condition is given. If this initial Wigner function is Gaussian, then this result shows that at an arbitrary time $t > 0$ the solution is also a Gaussian (with time dependent coefficients in the exponent). The Wigner function and $\rho(x, y, t)$ are connected by Wigner-Weyl transformation which maps a Gaussian function to Gaussian ones. Consequently, if we choose $\rho(x, y, t = 0)$ to be Gaussian it will be Gaussian at later times too, but with time dependent coefficients. More concretely, we consider the following Gaussian in the position representation

$$
\rho(x, y, t) = \exp\{-A(t)(x - y)^2 - B(t)(x^2 - y^2)
- C(t)(x + y)^2 - ID(t)(x - y) - E(t)(x + y) - N(t)\},
$$

(7)

where the time-dependent parameters $A, B, C, D, E$ and $N$ are real, because $\dot{\rho}$ is self-adjoint. Assuming positive $A(t)$ and $C(t)$ the eigenvalue problem in the position representation for a fixed $t$

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

(8)

has been considered in detail by Ref. [24]. The spectrum $\{\lambda_n\}_{n \in \mathbb{N}_0}$ of (7) depends only on $A$ and $C$ for all $t \geq 0$:

$$
\lambda_n = \lambda_0\lambda^n,
\lambda_0 = \frac{2\sqrt{C}}{\sqrt{A + \sqrt{C}}},
\lambda = \sqrt{A - \sqrt{C}}.
$$

If $0 < A < C$ some of the eigenvalues are negative, which means the Gaussian density matrix violates positivity. Clearly, all eigenvalues are in the interval $[0,1]$ iff

$$
A \geq C \geq 0.
$$

(9)

If (9) is not true at a given time $t$, then the Gaussian function $\rho(x, y, t)$ has no physical interpretation (i.e., if (9) fails it is a sufficient and necessary condition to detect unphysical behavior). We are going to test its validity by investigating $A/C$. Note that the purity is given by $\text{Tr} \rho^2 = \sqrt{C/A}$.

The time-dependent coefficients $A, B, C, D,$ and $E$ obey a system of non-linear non-autonomous differential equations. However, using the transformation

$$
\rho(k, \Delta, t) = \int_{-\infty}^{\infty} dx e^{ikx} \rho\left(x + \frac{\Delta}{2}, x - \frac{\Delta}{2}, t\right),
$$

(10)

given in [17, 24] we obtain the equation of motion for $\rho(k, \Delta, t)$

$$
\begin{align*}
\frac{\partial}{\partial t} \rho(k, \Delta, t) &= \left(\frac{\hbar k}{m} \frac{\partial}{\partial \Delta} - \frac{m\omega^2(t)}{\hbar} \frac{\partial}{\partial k} - \frac{D_{pp}(t)}{\hbar}\Delta^2 \right.
- 2\lambda(t)\Delta \left(\frac{\partial}{\partial \Delta} - 2D_{px}(t)k\Delta\right) \rho(k, \Delta, t).
\end{align*}
$$

Note that the above equation of motion contains only first order derivatives and therefore it is easier to construct its solutions. In this representation the Gaussian form of (7) is preserved and reads:

$$
\rho(k, \Delta, t) = \exp\{-c_1(t)k^2 - c_2(t)k\Delta - c_3(t)\Delta^2
- ic_4(t)k - ic_5(t)\Delta - c_6(t)\},
$$

(11)

where the time-dependent coefficients $c_1, c_2, c_3, c_4, c_5$ and $c_6$ are also real and obey the following system of linear differential equations:

$$
\begin{align*}
\dot{c}_1 &= \frac{\hbar c_2}{m},
\dot{c}_2 &= 2D_{px}(t) + \frac{2\hbar c_3}{m} - \frac{2m\omega^2(t)}{\hbar}c_1 - 2\lambda(t)c_2,
\dot{c}_3 &= \frac{D_{pp}(t)}{\hbar} - \frac{m\omega^2(t)}{\hbar}c_2 - 4\lambda(t)c_3,
\dot{c}_4 &= \frac{hc_5}{m},
\dot{c}_5 &= -\frac{m\omega^2(t)}{\hbar}c_4 - 2\lambda(t)c_5,
\dot{c}_6 &= 0.
\end{align*}
$$

(12)

The first three and the last three equations decouple. The first three can be written compactly as follows:

$$
\dot{c}(t) = M(t)c(t) + v(t),
$$

(13)

where $c^T(t) = (c_1, c_2, c_3)$ (the superscript $T$ denotes the transposition),

$$
M(t) = \begin{pmatrix}
0 & \frac{\hbar}{m} & 0 \\
-2\lambda(t) & -2\lambda(t) & \frac{2\hbar}{m} \\
0 & \frac{m\omega^2(t)}{\hbar} & -4\lambda(t)
\end{pmatrix},
$$

(14)

and

$$
v(t) = \begin{pmatrix}
0 \\
2D_{px}(t) \\
D_{pp}(t)/\hbar
\end{pmatrix}.
$$

The coefficients $A, B,$ and $C$ are related to $c$ through the transformation (10) as

$$
A = c_3 - \frac{c_2^2}{4c_1},
B = -\frac{c_2}{4c_1},
C = \frac{1}{16c_1}.
$$

(15)

We can already see the advantage of the new phase space representation $\rho(k, \Delta)$, because solving (13) is better suited for our subsequent investigation of the ratio $A/C$. However, the solution of (13) is still not simple, because the matrices $M(t)$ and $M(t')$ do not commute at different times $t \neq t'$ and the vector $v(t)$ is also time dependent. A formal solution with the help of a time-ordered exponential can be given, but does not seem to be helpful for us. Therefore, we are going to focus on the numerical solutions of (13) and to carry out a brief analysis on the stationary state.
III. A BRIEF ANALYTICAL STUDY OF THE STATIONARY STATE

In this section, we investigate the positivity of the stationary state. After a long time a Markovian limit is obtained, which yields

$$\omega_p^2(t \to \infty) = \left(\omega_p^{(M)}\right)^2, \quad \lambda(t \to \infty) = \lambda^{(M)},$$

$$D_{px}(t \to \infty) = D_{px}^{(M)}, \quad D_{pp}(t \to \infty) = D_{pp}^{(M)},$$

where the details about Markovian values (denoted with superscripts $M$) are given in Appendix A. Thus, $M(t)$ and $v(t)$ tend to constants $M^{(M)}$ and $v^{(M)}$. The stationary solution of $c(t)$ can be expressed as:

$$c^{(M)} = -[M^{(M)}]^{-1}v^{(M)}.$$ 

Approaching the stationary state is governed by the three eigenvalues of $M$, which are $(-2) \cdot \lambda(t)$ and $(-2) \cdot \left(\lambda(t) \pm \sqrt{\lambda^2(t) - \omega_p^2(t)}\right)$. For $t > 0$ the real part of all three eigenvalues is negative, thus $M(t)$ is contractive, which ensures that starting from arbitrary initial conditions $c(0)$ the trajectory $c(t)$ tends to its Markovian limit. In the asymptotic region $\lambda(t)$ and $\omega_p(t)$ must be replaced by their respective Markovian values.

reached their stationary values, the test $A/C \geq 1$ can be written as

$$A^{(M)} \div C^{(M)} = \left(\frac{D_{pp}^{(M)}}{m^2} \Gamma(\lambda^{(M)}) \cdot \Gamma(\omega^{(M)})\right)^2.$$ 

On the critical line $A^{(M)} \div C^{(M)} = 1$ the damping factor $\gamma$ can be expressed as

$$\gamma = \gamma_{\text{crit}}(\Omega, k_B T, \omega_0) = \frac{\Omega^2 + \omega_0^2}{\Omega^2} \cdot \coth^2 \left(\frac{\hbar \omega_0}{2 \pi k_B T}\right) - 1,$$

where

$$Z(\Omega, k_B T, \omega_0) = 2 - 4 \frac{k_B T}{\hbar \omega_0} \coth \frac{k_B T}{2 \pi k_B T} \left[-1 + \frac{\Omega}{2 \pi k_B T} \times \right.$$

$$\left.\times \Psi \left(\frac{i \hbar \omega_0}{2 \pi k_B T}\right) + \Psi \left(-\frac{i \hbar \omega_0}{2 \pi k_B T}\right) - 2 \Psi \left(\frac{\hbar \Omega}{2 \pi k_B T}\right)\right]$$

and $\Psi$ is the digamma function [28]. The denominator $Z(\Omega, k_B T, \omega_0)$ has a zero if we vary $k_B T$, thus there exist a certain temperature $\tilde{T}$ at which the damping factor $\gamma$ tends to infinity on the critical line, see Fig. 1. Clearly, above $\tilde{T}$ the stationary solution is a density operator for any damping factor $\gamma$, see region III. on Fig. 1. The stationary solution is not a density operator in region I., i.e., $T < \tilde{T}$ and $\gamma > \gamma_{\text{crit}}$. In this parameter region we can choose any initial condition the time evolution for $\hat{\rho}(t)$ violates the positivity of the density operator eventually. Regions II. and III. of Fig. 1 guarantee that the asymptotic state is physically allowed, but this does not guarantee that the full time evolution is physical. Problematic time evolution might appear for several kind of initial conditions, especially if we choose the parameters of the master equations close to the critical line $\gamma_{\text{crit}}$.

Analytical approximations for the critical line can be done in two cases. If $\Omega \gg \omega_0$ one can expect (See Fig. 1) that $k_B \tilde{T}$ is on the $h\Omega$ scale. Let us introduce the quantity $x = k_B \tilde{T} / (h\Omega)$. If $\Omega \gg \omega_0$ looking for the zeros for $Z$ in Eq. (19) the leading terms are:

$$0 = \pi x + \gamma_{\text{EM}} + \Psi \left(\frac{1}{2 \pi x}\right),$$

where $\gamma_{\text{EM}}$ is the Euler-Mascheroni constant, which is approximately $0.577$. Solving (20) for $x$ one gets $k_B \tilde{T} \approx 0.240395 \cdot h\Omega$ for large $\Omega$. It should be noted that this result has been previously found by Ref. [29], where the stationary state has been investigated from the point of view of Heisenberg uncertainty principle. In the case of Gaussian density operators the Heisenberg uncertainty principle and our test condition $A/C \geq 1$ are the same constraints on the parameter space of the master equation.

A different approximation is possible for $\gamma_{\text{crit}}$ at very low temperature. Keeping the leading order terms in Eq. (15) for $k_B T \ll \hbar \omega_0$ and $k_B T \ll h\Omega$ one gets the

![FIG. 1: Parameter space plot of $k_B T/(\hbar \omega_0)$ versus $\gamma/\omega_0$ at fixed $\Omega/\omega_0 = 20$. Continuous thick line shows the critical line $\gamma = \gamma_{\text{crit}}(k_B T)$. Dashed line indicates the temperature $\tilde{T}$. Regions I., II. and III. are discussed in the main text. Crosses indicate the parameters used in Figs. 2, 11.](image-url)
FIG. 2: Parameters used: $\gamma = \omega_0$, $\Omega = 20\omega_0$, $k_B T = 10h\omega_0$. Initial conditions are: $w = 1$, $(c_1(0), c_2(0), c_3(0)) = (d_0^2/4, 0, 1/(4d_0^2))$. Left panel: $A d_0^2$ and $C d_0^2$ as a function of $\omega_0 t$, where $d_0$ is width of the quantum harmonic oscillator’s ground state. Main figure shows the non-Markovian time evolution, the inset shows the Markovian time evolution. Right panel: $A/C$ as a function of $\omega_0 t$. Solid and dashed dotted line show this ratio for the non-Markovian and the Markovian case, respectively. Horizontal thin lines indicate the asymptotic values on both panels.

FIG. 3: The same as for Fig. 2. Parameters used: $\gamma = \omega_0$, $\Omega = 20\omega_0$, $k_B T = h\omega_0$. Initial conditions are: $w = 1$, $(c_1(0), c_2(0), c_3(0)) = (d_0^2/4, 0, 1/(4d_0^2))$. Positivity violations occur for $\omega_0 t > 0.79$ (Markovian case) and for $\omega_0 t > 2.03$ (non-Markovian case).

Limiting behavior

$$\gamma_{\text{crit}} \approx 4 \frac{\Omega^2 + \omega_0^2}{\Omega^2} \exp \left\{ \frac{h\omega_0}{k_B T} \right\} \equiv C \cdot e^{-\frac{a}{T}},$$  \hspace{1cm} \text{(21)}$$

where $C$ and $a$ are constants. Clearly, this function is non-analytical in $T$, and approaches the origin in Fig. 1 with infinite slope. Inverting (21) one has on the critical line

$$T \approx \frac{a}{\log\left( \frac{C}{\gamma_{\text{crit}}} \right)},$$  \hspace{1cm} \text{(22)}$$

for small $\gamma_{\text{crit}}$.

As we indicated earlier, one can experience positivity violations during the time evolution. In the following we show a few time evolutions which might be interesting for the reader. In the numerics we limit ourselves to Gaussian density operators, which means that we have
FIG. 4: The same as for Fig. 2. Parameters used: $\gamma = 0.1\omega_0$, $\Omega = 20\omega_0$, $k_BT = 0.01\hbar\omega_0$. Initial conditions are: $w = 1$, $(c_1(0), c_2(0), c_3(0)) = (d_0^2/4, 0, 1/(4d_0^2))$. Positivity violations for $\omega_0t > 0$ (Markovian case) and for $\omega_0t > 3.28$ (non-Markovian case).

FIG. 5: The same as for Fig. 2. Parameters used: $\gamma = 10\omega_0$, $\Omega = 20\omega_0$, $k_BT = 0.01\hbar\omega_0$. Initial conditions are: $w = 1$, $(c_1(0), c_2(0), c_3(0)) = (d_0^2/4, 0, 1/(4d_0^2))$. Positivity violations for $\omega_0t > 0$ (Markovian case) and for $\omega_0t > 0.23$ (non-Markovian case). For the non-Markovian case $A$ changes sign at $\omega_0t \approx 0.36$. $A$ and $C$ diverge at $\omega_0t \approx 0.44$.

to follow only the time evolution of $c(t)$, from which we extract $A$ and $C$ via (15) and check the validity of (9) numerically.

IV. NUMERICAL RESULTS

In the previous section we have discussed the validity of the stationary solution, which gives a constraint on the parameters of the master equation. We consider three different types of initial conditions of (13) namely, coherent, squeezed and thermal states. For the sake of completeness we hereby reformulate these well-known initial states to our representation.

Coherent state. This state is defined through the complex parameter $\alpha$

$$|\alpha\rangle = \sum_{n=0}^{\infty} e^{-\frac{\alpha^2}{2}} \frac{\alpha^n}{\sqrt{n!}} |n\rangle, \quad |\alpha\rangle = |\alpha| e^{i\phi},$$

(23)

where $|n\rangle$ ($n \in \mathbb{N}_0$) are the number states and $\phi$ is the complex phase of $\alpha$. The Wigner function of this coherent state reads

$$W(x, p) = \frac{1}{\pi\hbar} e^{-x^2/2 - \sqrt{\text{Re}(|\alpha|^2)}^2 - (p/\hbar - \sqrt{\text{Im}(|\alpha|^2)}^2}$
FIG. 6: The same as for Fig. 2. Parameters used: \( \gamma = 0.755 \omega_0, \Omega = 20 \omega_0, k_B T = \hbar \omega_0 \). Initial conditions are: \( w = 1, (c_1(0), c_2(0), c_3(0)) = (d_0^2/4, 0, 1/4d_0^2) \). The Markovian behavior is unphysical for \( 1.26 < \omega_0t < 2.68 \).

FIG. 7: The same as for Fig. 2(b). Parameters used: \( \gamma = 0.755 \omega_0, \Omega = 20 \omega_0, k_B T = \hbar \omega_0 \). Initial conditions are: \( w = 1/\sqrt{10}, (c_1(0), c_2(0), c_3(0)) = (d_0^2/(40), 0, 10/(4d_0^2)) \). The Markovian behavior is unphysical for \( 0 < \omega_0t < 0.17 \).

where \( d \) is a length and can be taken as

\[
d = w \sqrt{\frac{\hbar}{m \omega_0}} \equiv wd_0.
\]

\( w \) is a dimensionless positive number and \( d_0 \) is the width of the quantum harmonic oscillator’s ground state. Due to the relation

\[
W(x, p) = \left( \frac{1}{2\pi} \right)^2 \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} d\Delta e^{-i(kx + \Delta p/\hbar)} \rho(k, \Delta)
\]

we obtain

\[
c_{\text{coh}}(0) = \left( \frac{d^2}{4}, 0, \frac{1}{4d^2} \right).
\]  

Squeezed state. In this case the state is characterized by two complex parameters \( \alpha \) and \( \zeta = |\zeta|e^{i\phi} \). Introducing the creation \( a^\dagger \) and annihilation \( a \) operators of the quantum harmonic oscillator a squeezed state is given by

\[
|\alpha, \zeta\rangle = \hat{D}(\alpha)\hat{S}(\zeta)|0\rangle
\]

where \( \hat{D}(\alpha) = \exp(a\hat{a}^\dagger - \alpha^* \hat{a}) \) is the displacement and \( \hat{S}(\zeta) = \exp\left[\frac{\zeta}{2}(\hat{a}^\dagger \hat{a}^2 - \hat{a} \hat{a}^\dagger)^2\right] \) is the squeezing operator. After a lengthy but standard calculation the Wigner function yields

\[
W(x, p) = \frac{1}{\pi\hbar} e^{-\left(\frac{x}{d} - \sqrt{2}\text{Re}(\alpha)\right)^2 t_1 - \left(\frac{pt}{\hbar} - \sqrt{2}\text{Im}(\alpha)\right)^2 t_2}
\]

\[
\times \exp\left[\left(\frac{\zeta}{2} - \zeta^*\frac{x}{d} + \frac{\zeta^*}{2} x^2 + \frac{\zeta}{2} p^2 + \frac{\zeta^*}{2} p^2\right)\right] e^{-2\zeta}\sin\phi.
\]

Finally, with the help of (24) we get

\[
c_{\text{coh}}(0) = \left( \frac{d^2}{4}, \frac{1}{4d^2}, \frac{1}{4d^2} t_1 \right).
\]  

Thermal state. This is a Gibbs state characterized by the thermal equilibrium temperature \( T' \), which in the number state representation reads

\[
\hat{\rho} = \sum_n \frac{n!}{(1 + n_{\text{th}})^n} |n\rangle \langle n|.
\]
with the mean excitation number

$$n_{th} = \left[ \exp\left( \frac{\hbar \omega_0}{k_B T'} \right) - 1 \right]^{-1}.$$

We have for the Wigner function

$$W(x, p) = \frac{1}{\pi \hbar} e^{-\frac{x^2}{2 n_{th} + 1}} e^{-\frac{p^2}{2 n_{th} + 1}}.$$

Note that the coherent state with $w = 1$ corresponds to the ground state of the quantum harmonic oscillator and is contained as trivial special cases of the thermal and squeezed states.

FIG. 8: The same as for Fig. 2. Parameters used: $\gamma = 0.1 \omega_0$, $\Omega = 20 \omega_0$, $k_B T = 0.397055 \hbar \omega_0$. Initial conditions are: $w = 1$, $(c_1(0), c_2(0), c_3(0)) = (d_0^2/4, 0, 1/4d_0^2)$. Several positivity violations are for the Markovian case.

FIG. 9: $(A - C)d_0^2$ as a function of $\omega_0 t$. Parameters used: $\gamma = 0.1 \omega_0$, $\Omega = 20 \omega_0$, $k_B T = 0.397055 \hbar \omega_0$. Initial conditions are: $w = 1$, $(c_1(0), c_2(0), c_3(0)) = (d_0^2/4, 0, 1/4d_0^2)$. Solid line: non-Markovian case, dashed dotted line: Markovian case. The horizontal line is drawn at zero. One can observe several positivity violations for the Markovian case.

FIG. 10: Positivity violations in the Markovian runs for different squeezed initial conditions characterized by the complex $\zeta$. White region: no positivity violations, dark region: positivity violations. Parameters used: $\gamma = 0.755 \omega_0$, $\Omega = 20 \omega_0$, $k_B T = \hbar \omega_0$, $w = 1$. Time evolutions for points at $|\zeta| = 1$, $\phi = \pm \pi/4$ will be shown on Fig. 11.
non-Markovian time evolutions. Parameters used: $\gamma = 0.755\omega_0$, $\Omega = 20\omega_0$, $k_B T = \hbar\omega_0$. Initial conditions are: $w = 1$, $\xi = 1$, $\phi = \pm \pi/4$. $(c_1(0), c_2(0), c_3(0)) = (0.299405 d_0^2, 1.282289, 1.581693/d_0^2)$. Positivity violation is in the interval $0 < \omega_0 t < 1.85$ for the Markovian case, with $\phi = -\pi/4$. No violation is on the right panel.

FIG. 11: $A(t)/C(t)$ for selected squeezed initial states. Left Panel: Markovian time evolutions, right panel: non-Markovian time evolutions. Parameters used: $\gamma = 0.755\omega_0$, $\Omega = 20\omega_0$, $k_B T = \hbar\omega_0$. Initial conditions are: $w = 1$, $\xi = 1$, $\phi = \pm \pi/4$. $(c_1(0), c_2(0), c_3(0)) = (0.299405 d_0^2, 1.282289, 1.581693/d_0^2)$. Positivity violation is in the interval $0 < \omega_0 t < 1.85$ for the Markovian case, with $\phi = -\pi/4$. No violation is on the right panel.

In all subsequent numerical cases we will compare the time evolution of (13) with its Markovian version which is obtained by replacing all time-dependent coefficient functions with their respective limits as $t \to \infty$ i.e.,

$$\omega_p(t) \to \omega_p^{(M)}, \quad \lambda(t) \to \lambda^{(M)},$$

$$D_{px}(t) \to D_{px}^{(M)}, \quad D_{pp}(t) \to D_{pp}^{(M)}.$$

The result of a typical, physically valid time evolution can be seen on Fig. 12. Here the parameters are chosen so that the density operator is physical for any time, i.e., $A$ and $C$ are positive and $A \geq C$. One can observe very similar behavior if one starts from a squeezed or a thermal state, except $A/C$ starts from a number bigger than 1 for a thermal state. In the figures we use dimensionless units, $A$ and $C$ are multiplied with $d_0^2$, where $d_0$ is the width of the quantum harmonic oscillator’s ground state.

On Fig. 12(b) both curves are already below the horizontal line at $\omega_0 t \approx 2$, however, the duration of the physical behavior is longer for the non-Markovian case at the beginning. The parameters in Fig. 4 are also from Region I., however the comparison with the previous case shows that for smaller temperature $k_B T / \hbar\omega_0$ and damping factor $\gamma / \omega_0$ we can see a few oscillations. The non-Markovian evolution is physical up to $\omega_0 t \approx 3.28$ and later it becomes unphysical because $A/C$ gets smaller than one. The Markovian evolution promptly becomes unphysical at $t = 0$ and remains for all times. We note that the parameters $\gamma/\omega_0$, $\Omega/\omega_0$, $k_B T / \hbar\omega_0$ are chosen to be the same as for the bottom subfigure of Figure (10.7) in the book of Breuer and Petruccione [9].

In Fig. 12 we choose a bigger $\gamma$ than in Fig. 12. All the other parameters and initial conditions are the same. Parameters still belong to Region I. Here something more drastically happens in both cases. First the ratio of $A/C$ goes below 1 (indicating positivity violation) and at a later time $A$ changes sign and even at a further time $A$ and $C$ diverge changing signs anew. The Markovian evolution is still unphysical for the whole time evolution, while non-Markovian evolution shows physical behavior until $A/C$ goes below one. If any of $A$ and $C$ become negative the corresponding Wigner function and $\text{Tr} \hat{\rho}$ do not exist.

In Fig. 12 we used the same parameters as in Fig. 12 ex-
cept that $\gamma$ has been decreased in such a way that the parameters are now in Region II. The non-Markovian evolution is physical for all time. The Markovian evolution gets unphysical but bounces back into the $A/C \geq 1$ region and remains physical at later times.

For Fig. 6 the initial condition is a coherent state with $w = 1$ in Eq. (24). It is interesting to note that if we vary $w$ for example to $w = 1/\sqrt{70}$ the initial behavior of the Markovian run is completely different (See Fig. 7): the positivity is promptly violated at $t = 0^+$ and at a later time the system returns back to a physically allowed state. The non-Markovian time evolution remains physical for all the time even for this initial condition.

An interesting regime is when $\gamma/\omega_0$ and $k_B T/\hbar \omega_0$ are small. Here we expect a few damped oscillations. In Figs. 8 and 10 our parameters are close to the critical line but still in Region II. The non-Markovian time evolution is already physical at any time. However, the Markovian run shows several time intervals where the curve of $A/C$ gets values smaller than one. The same can be monitored also in the quantity $A - C$ (See Fig. 4).

Let us discuss a few facts about squeezed initial states. Choosing $\gamma$, $\Omega$ and $k_B T$ as in Fig. 6 we have found strong dependence on the initial conditions of the positivity violation. On Fig. 10a large dark region corresponds to the complex $\zeta$’s for which positivity violations can happen for the Markovian runs. This is further supported on Fig. 11 where two individual time evolutions are shown with the same $|\zeta|$ but opposite sign of $\phi$. For $\phi = -\pi/4$ the quotient $A/C$ shows a strong positivity violation, namely in a small time interval it becomes negative. There is no violation for $\phi = \pi/4$. This particular situation is explained by inequality (22) at $t = 0$ (see Appendix C). In fact, $c_2(0)$ flips sign for the change $\phi \rightarrow -\phi$. In the non-Markovian case, we found no positivity violations at all for this family of initial conditions if the stationary solution is physical.

Next, we discuss what can happen if one starts from a thermal state (which is not a pure initial state for $T' > 0$). Let us consider Fig. 12. We plot the minimal values of $A/C$ for individual Markovian runs starting from thermal initial states. Different curves belong to different damping factors $\gamma$. At $T' = 0$ we start from a coherent state. All relevant parameters belong to Region II. The figure clearly supports the expectation that if one increases the width of the initial Gaussian one can avoid positivity violations. Curves with decreasing $\gamma$ are further away from the critical line. Choosing $\gamma$ to be bigger than 0.72 there is no positivity violation even for $T' = 0$.

These numerical investigations suggest that the non-Markovian evolution becomes unphysical, i.e., $A/C < 1$, only when the stationary state is unphysical. This has been investigated in detail in Sec. 11 and results in constraints on the choice of the parameters of the model. However, this is not true for the Markovian evolution, which may show for certain times of the evolution unphysical behavior. It is indeed true that the non-Markovian evolution is still more reliable than the Markovian one.

V. SUMMARY AND FINAL REMARKS

Summarizing, we have investigated a non-Markovian master equation of the Caldeira-Leggett model with a central quantum harmonic oscillator, where we have considered the weak coupling limit and second order expansion in the coupling strength. Our goal has been to identify unphysical behavior of this master equation by means of following time evolutions of initial density operators and examining whether the evolving density operators lose its positivity. This is a very delicate problem for general initial density operators, because the time evolution is usually followed in the phase space representation and the study of positivity properties of the Weyl transformed operators is still an open problem [22]. Therefore, we have focused only on Gaussian states, where the spectrum can be completely identified from the phase space solutions of the master equation. It is very important to note that the master equation can be fulfilled with Gaussians for which the main coefficients $A$ and $C$ are negative. Similarly, at finite time divergent solutions exist for more general initial state.

As a first step, in Section II we have transformed the whole problem into a phase space representation where the evolution is described by a linear differential equation system. Then, we have identified algebraic relations between the evolving coefficients of this phase space representation and the spectrum of the evolving operator, which may not always be a density operator. We have used numerical simulations to follow the evolving spectrum. We have compared the non-Markovian evolution to a Markovian one, which we have obtained by taking the coefficients in the $t \rightarrow \infty$ limit, see (16). We have showed for coherent, squeezed and thermal initial conditions that the positivity violations in the non-Markovian evolution occur when the stationary solution is also not a physical state anymore. Therefore, a positivity check on the stationary solution is necessary, which puts important constraints on the parameters of our theory. Therefore, we have carried out an analysis on the stationary solution in Section III, where we have also found arguments known to the community, see for example [29]. However, it also worth to mention that not all published material handles this positivity issue very carefully, see for example Fig. 10.7 in [30]. In contrast to the non-Markovian evolution, we have found in Section IV both for short (occurring at $t = 0^+$) and intermediate (occurring at finite $t > 0$) time evolutions positivity violations in the Markovian case. Our numerical investigations suggest that the rapid growth the diffusion coefficient $D_{pp}(t)$ compared to the growth of $D_{pp}(t)$ is the reason, why the non-Markovian master equation avoids positivity violations.

We have only considered Ohmic spectral density with
a Lorentz-Drude cutoff function, but one may ask what can happen for other type of spectral densities. At least we now from [14] that in cases of so-called supra- and subohmic spectral densities $D_{pp}(t)$ is growing faster than $D_{xx}(t)$ for short times and together with our results we conjecture that non-Markovian evolutions for these spectral densities also cannot exhibit positivity violations for Gaussian initial states and physical stationary states.

If one follows the time evolution 11 starting from an arbitrary (not necessarily Gaussian) physically allowed initial density operator, then one can state the following: for parameters belonging to Region I. of our figure 1 starting from any initial condition there must be positivity violation both for non-Markovian and Markovian runs. This can be explained as follows. For parameters in Region I the asymptotic state is non-physical. However, this state is unique and corresponds to the asymptotic Gaussian state of any initially physical state, e.g., see [19, 29].

This can be explained as follows. For parameters in Region I the asymptotic state is non-physical. However, this state is unique and corresponds to the asymptotic Gaussian state of any initially physical state, e.g., see [19, 29], discussed in Section III. If this state is non-physical, then positivity violation must occur at least asymptotically. For parameters in Regions II and III one might find positivity violations for appropriately chosen non-Gaussian initial density operators as in the case for Gaussian initial density operators.

Numerically, the non-Markovian evolution does not seem to show any signs of positivity violations for physical stationary states. Unfortunately this is not always the case for the Markovian evolution. Therefore, we may say the non-Markovian evolution is superior to the Markovian one, which is vaguely speaking due to the rapid growth of $D_{pp}(t)$ compared to that of $D_{xx}(t)$. We managed to prove in Appendix A that there is no short time positivity violation for arbitrary Gaussian initial state and model parameter set. This remains true even when the stationary solution is unphysical. This finding seems to be connected with the so-called initial “jolt” found by Refs. [14, 17].

Several questions concerning this subject remain still open problems, even though the application of these master equations is very frequent. Here, we have investigated thoroughly a Markovian and a non-Markovian master equation of the Caldeira-Leggett model for initial Gaussian density operators and identified the boundaries of the physically interpretable solutions of the time evolutions. Therefore, our results provide a key step in establishing the range of applicability of these master equations.

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**Appendix A: Expressions for the coefficients $D_{pp}(t)$ and $D_{xx}(t)$**

Expanding the coth function in eq. (11) as

$$\coth \pi x = \sum_{n=-\infty}^{\infty} \frac{x}{\pi(x^2 + n^2)} = \frac{1}{\pi x} + \frac{2\pi}{\pi} \sum_{n=1}^{\infty} \frac{1}{(x^2 + n^2)}$$

and integrating term by term one gets for $s > 0$

$$D_1(s) = \frac{4m\gamma k_B T \Omega^2}{\hbar} \left[ e^{-\Omega s} \frac{1}{\Omega} + 2 \sum_{n=1}^{\infty} \frac{\Omega e^{-\Omega s} - \nu_n e^{-\nu_n s}}{\Omega^2 - \nu_n^2} \right],$$

(A1)

where $\nu_n$’s are the bosonic Matsubara frequencies:

$$\nu_n = 2\pi n k_B T/\hbar.$$  (A2)

The first part in the square brackets of (A1) can be transformed using the identity

$$e^{-\Omega s} \left[ \frac{1}{\Omega} + 2 \sum_{n=1}^{\infty} \frac{\Omega}{\Omega^2 - \nu_n^2} \right] = \frac{\pi}{\nu_1} \cot \left( \frac{\Omega \pi}{\nu_1} \right) e^{-\Omega s},$$

where $\nu_1 = 2\pi k_B T/\hbar$ is the first bosonic Matsubara-frequency. The other part in the square brackets of (A1) can be expressed as

$$\sum_{n=1}^{\infty} \frac{\nu_n e^{-\nu_n s}}{\Omega^2 - \nu_n^2} = -\frac{e^{-\nu_1 s}}{2\nu_1} \times$$

$$\left( G \left( e^{-\nu_1 s}, 1, 1 - \frac{\Omega}{\nu_1} \right) + G \left( e^{-\nu_1 s}, 1, 1 + \frac{\Omega}{\nu_1} \right) \right),$$

(A3)

where $G(z, a, b)$ denotes the so-called Lerch transcendent or HurwitzLerchPhi[z, a, b] in Mathematica. 30.

A similar but different sum also appear later

$$\sum_{n=1}^{\infty} \frac{\nu_n e^{-\nu_n s}}{\omega_0^2 + \nu_n^2} =$$

$$\frac{e^{-i \omega_0 s} F \left( e^{-\nu_1 s}, \frac{\omega_0 - \omega_0 \nu_1}{\nu_1}, -1 \right) + e^{i \omega_0 s} F \left( e^{-\nu_1 s}, \frac{\omega_0 + \omega_0 \nu_1}{\nu_1}, -1 \right)}{2i \omega_0},$$

where $F(z, a, b)$ is the so-called incomplete beta function Beta[z, a, b] (we also use the terminology of Wolfram Mathematica).

We need also two more sums over the Matsubara-frequencies, however, those ones can be calculated via the useful formulas

$$\sum_{n=1}^{\infty} \frac{\nu_n^2 e^{-\nu_n s}}{\Omega^2 - \nu_n^2} = -\frac{\partial}{\partial s} \left( \sum_{n=1}^{\infty} \frac{\nu_n e^{-\nu_n s}}{\Omega^2 - \nu_n^2} \right),$$
\[
\sum_{n=1}^{\infty} \frac{\nu_n^2 e^{-\nu_n s}}{\omega_0^2 + \nu_n^2} = \frac{\partial}{\partial s} \left( \sum_{n=1}^{\infty} \frac{\nu_n e^{-\nu_n s}}{\omega_0^2 + \nu_n^2} \right).
\]

Inserting the series [A1] into eq. [2] the integral over \( s \) is trivial, but the final forms for the diffusion coefficients are lengthy:

\[
D_{pz}^{(2)}(t) = \left( k_B T \gamma \Omega^2 \right) \left\{ \begin{array}{l}
\omega_0 \cdot \left( \frac{1}{\Omega} + 2 \sum_{n=1}^{\infty} \frac{\Omega}{\Omega^2 - \nu_n^2} - 2 \sum_{n=1}^{\infty} \left[ \frac{\nu_n}{\Omega^2 - \nu_n^2} + \frac{\nu_n^2}{\omega_0^2 + \nu_n^2} \right] \right)
- \omega_0 \cos (\omega_0 t) \cdot \left( \frac{e^{-\nu_1 t}}{\Omega} + 2 \sum_{n=1}^{\infty} \frac{\Omega e^{-\nu_n t}}{\Omega^2 - \nu_n^2} - 2 \sum_{n=1}^{\infty} \left[ \frac{\nu_n e^{-\nu_n t}}{\Omega^2 - \nu_n^2} + \frac{\nu_n^2 e^{-\nu_n t}}{\omega_0^2 + \nu_n^2} \right] \right)
- \sin (\omega_0 t) \cdot \left( e^{-\nu_1 t} + 2 \sum_{n=1}^{\infty} \frac{\Omega e^{-\nu_n t}}{\Omega^2 - \nu_n^2} - 2 \sum_{n=1}^{\infty} \left[ \frac{\nu_n e^{-\nu_n t}}{\Omega^2 - \nu_n^2} + \frac{\nu_n^2 e^{-\nu_n t}}{\omega_0^2 + \nu_n^2} \right] \right)
\end{array} \right\}. \tag{A4}
\]

\[
D_{pp}^{(2)}(t) = \frac{2 k_B T m \gamma \Omega^2}{\hbar (\omega_0^2 + \Omega^2)} \left\{ \begin{array}{l}
\left( 1 + 2 \sum_{n=1}^{\infty} \frac{\Omega^2}{\Omega^2 - \nu_n^2} - 2 \sum_{n=1}^{\infty} \left[ \frac{\nu_n^2}{\Omega^2 - \nu_n^2} + \frac{\nu_n^2}{\omega_0^2 + \nu_n^2} \right] \right)
+ \omega_0 \sin (\omega_0 t) \cdot \left( \frac{e^{-\nu_1 t}}{\Omega^2} + 2 \sum_{n=1}^{\infty} \frac{\Omega e^{-\nu_n t}}{\Omega^2 - \nu_n^2} - 2 \sum_{n=1}^{\infty} \left[ \frac{\nu_n e^{-\nu_n t}}{\Omega^2 - \nu_n^2} + \frac{\nu_n^2 e^{-\nu_n t}}{\omega_0^2 + \nu_n^2} \right] \right)
- \cos (\omega_0 t) \cdot \left( e^{-\nu_1 t} + 2 \sum_{n=1}^{\infty} \frac{\Omega e^{-\nu_n t}}{\Omega^2 - \nu_n^2} - 2 \sum_{n=1}^{\infty} \left[ \frac{\nu_n e^{-\nu_n t}}{\Omega^2 - \nu_n^2} + \frac{\nu_n^2 e^{-\nu_n t}}{\omega_0^2 + \nu_n^2} \right] \right) \end{array} \right\}. \tag{A5}
\]

We used the above formulas in our numerical works. The Markovian values for \( \omega_p^2 \) and \( \lambda \) are

\[
\left( \omega_p^{(M)} \right)^2 = \omega_0^2 + 2 \gamma - \frac{2 \gamma \Omega^3}{\Omega^2 + \omega_0^2}, \quad \lambda^{(M)} = \frac{\gamma \Omega^2}{\Omega^2 + \omega_0^2}. \tag{A6}
\]

The asymptotic Markovian values for the diffusion coefficients can be read off from the first lines of eqs. [A4] and [A5]. Performing the Matsubara sums they can be given as

\[
D_{pp}^{(M)} = m \gamma \omega_0 \frac{\Omega^2}{\omega_0^2 + \Omega^2} \coth \left( \frac{\hbar \omega_0}{2 k_B T} \right), \tag{A7}
\]

\[
D_{pz}^{(M)} = \frac{\gamma \Omega^2}{\Omega^2 + \omega_0^2} \left[ \frac{k_B T}{\hbar \Omega} - \frac{1}{2 \pi} \left\{ 2 \Psi \left( \frac{\hbar \Omega}{2 \pi k_B T} \right) - \Psi \left( \frac{\hbar \omega_0}{2 \pi k_B T} \right) - \Psi \left( \frac{-i \hbar \omega_0}{2 \pi k_B T} \right) \right\} \right], \tag{A8}
\]

where \( \Psi(x) \) is the digamma function. The Markovian values [A4]-[A8] fully determine the asymptotic matrix \( M^{(M)} \) and the asymptotic vector \( v^{(M)} \).

Appendix B: Behavior of \( D_{pp}(t) \) and \( D_{pz}(t) \) for small time \( t \)

At very small temperature the hyperbolic cotangent factor in Eq. [4] can be well approximated by one:

\[
D_1(s)|_{t=0} = \frac{2 \gamma m \Omega^2}{\pi} \int_0^\infty \frac{\omega}{\Omega^2 + \omega^2} \cos (\omega s) d\omega = \frac{2 \gamma m \Omega^2}{\pi} \left( \sinh (\Omega s) \text{Shi} (\Omega s) - \cosh (\Omega s) \text{Chi} (\Omega s) \right), \tag{B1}
\]

where

\[
\text{Chi} (z) = \gamma_{EM} + \log (z) + \int_0^z \frac{(\cosh (t) - 1)}{t} dt, \tag{B2}
\]

is the function \( \text{CoshIntegral}[x] \) and

\[
\text{Shi} (z) = \int_0^z \frac{\sinh (t)}{t} dt \tag{B3}
\]

is the function \( \text{SinhIntegral}[x] \) in Mathematica. For short times \( s \) the dominant behavior in \( D_1(s) \) is the logarithm function. By Eqs. [2], [12] and [13] the coefficients \( D_{pp}(t) \) and \( D_{pz}(t) \) behave as

\[
D_{pp}(t) = \frac{2 \gamma m \Omega^2}{\pi} (1 - \gamma_{EM} - \log \Omega t) t + O(t^3), \tag{B4}
\]

\[
D_{pz}(t) = \frac{\gamma \Omega^2}{4 \pi} (1 - 2 \gamma_{EM} - 2 \log \Omega t) t^2 + O(t^4). \tag{B5}
\]

for small \( t \) and \( T = 0 \).
At finite temperature one can make the decomposition
\[ D_1(s) = D_1(s)\big|_{T=0} + \frac{2\gamma m \Omega^2}{\pi} \int_0^\infty \frac{\omega}{\Omega^2 + \omega^2} \left[ \coth\left( \frac{\hbar \omega}{2k_BT} \right) - 1 \right] d\omega, \]
where the first term on the right hand side is discussed above and behaves as \( \sim \log(\Omega s) \), while the second is finite even for \( s = 0 \). By Eq. (2) at finite temperature the short time dominant behavior of \( D_{px}(t) \) and \( D_{pp}(t) \) are still:
\[ D_{pp}(t) \simeq -\frac{2\gamma m \Omega^2}{\pi} t \log(\Omega t), \tag{B6} \]
\[ D_{px}(t) \simeq -\frac{\gamma \Omega^2}{2\pi} t^2 \log(\Omega t). \tag{B7} \]

**Appendix C: Analysis of small time behavior**

In this appendix, we show how a differential equation for the quotient \( A(t)/C(t) \) can be used to prove small time positivity violation/nonviolation. We begin with the non-Markovian case. Using the notations of Section III, we set \( Q(t) = A/C = 16c_1c_3 - 4c_2^2 \), and via the system (13) we arrive at
\[ \dot{Q} + 4\lambda(t)Q = 16\frac{D_{pp}(t)}{\hbar} c_1(t) - 16D_{px}(t)c_2(t). \]
The general solution of which is given by the variation of constants formula
\[ Q(t) = \frac{Q(0)}{\Lambda(t)} + 16\int_0^t \Lambda(s) \left[ \frac{D_{pp}(s)}{\hbar} c_1(s) - D_{px}(s)c_2(s) \right] ds, \]
where we have let \( \Lambda(t) = \exp\left( 4 \int_0^t \lambda \right) \) for convenience. Using this, the condition \( Q(t) \geq 1 \) is clearly equivalent to \( F(t) \geq 0 \), where
\[ F(t) = \int_0^t \Lambda(s) \left[ \frac{D_{pp}(s)}{\hbar} c_1(s) - D_{px}(s)c_2(s) \right] ds - \frac{\Lambda(t) - Q(0)}{16}. \]
Note that \( F(0) = \frac{Q(0) - 1}{\hbar} \geq 0 \). Therefore, a sufficient condition for \( F(t) \geq 0 \) for small \( t \) to hold is simply that \( F'(t) \geq 0 \), i.e.,
\[ \frac{D_{pp}(t)}{\hbar} c_1(t) - D_{px}(t)c_2(t) \geq \frac{\lambda(t)}{4}. \tag{C1} \]
We note in passing that for pure initial states, \( F(0) = 0 \), so \( F'(t) \geq 0 \) is actually equivalent to \( Q(t) \geq 1 \) for sufficiently small \( t \). In fact, \( c_1 \) is always positive, and on the left hand side the first term is bigger in modulus than the second term. In the first term the logarithm ensures that the inequality is true for small \( t \), and for any positive \( c_1 \). This shows that the non-Markovian time evolution never violates positivity at \( t = 0^+ \).

In the Markovian case, a completely analogous condition to (C1) can be derived with \( D_{pp}(t), D_{px}(t) \) and \( \lambda(t) \) replaced by their Markovian counterparts \( D_{pp}^{(M)}, D_{px}^{(M)} \) and \( \lambda^{(M)} \), viz.
\[ \frac{D_{pp}^{(M)}}{\hbar} c_1(t) - D_{px}^{(M)}c_2(t) \geq \frac{\lambda^{(M)}}{4}. \tag{C2} \]
Now consider squeezed initial states \( c_{\text{eq}}(0) \), for which clearly \( Q(0) = 1 \). Evaluating the preceding inequality at \( t = 0 \), we obtain a set of initial states \( c_{\text{eq}}(0) \) that is surely violating at \( t = 0^+ \). This constitutes a subset of the gray set in Figure 1C. Hence, we have shown that in the Markovian case, it is always possible to find a pure state that violates positivity at \( t = 0^+ \).

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