An entropy production based method for determining the position diffusion’s coefficient of a quantum Brownian motion

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Abstract. Quantum Brownian motion of a harmonic oscillator in the Markovian approximation is described by the respective Caldeira-Leggett master equation. This master equation can be brought into Lindblad form by adding a position diffusion term to it. The coefficient of this term is either customarily taken to be the lower bound dictated by the Dekker inequality or determined by more detailed derivations on the linearly damped quantum harmonic oscillator. In this paper, we explore the theoretical possibilities of determining the position diffusion term’s coefficient by analysing the entropy production of the master equation. It is shown that the obtained value has a linear dependence on the temperature, which is in marked contrast to previous studies.

Keywords: Quantum Brownian motion, entropy production, position diffusion
1. Introduction

Origins of the quantum Brownian motion lie in the question of how to reconcile damped equation of motion, e.g., Langevin equation for Brownian motion, with the process of quantization [1]. Over the past decades, the method of quantizing dissipative systems has received a lot of attention [2] and derivations with respect to the quantum Brownian motion’s master equation have been thoroughly scrutinized, see for example Refs. [3, 4, 5, 6] (the literature on the topic is considerable). A Markovian master equation is expected to be in Lindblad form [7, 8] in order to generate a completely positive trace preserving (CPTP) semigroup. However, the so-called Caldeira-Leggett master equation of Ref. [1], which is based on functional integral description of damped quantum systems [9], is found not to be in Lindblad form [10, 11]. Another approach to the quantization of a damped harmonic oscillator [12, 13, 14], where a weak coupling is considered between the harmonic oscillator and the reservoir, has resulted in a similar master equation to Ref. [1], but for this time in Lindblad form. The master equation in Ref. [1] with momentum diffusion and damping terms is now extended with two diffusion terms, where one of them describes position diffusion and the other term is a double commutator involving both position and momentum operator. The coefficients of the four diffusion terms must satisfy the Dekker inequality [14] to ensure that the master equation generates a CPTP semigroup. However, if one wanted to determine the value of one of the coefficients, provided that the other three coefficients are known, the Dekker inequality would result only in a lower bound. Therefore, in the context of bringing the Caldeira-Leggett master equation in Lindblad form, the coefficients of the added diffusion terms are not exactly determined which is a curious fact and deserves attention. A possible approach to this question is to reconsider the approximations within the microscopic model and derive a new master equation. Ref. [15] has extended the derivation of Ref. [1] to medium temperatures, thus obtaining all coefficients by neglecting quadratic and higher orders in inverse temperature. In a different approach, H. Dekker has obtained these coefficients by applying a quasi-canonical phase space quantization procedure to the linearly damped harmonic oscillator [16].

The purpose of this paper is to present a method, which is also capable of determining the value of the position diffusion’s coefficient. We consider the master equation of Ref. [1] with the two coefficients of momentum diffusion and damping obtained by assuming that the environment has Ohmic spectral density with a high frequency cutoff. The position and momentum mixed diffusion term can be neglected due to this consideration [15]. Therefore, we extend the Caldeira-Leggett master equation only with the position diffusion term and by thus assuring the mathematical consistency. In fact, we use most of the arguments of Ref. [15] and only neglect the result on the coefficient of the position diffusion term, which we consider to be unknown. We simply pose the question: Is it possible to determine this value only from the mathematical structure of the master equation? We will show with the help of the entropy production that the answer is affirmative.
The generator of the extended Caldeira-Leggett master equation is an unbounded operator and it is important to note this, because the proof of Lindblad [8] is based on uniformly continuous semigroups. Therefore, we use a Gaussian ansatz for the density matrix, which is in the domain of the generator, and furthermore, Gaussian states are mapped into Gaussian states during the whole time evolution. In this context, the resulting density matrix equations enable investigations on the relative entropy between any evolving state and the steady state of the master equation. Now, taking the negative time derivative of this special relative entropy functional at $t = 0$, we get the entropy production [17]. As the entropy production is a convex functional on the set of Gaussian states, one is able to show the so-called principle of minimal entropy production [18] (for an extended view see Ref. [19]). Here, we make use of this principle and investigate entropy production rates for unitarily transformed steady states. These rates are positive and depend on the unknown value of the position diffusion’s coefficient. We show that the characteristic frequencies of the master equation’s exponential decaying mechanism are independent of this coefficient. Therefore, by fixing the values of these characteristic frequencies the entropy production indicates how fast the system returns to its steady state. As a guiding principle we consider that this unknown coefficient obtains its physical value when the system is brought back to its steady state as fast as possible. In other words, the position of the global maximum of the entropy production on the allowed set of the position diffusion’s coefficients, defined by the Dekker inequality, determines the unknown value.

The paper is organised as follows. In Sec. 2 we discuss the solutions of the master equation and give the analytical formula of the relative entropy between an arbitrary Gaussian state and the Gaussian steady state. In Sec. 3 we derive the formula for the entropy production rate and explore its properties. We show that the coefficient of the position diffusion term can be obtained by solving a transcendental equation. We conduct numerical investigation in Sec. 4 in order to determine the coefficient’s value. Detailed derivations supporting the main text are collected in two appendices.

2. Master equation and relative entropy

Let us consider the extended Caldeira-Leggett master equation [11, 13] of a quantum harmonic oscillator with mass $m$ and frequency $\omega$ ($\hbar = 1$)

$$\frac{d\hat{\rho}}{dt} = -i \left[ \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2}, \hat{\rho} \right] - D_{pp}[\hat{x}, [\hat{x}, \hat{\rho}]] - i\gamma[\hat{x}, \{\hat{p}, \hat{\rho}\}] - D_{xx}[\hat{p}, [\hat{p}, \hat{\rho}]],$$  \hspace{1cm} (1)  

subject also to a position diffusion with coefficient $D_{xx}$ and where $[,]$ stands for commutators while $\{,\}$ for the anti-commutators. $\gamma$ is the relaxation constant and $D_{pp}$ stands for the momentum diffusion coefficient. The diffusion term $[\hat{p}, [\hat{p}, \hat{\rho}]]$ has already been derived, for instance, in the pioneering stage of the quantization of dissipative systems [13], or later as an extension of the Caldeira-Leggett model to medium temperatures [15]. It is worth to mention that these derivations contain an
extra term \([\hat{p}, [\hat{x}, \hat{\rho}]]\), which will be neglected in this paper. We shall return to this point later on, when we discuss the derivation of \(D_{pp}\) for an environment with Ohmic spectral density.

The master equation \([1]\) in position representation reads

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

In order to solve this equation of motion we make use of the following Gaussian ansatz

\[
\rho(x, y, t) = \exp\{-A(t) (x - y)^2 - i B(t) (x - y) (x + y) - C(t) (x + y)^2 - i D(t)(x - y) - E(t)(x + y) - N(t)\},
\]

where all the time-dependent parameters \(A(t), B(t), C(t), D(t), E(t)\) and \(N(t)\) are real. As these real parameters obey a non-linear system of ordinary differential equations, it is worth to transform the whole problem into a picture, where the solutions of the equation of motion can be found much easier. Thus, in the next step we consider a representation of the density matrix in \([1]\) with the help of a double Fourier transform

\[
\rho(k, \Delta, t) = \text{Tr}\{\hat{\rho}(t) \exp\{ik\hat{x} + i\Delta\hat{\rho}\}\}.
\]

The equation of motion for \(\rho(k, \Delta, t)\) reads

\[
\frac{\partial}{\partial t} \rho(k, \Delta, t) = \left( \frac{k}{m} \frac{\partial}{\partial k} - m \omega^2 \frac{\partial}{\partial \Delta} - D_{pp} \Delta^2 - 2 \gamma \Delta \frac{\partial}{\partial \Delta} - D_{xx} k^2 \right) \rho(k, \Delta, t),
\]

where we used the relations

\[
e^{i k \hat{x} + i \Delta \hat{\rho}} = - \left( i \frac{\partial}{\partial \Delta} + \frac{k}{2} \right) e^{i k \hat{x} + i \Delta \hat{\rho}}, \quad \hat{\rho} e^{i k \hat{x} + i \Delta \hat{\rho}} = - \left( i \frac{\partial}{\partial \Delta} - \frac{k}{2} \right) e^{i k \hat{x} + i \Delta \hat{\rho}}.
\]

The above equation of motion contains only first order derivatives and therefore is easier to construct its solutions. Now, the Gaussian ansatz has the following form

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

where the parameters \(c_1, c_2, c_3, c_4, c_5\) and \(c_6\) are real and they obey the following linear differential equations

\[
\dot{c}_1 = D_{xx} + \frac{c_2}{m}, \quad \dot{c}_2 = \frac{2c_3}{m} - 2m \omega^2 c_1 - 2 \gamma c_2, \quad \dot{c}_3 = D_{pp} - m \omega^2 c_2 - 4 \gamma c_3, \quad \dot{c}_4 = \frac{c_5}{m}, \quad \dot{c}_5 = -m \omega^2 c_1 - 2 \gamma c_5, \quad \dot{c}_6 = 0.
\]

These differential equations can be solved by standard methods (see Appendix A), but the general solutions are not required for our study. We only present here the steady state solutions (see also \([A,1]\)):

\[
\begin{align*}
\hat{c}^{\text{st}}_1 &= \frac{m^2 (4 \gamma^2 + \omega^2) D_{xx} + D_{pp}}{4 \gamma m^2 \omega^2}, & \hat{c}^{\text{st}}_2 &= -m D_{xx}, \\
\hat{c}^{\text{st}}_3 &= \frac{m^2 \omega^2 D_{xx} + D_{pp}}{4 \gamma}, & \hat{c}^{\text{st}}_4 &= \hat{c}^{\text{st}}_5 = 0, & \hat{c}^{\text{st}}_6 &= c_6(0).
\end{align*}
\]
The eigenvalues of the density matrix \( \hat{\rho} \) are obtained in the position representation, which is discussed in Appendix B. Applying the transformation (A.2) between the coefficients of \( \rho(x, y) \) and \( \rho(k, \Delta) \) these eigenvalues yield

\[
\lambda_n = \frac{2}{2\sqrt{4c_1c_3 - c_2^2} + 1} \left( \frac{2\sqrt{4c_1c_3 - c_2^2} - 1}{2\sqrt{4c_1c_3 - c_2^2} + 1} \right)^n, \quad n \in \mathbb{N}_0.
\]

Recall that thermal states of a quantum harmonic oscillator in the Fock representation have the form

\[
\hat{\rho}_{\text{th}} = \frac{1}{\bar{n} + 1} \sum_{n=0}^{\infty} \left( \frac{n}{\bar{n} + 1} \right)^n \langle n \rangle \langle n \rangle,
\]

where \( \bar{n} \) is the mean photon number. Thus, our state \( \hat{\rho} \) with

\[
\bar{n} = \frac{2\sqrt{4c_1c_3 - c_2^2} - 1}{2}
\]

is nothing else than a unitarily transformed thermal state. Furthermore, \( \rho(k, \Delta) \) is also the symmetric characteristic function \( \chi(\lambda, \lambda^*) \) of \( \hat{\rho} \)

\[
\rho(k, \Delta) = \text{Tr} \left\{ \hat{\rho} \exp \{ik\hat{x} + i\Delta\hat{p} \} \right\} = \chi(\lambda, \lambda^*),
\]

\[
k = -\frac{i}{\sqrt{2}}(\lambda - \lambda^*), \quad \Delta = -\frac{1}{\sqrt{2}}(\lambda + \lambda^*),
\]

where \( \hat{a} (\hat{a}^\dagger) \) is the annihilation (creation) operator. A simple transformation yields

\[
\chi(\lambda, \lambda^*) = \exp \left\{ -(c_1 + c_3)|\lambda|^2 - \frac{-c_1 + c_3 + ic_2}{2}\lambda^2 - \frac{-c_1 + c_3 - ic_2}{2}(\lambda^*)^2 \right. \\
+ \left. \frac{-c_4 + ic_5}{\sqrt{2}} \lambda - \frac{-c_4 - ic_5}{\sqrt{2}} \lambda^* - c_6 \right\},
\]

which shows that \( \hat{\rho} \) with the Gaussian ansatz in the \( (k, \Delta) \) representation is a displaced squeezed thermal state (DSTS) [20]. Nevertheless, due to the evolution in (1) and by choosing an initial Gaussian density matrix, \( \hat{\rho} \) remains a DSTS at all times.

Our next aim is to calculate the relative entropy between \( \hat{\rho}(t) \) and the stationary solution \( \hat{\rho}_{\text{st}} \) for any \( t \geq 0 \). The relative entropy between the two arbitrary states \( \hat{\rho} \) and \( \hat{\sigma} \) is defined as [21]

\[
S(\hat{\rho} | \hat{\sigma}) = \begin{cases} 
\text{Tr} \{ \hat{\rho}(\log \hat{\rho} - \log \hat{\sigma}) \}, & \text{supp}(\rho) \subseteq \text{supp}(\sigma) \\
+\infty, & \text{otherwise}.
\end{cases}
\]

The support of a state \( \hat{\rho} \) is the complement of its kernel, i.e., a subspace of the Hilbert space where \( \hat{\rho} \) does not have eigenvalues equal to zero.

According to Ref. [20] the relative entropy between two DSTS state has an analytical form and can be expressed as a function of the two characteristic functions’
parameters. Employing this formula we obtain the following relation:

\[
S(\hat{\rho}(t) | \hat{\rho}^{st}) = -(\bar{n}(t) + 1) \log(\bar{n}(t) + 1) + \bar{n}(t) \log \bar{n}(t) + \frac{\log [(\bar{n}^{st} + 1)\bar{n}^{st}]}{2} \\
+ \frac{2 \log (\bar{n}^{st} + 1)}{2\bar{n}^{st} + 1} \left[ 2(c_1(t)c_3^{st} + c_3(t)c_1^{st}) - c_2(t)c_2^{st} + c_1^{st}c_5^2(t) + c_3^{st}c_4^2(t) \\
- c_4(t)c_5(t)c_2^{st} \right],
\]

where we have used the relation (8) to define

\[
\bar{n}(t) = \frac{2\sqrt{4c_1(t)c_2(t) - c_3^2(t)} - 1}{2}, \quad \bar{n}^{st} = \frac{2\sqrt{4c_1^{st}c_3^{st} - (c_2^{st})^2} - 1}{2}.
\]

We remark that (12), cast in an analytical form, is better suited for our subsequent investigation.

3. Entropy production and position diffusion

In this section we present and investigate an entropy production based method, which is capable of identifying the coefficient of the position diffusion term in (1). The other parameters of the model can be derived from a microscopic model consisting an environment with Ohmic spectral density and a high frequency cutoff (see e.g. Ref. [1]). This considerations yield the following relations

\[
\gamma = \frac{\eta}{2m}, \quad D_{pp} = \eta k_B T,
\]

where \(\eta\) is the viscosity coefficient in a Quantum Brownian motion and \(T\) is the temperature of the environment. We immediately have that \(D_{pp} = 2m\gamma k_B T\). We have mentioned in Sec. [2] that the terms \([\hat{p}, [\hat{x}, \hat{\rho}]]\) is going to be neglected in Eq. (1). Ref. [22] has already demonstrated that the coefficients of these terms are negligible under assumptions of the Born-Markov approximation and slow motion of the central system in comparison to the bath correlation time. These coefficients can also be determined from an extension of the Caldeira-Leggett model to medium temperatures (see Ref. [15]), however even in that case are found to be very small.

The Caldeira-Leggett model is not in the Lindblad form [7, 8], which presents a mathematical difficulty since the Lindblad form would ensure that the master equation generates a quantum dynamical or CPTP semigroup. This semigroup maps quantum states to quantum states and furthermore the map is also completely positive. We shall not discuss here the properties and applications of quantum dynamical semigroups, instead we refer to the book [22]. So the Caldeira-Leggett model can be put in Lindblad form by adding \(-D_{xx}[\hat{p}, [\hat{p}, \hat{\rho}]]\) and we already know that \(D_{xx}\) can be defined through the Dekker inequality [14]

\[
D_{pp}D_{xx} \geq \frac{\gamma^2}{4},
\]

(15)
obtained by imposing the condition that Eq. (1) preserves the uncertainty principle. Combining this with (14) we find that the minimal value for $D_{xx}$ is

$$D^\text{min}_{xx} = \frac{\gamma}{8mk_B T}. \quad (16)$$

Inequality (15) is also a fundamental constraint, which must be satisfied in order to write the master equation (1) in Lindblad form. In Ref. [15], a value of $D_{xx} = 4D^\text{min}_{xx}/3$ was obtained for large and medium temperatures by using Markovian approximation in a path integral formalism. This method neglected the quadratic and higher powers of the inverse temperature $1/T$. 

In order to find possible values for $D_{xx}$ satisfying inequality (15), we consider a different method. It has been shown by Refs. [23, 24] that for a CPTP map $\Phi$,

$$S(\hat{\rho} \mid \hat{\sigma}) \geq S(\Phi(\hat{\rho}) \mid \Phi(\hat{\sigma})), \quad (17)$$

i.e. the monotonicity of the quantum relative entropy holds. Now, rewriting Eq. (1) as

$$\frac{d\hat{\rho}}{dt} = \mathcal{L}\hat{\rho}, \quad \text{with} \quad \Phi = e^{\mathcal{L}t},$$

we have that the time-dependent function

$$S(e^{\mathcal{L}t}\hat{\rho}(0) \mid e^{\mathcal{L}t}\hat{\rho}^\text{st}) = S(e^{\mathcal{L}t}\hat{\rho}(0) \mid \hat{\rho}^\text{st}) \quad (18)$$

is monotonically decreasing in time and continuous from the right (see Ref. [17]). This time dependence is depicted in Figs. 1a and 1b for two types of initial conditions, a coherent state and a thermal state. For the underdamped $\gamma/\omega < 1$ and overdamped $\gamma/\omega > 1$ cases the relative entropy approaches 0 slower than in the critically damped case $\gamma/\omega = 1$. This is due to the characteristic frequencies present in the evolution $e^{\mathcal{L}t}\hat{\rho}$ (see Appendix A): $-2\gamma/\omega \pm 2\sqrt{(\gamma/\omega)^2 - 1}$, $-\gamma/\omega \pm \sqrt{(\gamma/\omega)^2 - 1}$, and $-2\gamma$. When we have an underdamped case then the frequencies have small real parts, thus the relative entropy approaches zero slowly. In the overdamped case, the frequencies $-\gamma/\omega + \sqrt{(\gamma/\omega)^2 - 1}$ and $-2\gamma/\omega + 2\sqrt{(\gamma/\omega)^2 - 1}$ are again small, which results in a slow exponential decay.

The entropy production is defined as the negative time-derivative of (18) at $t = 0$,

$$\sigma = -\frac{d}{dt}S(e^{\mathcal{L}t}\hat{\rho}(0) \mid \hat{\rho}^\text{st})\bigg|_{t=0}, \quad (19)$$

which is a nonnegative convex functional. We argue here that $D_{xx}$ can be determined from $\sigma$. It is clear from the characteristic frequencies that $D_{xx}$ does not influence the decaying mechanism of the time evolution and therefore for a fixed value of $\gamma/\omega$ the entropy production $\sigma$ indicates how fast the system is approaching its steady state. Therefore, we consider that a time evolution which wants to turn back the system to its steady state as fast as possible, i.e., for which the entropy production $\sigma$ has the largest value, is the one which determines the value of $D_{xx}$. This search for the maximum entropy production should not be confused with the principle of minimal entropy production, which is satisfied in this paper (see Lemma 5 in Ref. [17]).
In order to investigate the entropy production rate we express $\sigma$ as the function of $\gamma$, $D_{pp}$, and $D_{xx}$. First, we substitute the relations

\[ \dot{c}_1(0) = D_{xx} + \frac{c_2(0)}{m}, \quad \dot{c}_2(0) = \frac{2c_3(0)}{m} - 2m\omega^2c_1(0) - 2\gamma c_2(0), \]
\[ \dot{c}_3(0) = D_{pp} - m\omega^2c_2(0) - 4\gamma c_3(0), \quad \dot{c}_4(0) = \frac{c_5(0)}{m}, \]
\[ \dot{c}_5(0) = -m\omega^2c_1(0) - 2\gamma c_5(0) \]

into (19), where we make use of Eqs. (5) and (12). We finally find that

\[ \frac{\sigma}{\omega} = \frac{4D'_{pp}c'_1(0) + 4D'_{xx}c'_3(0) - \gamma'(2\bar{n}(0) + 1)^2}{2\bar{n}(0) + 1} \log\left(\frac{\bar{n}(0) + 1}{\bar{n}(0)}\right) \]
\[ - \log\left(\frac{\bar{n}_{st} + 1}{\bar{n}_{st}}\right) \left[ 4D'^2_{pp} + \frac{D'^2_{xx}}{4} + 2D'_{pp}D'_{xx}(2\gamma'^2 + 1) - 8\gamma'D'_{pp}(2c'_3(0) + c'_5(0)) \right. \]
\[ - \gamma'D'_{xx} \left( c'_1(0) + 4\gamma'c'_2(0) + 16\gamma'^2c'_3(0) + \frac{(c'_4(0) + 4\gamma'c'_5(0))^2}{2}\right) \left( \frac{1}{\gamma'(2n_{st} + 1)} \right) \]

Here we have introduced the following dimensionless parameters

\[ D'_{pp} = \frac{D_{pp}x_0^2}{\omega}, \quad \gamma' = \frac{\gamma}{\omega}, \quad D'_{xx} = \frac{D_{xx}x_0^2}{\omega}, \]
\[ c'_1 = \frac{c_1}{x_0^2}, \quad c'_2 = c_2, \quad c'_3 = c_3x_0^2, \quad c'_4 = \frac{c_4}{x_0}, \quad c'_5 = c_5x_0, \]

where $x_0 = 1/\sqrt{2m\omega}$ is the width of the quantum harmonic oscillator’s ground state wave function. It is worth mentioning that $n_{st}$ and $n(t)$ ($t \geq 0$) are invariant under the above transformations.
First, we investigate those cases where the entropy production approaches infinity. These cases are inconclusive and one cannot infer any information about $D'_{xx}$. We would like to keep all our parameters finite and therefore it can be seen that there are two cases: whenever either $n(0)$ or $n^{st}$ approaches zero the entropy production rate approaches infinity. These limit cases can be regarded as the system is either initially or stationarily in a pure state. The latter one is equivalent to

$$4c_1^{st}c_3^{st} - (c_2^{st})^2 = \frac{1}{4}$$

(22)

and substituting (5) into it we obtain a quadratic equation for $D'_{xx}$, which has two real roots:

$$D_{xx}^{\pm} = -4D'_{pp}(1 + 2\gamma'^2) \pm 2\gamma'\sqrt{1 + 16D'_{pp}(1 + \gamma'^2)}.$$  

(23)

Now, comparing the bigger root $D_{xx}^{+}$ with the minimum of $D'_{xx}$ allowed by (15) we have

$$D_{xx}^{\min} = \frac{\gamma'^2}{4D'_{pp}} \geq D_{xx}^{+},$$

which is equivalent to

$$(\gamma'^2 - 16D'^2_{pp})^2 + 64\gamma'^4D'^2_{pp} \geq 0.$$  

This expression is always true and the equality is obtained only for $\gamma' = D'_{pp} = 0$, which is an uninteresting case for our study. Hence, from now on we shall investigate the entropy production only on the interval $[D_{xx}^{\min}, \infty)$.

We make also the observation that

$$\lim_{D_{xx} \to \infty} \frac{\sigma}{\omega D'_{xx}} = \frac{4c_3'(0)}{2\bar{n}(0) + 1} \log \left( \frac{\bar{n}(0) + 1}{\bar{n}(0)} \right) = a,$$

(24)

and

$$\lim_{D_{xx} \to \infty} \frac{\sigma}{\omega} - aD'_{xx} = \frac{4D'_{pp}c_3'(0) - \gamma'(2\bar{n}(0) + 1)^2}{2\bar{n}(0) + 1} \log \left( \frac{\bar{n}(0) + 1}{\bar{n}(0)} \right) - 2\gamma' = b,$$

(25)

which means that $\sigma/\omega$ as a function of $D'_{xx}$ is asymptotic to the line $aD'_{xx} + b$.

Now, our main goal is to find a value for $D'_{xx}$ by searching for the global maximum of the entropy production $\sigma$. At this stage it is clear that $\sigma$ has a global maximum when $D'_{xx} \to \infty$ and in order to circumvent this issue we consider that

$$c_1'(0) = c_1^{st}, \quad c_2'(0) = c_2^{st}, \quad c_3'(0) = c_3^{st},$$

(26)

which directly yields that $n(0) = n^{st}$ and

$$\lim_{D_{xx} \to \infty} \frac{4}{2\bar{n}(0) + 1} \log \left( \frac{\bar{n}(0) + 1}{\bar{n}(0)} \right) = 0.$$  

(27)

The above assumptions ensure that the global maximum of $\sigma$ at $D'_{xx} \to \infty$ disappears, as is shown in Figs. 2a and 2b. In particular, Fig. 2b shows that the
Figure 2: Entropy production $\sigma/\omega$ as a function of $D'_{xx}$ according to Eqs. (20) and (28). We set $c'_4(0) = c'_5(0) = 2$ and $D'_{pp}/\gamma' = 2$ for all three type of curves: $\gamma' = 0.8$ (solid), $\gamma' = 1$ (dashed), and $\gamma' = 1.2$ (dotted). The figures are displayed for two different initial conditions: an initial state with $n_{1}(0) \neq n_{\text{st}}$, and a displaced steady state, i.e., $c'_1(0) = c'_{\text{st}}$, $c'_2(0) = c'_{\text{st}}$, and $c'_3(0) = c'_{\text{st}}$. In both figures the curves start at the minimum allowed value $\gamma'^2/(4D'_{pp})$ in accordance with (15).

The condition (26) also means that our initial condition is a displaced steady state. Nonetheless, it must be admitted that this is not the most general way to get rid of the global maximum at $D'_{xx} \to \infty$, because $n(0) = n_{\text{st}}$ would be enough, which does not imply (26). However, this leads to difficulties in the identification of all possible $c'_1(0), c'_2(0),$ and $c'_3(0)$. We neglect this general approach, for now. Finally, Eq. (20) under the conditions (26) is changed to

$$\sigma(D'_{xx})/\omega = \frac{16D'_{pp}c'^2_5(0) + D'_{xx}(c'_4(0) + 4\gamma'c'_5(0))^2}{4n_{\text{st}} + 2}\log\left(\frac{n_{\text{st}} + 1}{n_{\text{st}}}\right).$$

(28)

It is obvious from (28) that the entropy production becomes bigger as we increase $c'_4(0)$ and $c'_5(0)$, i.e., we displace further the steady state. We remind the reader that we are only interested in $D'_{xx} \in [D'_{\text{min}}, \infty)$, therefore we introduce a renormalized entropy production

$$\sigma_R(D'_{xx}, c'_4(0), c'_5(0)) = \frac{\sigma(D'_{xx})}{\sigma(D'_{xx})_{\text{min}}},$$

(29)

which has the following property

$$\frac{\sigma_R(D'_{xx}, c'_4(0), c'_5(0))}{\sigma_R(D'_{xx}, c'_4(0), c'_5(0) = 0)} = 1 + \frac{16D'_{pp}c'^2_5(0)(\gamma'^2 - 4D'_{pp}D'_{xx})}{D'_{xx}(\gamma'^2(c'_4(0) + 4\gamma'c'_5(0))^2 + 64D'^2_{pp}c'^2_5(0))} \leq 1,$$

because $\gamma'^2 - 4D'_{pp}D'_{xx} \leq 0$ due to (15). Figures in 3 show indeed that smaller $c'_5(0)$-s yield larger $\sigma_R$-s. Through the definition of this new quantity it is guaranteed that the
Figure 3: Renormalized entropy production $\sigma_R$ as a function of $D'_{xx}$ according to Eq. (29). We set $\gamma' = 1$ and $D'_{pp} = 2$ for all curves. Left panel: $c_4'(0) = 0.5$ and $c_5'(0) = 1$ (solid); $c_4'(0) = 0.5$ and $c_5'(0) = 1$ (dashed); $c_4'(0) = 1$ and $c_5'(0) = 0.5$ (dotted). Right panel: $c_4'(0) = 1$ and $c_5'(0) = 0.5$ (solid); $c_4'(0) = 1$ and $c_5'(0) = 0.4$ (dashed); $c_4'(0) = 1$ and $c_5'(0) = 0.3$ (dotted). In both figures the curves start at the minimum allowed value $\gamma'^2/(4D'_{pp})$ in accordance with (15).

In the subsequent discussion we investigate the global maximum of Eq. (30). First, we take into consideration the result of [1], namely that $D'_{pp}$ can be expressed as a function of $\gamma'$ and the temperature $T$ of the environment, and thus Eq. (14) in the primed coefficients reads

$$D'_{pp} = \gamma' \frac{k_B T}{\omega},$$

where $k_B T/\omega \geq 1$ in order that the central system is slow compared to the bath correlation times [15]. This argument must hold in order to be consistent with the neglection of $[\hat{p}, [\hat{x}, \hat{p}]]$ term in Eq. (1). On the other hand, the applicability of the Born-Markov approximations, which lead to (1), imposes that $k_B T/\omega \gg \gamma'$ [22].
Table 1: Our conventional symbols for the position diffusion’s coefficient used in this section.

| Symbol | Description |
|--------|-------------|
| $D_{xx}$ | General coefficient |
| $D_{xx}^{\text{min}}$ | Minimum coefficient value according to Dekker’s inequality in Eq. (15) |
| $D'_{xx}$ | General dimensionless coefficient |
| $D'_{xx}^{\text{min}}$ | Minimum dimensionless coefficient value |
| $D'_{xx}^\pm$ | The roots of the quadratic equation in (22) |
| $D'_{xx}$ | The dimensionless coefficient value that needs to be determined from the entropy production |

Figure 4: Location $D'_{xx}(\gamma', T')$ of the only global maximum of $f(\gamma', T', D'_{xx})$ in Eq. (32). Left panel: estimated analytical solution of the transcendental equation (33). Right panel: numerical solutions of the transcendental equation (33) on $10^6$ grid points.

4. Numerical results

Let us rewrite the maximum of renormalized entropy production in (30) as

$$f(\gamma', T', D'_{xx}) = \frac{D'_{xx}}{(2\bar{n}_{\text{st}} + 1)} \text{arcoth} \left(2\bar{n}_{\text{st}} + 1\right),$$

(32)

where $T' = k_B T / \omega$ and we have neglected the $D'_{xx}$ independent $C$. We search for the only global maximum of $f(\gamma', T', D'_{xx})$ and its position $D'_{xx}(\gamma', T')$ in the interval $[D'_{xx}^{\text{min}}, \infty)$. To achieve this goal, we need to solve the following transcendental equation within the required range:

$$\left. \frac{\partial f(\gamma', T', D'_{xx})}{\partial D'_{xx}} \right|_{D'_{xx}=D'_{xx}(\gamma', T')} = 0.$$  

(33)
Figure 5: $|D_{xx}^n(\gamma', T') - D_{xx}^{num}(\gamma', T')| / |D_{xx}(\gamma', T')|$ relative error between the numerical and the estimated solutions of Eq. (33) on $10^6$ grid points. The error is slightly increased on concentric curves due to the numerical errors, which are already present on the right panel of Fig. 4.

Numerical solutions of this equation suggest that the position of the global maximum can be estimated by

$$D_{xx}^*(\gamma', T') = D_{xx}^{min} + \gamma' \sqrt{(4T')^2 - 2} = \gamma' \left( \frac{1}{4T'} + \sqrt{(4T')^2 - 2} \right), \quad (34)$$

which is in accordance with the Dekker inequality (see Eq. (15))

$$D_{xx}^*(\gamma', T')D_{pp} = \gamma'^2 \left( \frac{1}{4} + T' \sqrt{(4T')^2 - 2} \right) \geq \frac{\gamma'^2}{4}, \quad (35)$$

if $T' \geq 1/(2\sqrt{2})$. This conditions hold true, because $T' \geq 1$ in order that the master equation in Eq. (1) is justified. Furthermore, for large temperatures $T' \gg 1$ the
approximative solution reads

\[ D_{xx}'(\gamma', T') \approx 4\gamma'T'. \] (36)

An important ingredient in the above method is to estimate the error between the approximating solution and the numerical data. For this purpose, we employ the relative error:

\[ \frac{|D_{xx}'(\gamma_n', T_m') - D_{xx}'_{\text{num}}(\gamma_n', T_m')|}{|D_{xx}'(\gamma_n', T_m')|}, \] (37)

where \( \gamma_n' = n \) and \( T_m' = m \) with \( 1 \leq n, m \leq 1000 \) (see also Fig. 4). Fig. 5 demonstrates that the relative error determined for each point separately is approximately at most \( 10^{-2} \). The \( L_2 \) relative error norm for the whole grid with \( 10^6 \) points yields

\[ \sqrt{\sum_{n,m=1}^{1000} |D_{xx}'(\gamma_n', T_m') - D_{xx}'_{\text{num}}(\gamma_n', T_m')|^2} = 9.8 \times 10^{-3}. \] (38)

This figure also shows that in the region where \( T' \) is larger than \( \gamma' \) the approximating solution is more accurate. If we recall now the condition of the Born-Markov approximation \( T' \gg \gamma' \) and the result in (34), thence it follows that the dimensionless coefficient of the position diffusion takes the value \( 4\gamma'T' \). Now, employing the transformation in (21) we obtain

\[ D_{xx}' = 2\gamma \frac{k_BT}{m\omega^2}. \] (39)

This is our main result and together with \( D_{pp} = 2m\gamma k_BT \), they fulfil the Dekker inequality (15), because \( k_BT/\omega \geq 1 \), i.e., the central system is slow compared to the bath correlation times.

| \( D_{xx}'(\gamma', T') \) | The dimensionless coefficient that needs to be determined from Eq. (33) |
| \( D_{xx}'_{\text{num}}(\gamma_n', T_m') \) | An estimated analytic solution of Eq. (33) |
| \( D_{xx}'_{\text{num}}(\gamma_n', T_m') \) | Numerical solution of Eq. (33) with dimensionless parameters at the grid points \( \gamma_n' \) and \( T_m' \) |
| \( D_{xx} \) | The coefficient value that maximizes the entropy production |

Table 2: Our conventional symbols for the position diffusion’s coefficient used in this section.

5. Conclusions

We have introduced a method to determine the coefficient of the position diffusion term in an extended Caldeira-Leggett master equation. This term is required to obtain a mathematically consistent master-equation in Lindblad form. The value of this coefficient is lower bounded via the Dekker inequality (15), and obtained by applying a quasi-canonical phase space quantization procedure (16) or extending the Caldeira-Leggett model to medium temperatures (15). The latter method heavily depends on the
expansion of environment’s correlation function with respect to the inverse temperature, where quadratic and higher order terms are neglected. In this paper, we have studied this coefficient by using the entropy production of the master equation. For simplicity, we have considered an environment with Ohmic spectral density and the central particle to be in a harmonic potential. Therefore, the parameters of the model are the temperature \( T \) of the environment, relaxation rate \( \gamma \), mass \( m \), and the frequency of the oscillator \( \omega \). Then, we have considered that the position diffusion’s coefficient is unknown in the extended Caldeira-Leggett master equation and investigated the entropy production as a function of the this parameter.

In fact, we have used Gaussian density matrices for the initial conditions, because during the time evolution the Gaussian form is preserved. Making use of the analytical form of the relative entropy between two Gaussian states, we have been able to determine analytically the entropy production. In general, the function of the entropy production is difficult to analyse, therefore without the need for completeness, we have restricted our calculation to states which are only unitarily displaced Gaussian steady states. This resulted in a simplification of our problem, because the entropy production now depends only on the temperature \( T \), relaxation rate \( \gamma \), mass \( m \), frequency of the oscillator \( \omega \), and the unknown value of the position diffusion’s coefficient \( D_{xx} \). Then, we have stated that the value of \( D_{xx} \) is defined by the position of the global maximum of the entropy production. The entropy production as a function of \( D_{xx} \) at its maximum is equivalent to the fastest exponential decay of the system towards the steady state. In order to determine the position of the maximum entropy production as a function of \( D_{xx} \), we have solved numerically a transcendental equation. We have estimated the solutions of this transcendental equation and studied the relative error between the approximating analytical solution and the numerical data. We have found that \( D_{xx} = 2\gamma k_B T/(m\omega^2) \), which is in contrast with the values obtained by taking the allowed minimum value of the Dekker inequality or considering the derivation of Ref. [15], because here at high temperatures the position diffusion stays a dominant source of decoherence. Furthermore, the obtained value is in agreement with the Dekker inequality.

In summary, we have determined the coefficient of the position diffusion in an extended Caldeira-Leggett master equation by studying the entropy production. In addition, we have applied the following guiding principle: the value of the unknown parameter is defined as the one for which the system returns to its steady state as fast as possible. This principle may be tested by verifying the findings in optomechanical systems [25] or superconducting tunnel junctions [26]. Moreover, the presented method is still open for further theoretical investigations.

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Appendix A. Solutions of Eq. (4)

A general solution of (4) can be obtained, for example, with the help of the Laplace transformation

\[ c_i(z) = \int_0^\infty c_i(t)e^{-zt} \, dt, \quad i \in \{1, 2, 3, 4, 5, 6\} \]

which transforms Eq. (4) with the initial condition \( c_i(0) \) into an algebraic equation for \( c_i(z) \). The first three coefficients \( c_1(z), c_2(z), \) and \( c_3(z) \) are coupled only to each other while \( c_4(z) \) and \( c_5(z) \) form also their own system of linear equations. \( c_6(z) \) is simply \( c_6(0)/z \). Inverting these solution with the help of the inverse relation

\[ c_i(t) = \frac{1}{2\pi i} \int_C e^{zt}c_i(z) \, dz, \quad i \in \{1, 2, 3, 4, 5, 6\} \]

we obtain the solution for \( c_i(t) \) and the path of integration \( C \) has to be chosen in such a way that all poles of \( c_i(z) \) are included. The poles of \( c_1(z), c_2(z), \) and \( c_3(z) \) are: \( z = 0, z = -2\gamma, z = -2\gamma - 2\sqrt{\gamma^2 - \omega^2}, \) and \( z = -2\gamma + 2\sqrt{\gamma^2 - \omega^2} \). The poles of \( c_4(z), \) and \( c_5(z) \) are: \( z = -\gamma - \sqrt{\gamma^2 - \omega^2} \) and \( z = -\gamma + \sqrt{\gamma^2 - \omega^2} \). In the following we employ the transformation \( \Omega = \sqrt{\gamma^2 - 1} \) and dimensionless time \( \tau = \omega t \), which allow us to present the solutions in a more concise form. The solutions to the first three transformed coefficients are:

\[
\begin{align*}
  c_1'(\tau) &= \frac{4D_{pp}' + D_{xx}'(4\gamma'^2 + 1)}{4\gamma'} \\
  &\quad + e^{-2\gamma'\tau} \frac{4D_{pp}' + D_{xx}' - 2\gamma'(c_1'(0) + 2\gamma'c_2'(0) + 4c_3'(0))}{4\gamma'O^2} \\
  &\quad + \sum_{y=\pm \Omega} e^{-2(\gamma' + y)\tau} \left[ \frac{-4D_{pp}' + D_{xx}'(1 - 2\gamma'^2 + 2\gamma'y) + 2c_1'(0)(\gamma' - y)}{8(\gamma' + y)y^2} 
  + \frac{2c_1'(0)(\gamma' + y) + c_2'(0)}{2(\gamma' + y)y^2} \right], \\
  c_2'(\tau) &= -\frac{D_{xx}'}{2} + e^{-2\gamma'\tau} \frac{-4D_{pp}' - D_{xx}' + 2\gamma'(c_1'(0) + 2\gamma'c_2'(0) + 4c_3'(0))}{4\Omega^2} \\
  &\quad + \sum_{y=\pm \Omega} e^{-2(\gamma' + y)\tau} \left[ \frac{4D_{pp}'(\gamma' + y) + D_{xx}'(\gamma' - y) - 2c_1'(0) - 4c_2'(0)(\gamma' + y)}{8(\gamma' + y)y^2} 
  + \frac{c_3'(0)(1 - 2\gamma'^2 - 2\gamma'y)}{(\gamma' + y)y^2} \right],
\end{align*}
\]
\[ c'_3(\tau) = \frac{4D'_{pp} + D'_{xx}}{16\gamma'} \]
\[ + e^{-2\gamma\tau} \frac{4D'_{pp} + D'_{xx} - 2\gamma' (c'_1(0) + 2\gamma'c'_2(0) + 4c'_3(0))}{16\gamma'\Omega^2} \]
\[ + \sum_{y=\pm\Omega} e^{-2(\gamma'+y)\tau} \left[ \frac{4D'_{pp}(1 - 2\gamma'^2 - 2\gamma'y) - D'_{xx} + 2c'_1(0)(\gamma' + y)}{32(\gamma' + y)y^2} \right. \]
\[ \left. - c'_2(0)(1 - 2\gamma'^2 - 2\gamma'y) + 2c'_3(0)(3\gamma' + y - 4\gamma'^3 - 4\gamma'^2y) \right] \],

where for \( \tau \to \infty \) we obtain the stationary values
\[ c'_1^{\text{st}} = \frac{4D'_{pp} + D'_{xx}(4\gamma'^2 + 1)}{4\gamma'}, \quad c'_2^{\text{st}} = -\frac{D'_{xx}}{2}, \]
\[ c'_3^{\text{st}} = \frac{4D'_{pp} + D'_{xx}}{16\gamma'}. \] (A.1)

The solutions to the other transformed coefficients are:
\[ c'_4(\tau) = e^{-(\gamma'+\Omega)\tau} c'_4(0)(\Omega - \gamma') - 2c'_5(0) + e^{-(\gamma'-\Omega)\tau} c'_4(0)(\gamma' + \Omega) + 2c'_5(0), \]
\[ c'_5(\tau) = e^{-(\gamma'+\Omega)\tau} \frac{2c'_3(0)(\gamma' + \Omega) + c'_4(0)}{4\Omega} + e^{-(\gamma'-\Omega)\tau} \frac{2c'_3(0)(\Omega - \gamma') - c'_4(0)}{4\Omega}, \]
\[ c'_6(\tau) = c'_6(0), \]

where for \( \tau \to \infty \) both \( c'_4(\tau) \) and \( c'_5(\tau) \) tend to the same stationary value, zero.

In the next step we transform all \( c \)'s back to the \( A, B, \ldots \) coefficients in the position representation [2] with the help of the following relation
\[ \rho(k, \Delta, t) = \int e^{i k x} \rho \left( x + \frac{\Delta}{2}, x - \frac{\Delta}{2} \right) dx. \]

Evaluating the above integral for the ansatz in the position representation (see Eq. (2)) we obtain the relations [27]
\[ A = \frac{1}{x_0^2} \left( c'_3 - \frac{c'_2^2}{4c'_1^2} \right), \quad B = -\frac{1}{x_0^2} \frac{c'_2}{4c'_1}, \quad C = \frac{1}{x_0^2} \frac{1}{16c'_1}, \]
\[ D = -\frac{1}{x_0} \left( \frac{c'_2 c'_4}{2c'_1} - c'_5 \right), \quad E = \frac{1}{x_0} \frac{c'_4}{4c'_1}, \]
\[ e^{-c'_6} = \sqrt{\frac{\pi}{4C}} \exp \left\{ \frac{E^2}{4C} - N \right\} = \text{Tr}\{\hat{\rho}\} = 1. \] (A.2)

These relation are very crucial for our study, because in the subsequent section it will demonstrated that the eigenvalues and the eigenvectors of the density matrix \( \hat{\rho} \) can be constructed with the help of the real parameters \( A(\tau), B(\tau), C(\tau), D(\tau), E(\tau) \) and \( N(\tau) \).
Appendix B. Eigenvalues and eigenvectors

The object of this section is to find the eigenvalues and eigenvectors of the Gaussian density matrix in Eq. (2)

\[
\rho(x, y) = \exp\{-A(x-y)^2 - iB(x-y)(x+y) - C(x+y)^2 - iD(x-y) - E(x+y) - N\},
\]

with

\[
e^{-N} = \sqrt{\frac{4C}{\pi}} e^{- \frac{N^2}{4}}.
\]

In order to solve this problem we introduce the generalized Hermite polynomials \(H_n(x, a)\) (see e.g. Ref. [28]), which are defined by their generating function

\[
\exp\{2xu - au^2\} = \sum_{n=0}^{\infty} H_n(x, a) \frac{u^n}{n!},
\]

for all \(a > 0\). These functions are related to the usual Hermite polynomials as \(H_n(x, a) = a^{n/2}H_n(a^{-1/2}x)\), so \(H_n(x) = H_n(x, 1)\). The eigenproblem

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

is solved by

\[
\phi_n(x) = H_n\left(x + \frac{E}{4C}, \frac{1}{4\sqrt{AC}}\right) \exp\left\{-x^2 \left(2\sqrt{AC} + iB\right) - x \left(\sqrt{A/C} E + iD\right)\right\},
\]

\[
\epsilon_n = \epsilon_0^n, \quad \epsilon_0 = \frac{2\sqrt{C}}{\sqrt{A + \sqrt{C}}}, \quad \epsilon = \frac{\sqrt{A - \sqrt{C}}}{\sqrt{A + \sqrt{C}}}
\]

First, we observe that \(A \geq C\), otherwise the density matrix has negative eigenvalues. Furthermore, \(C > 0\) in order to avoid that all eigenvalues are equal to zero. The other three parameters \(B, D,\) and \(E\) can be any real numbers. These parameter ranges guarantee that the Gaussian functions of form \(2\) are states of a quantum harmonic oscillator. In order that the eigenfunctions \(\phi_n(x)\) form an orthonormal basis, we divide each of them with the square root of the norm resulting a prefactor of \((16AC)^{n+1/2}/(\sqrt{\pi}2^{m}n!)\). The obtained formulas extend the result of Ref. [29].

In the following we present a detailed derivation of Eq. (B.2). We replace \(x\) by \(y\) in Eq. (B.1) and then shift \(y\) by \(y + \kappa\). Multiplying this transformed equality by \(\rho(x, y) \exp\{zy^2 + wy\}\) and integrating with respect to \(y\), we get

\[
\int_{-\infty}^{+\infty} \exp\{2(y + \kappa)u - au^2\} \rho(x, y) \exp\{zy^2 + wy\} dy =
\]

\[
= \sum_{n=0}^{\infty} \frac{u^n}{n!} \int_{-\infty}^{+\infty} \rho(x, y) H_n(y + \kappa, a) \exp\{zy^2 + wy\} dy.
\]

(B.3)
The left hand side integrates to
\[
2 \sqrt{\frac{C}{\tau_--z}} \exp \left\{ -\frac{E^2}{4C} + \frac{(\eta_--w)^2}{4(\tau_--z)} \right\} \times \\
\exp \left\{ 2xu \frac{\delta}{\tau_--z} + 2u \left( \kappa + \frac{\eta_- + \omega}{\tau_-} \right) - u^2 \left( a - \frac{1}{\tau_-} \right) \right\} \times \\
\exp \left\{ x^2 \left( \frac{\delta^2}{\tau_- - \tau_+} - \frac{x}{\tau_- - z} \right) + x \frac{\delta(\omega + \eta_-) - (\tau_- - z)\eta_+}{\tau_- - z} \right\},
\]
(B.4)
where
\[
\tau_\pm = A + C \pm iB, \quad \eta_\pm = iD \pm E, \quad \delta = A - C.
\]
In order that Eq. (B.3) is indeed an eigenvalue equation (see Eq. (B.2)) with the ansatz
eigenvector \( \phi_n(y) = H_n(y + \kappa, a) \exp\{zy^2 + wy\} \), we require that the coefficients of \( x^2 \) and \( x \) in (B.4) coincide with the coefficients of \( y^2 \) and \( y \) in \( \exp\{zy^2 + wy\} \). Thus, we can determine \( z \) and \( \omega \) from the following equations:
\[
z = \frac{\delta^2}{\tau_- - z} - \tau_+, \quad \omega = \frac{\delta(\omega + \eta_-) - (\tau_- - z)\eta_+}{\tau_- - z}.
\]
We obtain from the quadratic equation of \( z \) the solutions \( z = -iB \pm 2\sqrt{AC} \). As both \( A \) and \( C \) are positive real numbers the solution \( -iB + 2\sqrt{AC} \) renders the integral in (B.3) divergent. Therefore, we consider only \( z = -iB - 2\sqrt{AC} \). This yields that \( \omega = -\sqrt{A/C} E - iD \) and
\[
\exp \left\{ -\frac{E^2}{4C} + \frac{(\eta_- + w)^2}{4(\tau_- - z)} \right\} = \exp \left\{ -\frac{E^2}{4C} + \frac{E^2}{4C} \right\} = 1.
\]
Now, let \( u' = u\delta/(\tau_- - z) \), so that the exponent of second exponential factor in (B.4) reads
\[
2 \left( x + \frac{\kappa(\tau_- - z) + \eta_- + \omega}{\delta} \right) u' - \frac{a(\tau_- - z)^2 - (\tau_- - z)}{\delta^2} u^2.
\]
The exponent of the above expression has to coincide with the generating function of
\( H_n(x + \kappa, a) \), which results for \( \kappa \) and \( a \) the following equations:
\[
\kappa = \frac{\kappa(\tau_- - z) + \eta_- + \omega}{\delta}, \quad a = \frac{a(\tau_- - z)^2 - (\tau_- - z)}{\delta^2}.
\]
Substituting the values of \( z \) and \( \omega \) we get
\[
\kappa = \frac{E}{2C}, \quad a = \frac{1}{4\sqrt{AC}}.
\]
In summary, (B.4) reads
\[
\frac{2\sqrt{C}}{\sqrt{A} + \sqrt{C}} e^{2(x+\kappa)u' - au'^2} e^{-x^2(-iB-2\sqrt{AC}) - x \left( \sqrt{A/C} E + iD \right)}.
\]
Now, substituting the above expression into (B.3) and rewriting the generating function in terms of generalized Hermite polynomials, we get

\[
\sum_{n=0}^{\infty} \frac{u^n}{n!} \frac{2\sqrt{C}}{\sqrt{A} + \sqrt{C}} \left( \frac{\sqrt{A} - \sqrt{C}}{\sqrt{A} + \sqrt{C}} \right)^n H_n(x + \kappa, a) e^{-(iB-2\sqrt{AC})} e^{-(\sqrt{A/C} E + iD)}
\]

\[
= \sum_{n=0}^{\infty} \frac{u^n}{n!} \int_{-\infty}^{+\infty} \rho(x, y) H_n(y + \kappa, a) e^{-(iB-2\sqrt{AC})} e^{-(\sqrt{A/C} E + iD)} dy,
\]

where we have used the relation

\[
u' = \frac{u\delta}{(\tau_+ - z)} = \frac{\sqrt{A} - \sqrt{C}}{\sqrt{A} + \sqrt{C}}.
\]

We obtain the desired result by comparing the coefficients of \(u^n\) on each side of the equation.

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