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The approach to thermal equilibrium in the Caldeira–Leggett model

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Abstract

We compare the long time behaviour and approach to thermal equilibrium of the one-dimensional Caldeira–Leggett model for the master equation in Lindblad and non-Lindblad forms. We first solve the explicit time evolution for the free particle and harmonic oscillator systems and show that our results agree with previous such attempts, and then show that Lindblad and non-Lindblad cases lead to the same evolution when we take the limitations of the Caldeira–Leggett model into account.

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1. Introduction

The Caldeira–Leggett model [1] is a simple system–reservoir model that can explain the basic aspects of dissipation in solid state physics, and in the high temperature and weak coupling limit, can also account for quantum Brownian motion [1–6]. It consists of a particle, which is also called 'the system', that interacts with a heat bath of simple harmonic oscillators through a linear term.

Time evolution and long time behaviour of the Caldeira–Leggett model has been examined in the literature using various mathematical approaches such as path integration, stochastic calculus and others [5–14]. These studies have had a variety of physical motivations ranging from Caldeira and Leggett's initial aim of explaining the quantum Brownian motion to exploration of certain models of quantum measurement [7, 8].

In this study, our main aim will be investigating the long time behaviour of the Caldeira–Leggett master equation, more specifically the relations between the so-called Lindblad and non-Lindblad forms of the time evolution. We will first give an outline of the stationary solution of the Caldeira–Leggett model and its relationship with the thermal equilibrium density matrix in order to lay down what we expect to see in terms of these already known properties. Then we will calculate the exact time evolution of the Caldeira–Leggett model with a detailed discussion of the density matrix at long times. Our calculation of the time evolution of the density matrix forms the basis of our comparison of the Lindblad and non-Lindblad cases, thus we will spend considerable time on it. However, we should note that many basic aspects of this long time behaviour have been previously obtained in the aforementioned studies, and the novelty of our results mostly are in the comparison of Lindblad and non-Lindblad forms of the master equation. Details of our calculational tools and some further discussions can be found in the appendices.

2. The master equation and the stationary states

The Caldeira–Leggett model is defined by the following Hamiltonian:

$$H = \overbrace{\frac{1}{2m}p^2 + V(q)}^{H_S} + \overbrace{q^2\sum_n \frac{\kappa_n^2}{2m_n\omega_n^2}}^{H_c} + \overbrace{\sum_n\left(\frac{1}{2m_n}p_n^2 + \frac{1}{2}m_n\omega_n^2 q_n^2\right)}^{H_B} - \overbrace{q\sum_n \kappa_n q_n}^{H_I}$$
$$= \frac{1}{2m}p^2 + V(q) + \sum_n\left(\frac{1}{2m_n}p_n^2 + \frac{1}{2}m_n\omega_n^2(q_n - q)^2\right) \qquad \left(\kappa_n \equiv m_n\omega_n^2\right) \tag{1}$$

where q, p are the position and momentum operators of the system and $\{q_n\}$, $\{p_n\}$ are the position and momentum operators of the bath oscillators, respectively. H_S is the system Hamiltonian, H_I is the interaction term and H_B is the Hamiltonian for the reservoir. Inclusion of the counterterm H_c is to avoid a shift due to the coupling in the bare potential $V(q)$ [13, 15]. For our study, the reservoir oscillators are described by an Ohmic spectral density with a Lorentz–Drude cutoff function

$$J(\omega) = \frac{2m\gamma}{\pi}\omega\frac{\Omega^2}{\Omega^2 + \omega^2}. \tag{2}$$

In the high temperature, weak coupling quantum Brownian motion case in which we are interested, it can be shown through various methods that the Hamiltonian leads to the following master equation for the reduced density matrix of the system [1, 16–18]:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_t = -\frac{\mathrm{i}}{\hbar}[H_S, \rho_t] - \frac{2\gamma m k_B T}{\hbar^2}[q, [q, \rho_t]] - \mathrm{i}\frac{\gamma}{\hbar}[q, \{p, \rho_t\}]. \tag{3}$$

In this form, the time evolution is not a quantum-dynamical semigroup and it violates positivity on short timescales [19]. However, one can add a 'minimally invasive' term, $-\frac{\gamma}{8mk_BT}[p, [p, \rho_t]]$, which is negligible compared to the other terms in the high temperature limit and which brings the equation into the so-called Lindblad form

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_t = -\frac{\mathrm{i}}{\hbar}[H_S, \rho_t] - \frac{2\gamma m k_B T}{\hbar^2}[q, [q, \rho_t]] - \frac{\gamma}{8mk_BT}[p, [p, \rho_t]] - \mathrm{i}\frac{\gamma}{\hbar}[q, \{p, \rho_t\}], \tag{4}$$

with the relaxation rate γ and the Lindblad operator

$$A = \sqrt{\frac{4mk_BT}{\hbar^2}}x + \mathrm{i}\sqrt{\frac{1}{4mk_BT}}p, \tag{5}$$

which gives the Lindblad evolution [20, 21]

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_t = -\frac{\mathrm{i}}{\hbar}\left[H_S + \frac{\gamma}{2}(qp + pq), \rho_t\right] + \gamma\left(A\rho_t A^\dagger - \frac{1}{2}A^\dagger A\rho_t - \frac{1}{2}\rho_t A^\dagger A\right). \tag{6}$$

Justification of the introduction of the minimally invasive term has been further discussed by Diosi [22].

Certain conditions have to be met for (3) and (4) to be valid [1, 16–18, 23]:

(1) The typical timescale over which the state of the system changes appreciably, $\tau_R \sim 1/\gamma$, should be much larger than the typical decay time for the correlation functions of the bath oscillators, τ_B, which translates into

$$\hbar\gamma \ll \min\{\hbar\Omega, 2\pi k_B T\}, \tag{7}$$

(2) The typical system evolution time, $1/\omega_S$, should be large compared to τ_B

$$\hbar\omega_S \ll \min\{\hbar\Omega, 2\pi k_B T\}. \tag{8}$$

This condition is required for the validity of the introduction of the 'minimally invasive' term as well as for other steps in the derivation of the master equation. We expect $p \sim m\omega_S q$ for the typical momentum and position values, so the ratio of the momentum double commutator to the position double commutator in (4) is at the order $(\hbar\omega_S/k_B T)^2$. This means it is negligible under this condition, making the Lindblad form of the master equation valid.

We will stick to these conditions throughout our study. A discussion of the modifications to the master equation at lower temperatures can be found in [23].

The first step in understanding the implications of the master equation is studying the stationary solution, i.e. the solution with $\mathrm{d}\rho_t/\mathrm{d}t = 0$. The general expectation is that, in the long time limit, the density matrix is going to reach this solution irrespective of the initial condition. For the non-Lindblad case, (3), and for a potential $V(q)$ whose spatial variations are small, the stationary solution in the position representation is given by (see, for example [7])

$$\langle q_1|\rho|q_2\rangle \approx N \exp\left(-\frac{V((q_1+q_2)/2)}{k_B T} - \frac{m k_B T (q_1-q_2)^2}{2\hbar^2}\right), \tag{9}$$

which can also be obtained using basic techniques for partial differential equations [11, 24], where N is a normalization constant. Moreover, for the case of the quadratic potential or the free particle, this equation is exact.

For the free particle, $(V(q) = 0)$, equation (9) gives the exact thermal equilibrium state, which can be obtained transforming the familiar expression

$$\langle p_1|\rho_{\mathrm{th}}|p_2\rangle = \langle p_1|N\,\mathrm{e}^{-\frac{p^2}{2mk_BT}}|p_2\rangle \begin{cases} \sqrt{\dfrac{1}{2\pi m k_B T}}\,\mathrm{e}^{-\frac{p_1^2}{2mk_BT}} & p_1 = p_2 \\ 0 & \text{otherwise} \end{cases} \tag{10}$$

into the position representation, using the Fourier transform.

For the harmonic oscillator, $V(q) = \frac{1}{2}m\omega^2 q^2$, the thermal equilibrium density matrix is given by [25]

$$\langle q_1|\rho|q_2\rangle = N \exp\left[-\frac{m\omega}{2\hbar\tanh(\hbar\omega/k_BT)}\left(q_1^2+q_2^2\right) + \frac{m\omega}{\hbar\sinh(\hbar\omega/k_BT)}q_1q_2\right] \tag{11}$$

which clearly does not agree with (9). The source of this disagreement can be traced by expanding the exponent in (11) in powers of $\hbar\omega/k_BT$. To the leading order

$$\begin{aligned}\langle q_1|\rho|q_2\rangle &= N \exp\left[-\frac{mk_BT}{2\hbar^2}\left(\frac{\hbar\omega}{k_BT}\right)^2\frac{(q_1+q_2)^2}{4} - \frac{mk_BT}{2\hbar^2}\left(1+\frac{1}{12}\left(\frac{\hbar\omega}{k_BT}\right)^2\right)(q_1-q_2)^2\right] \\ &= N\exp\left[-\frac{m\omega^2}{8k_BT}(q_1+q_2)^2 - \frac{mk_BT}{2\hbar^2}(q_1-q_2)^2\right]\exp\left[-\frac{m\omega^2}{24k_BT}(q_1-q_2)^2\right],\end{aligned} \tag{12}$$

which agrees with (9) on the diagonal ($q_1 = q_2$), ignoring the higher order terms, but does not agree with it if we move away from the diagonal where $q_1 - q_2$ is comparable to $q_1 + q_2$ in magnitude. This should not be surprising, since the term in the exponent that causes the difference, $-\frac{m\omega^2}{24k_BT}(q_1 - q_2)^2$, is at the order $(\hbar\omega/k_BT)^2$ compared to $\frac{mk_BT}{2\hbar^2}(q_1 - q_2)^2$. Also, we expect $m\omega^2 q^2 \sim \hbar\omega$, which means $\frac{m\omega^2}{24k_BT}(q_1 - q_2)^2 \sim \frac{\hbar\omega}{k_BT}$. We already stated that our master equation is valid in the regime where $\hbar\omega/k_BT \ll 1$, thus it is expected that such terms are not captured by the stationary state of the non-Lindblad master equation. In other words, by agreeing to use (3) or (4) to investigate the Caldeira–Leggett model, we give up the prospect to have sensitivity to any higher order terms in $\hbar\omega/k_BT$.

To summarize, the stationary solution of the free particle Caldeira–Leggett master equation in the non-Lindblad case is the exact thermal equilibrium density matrix for the free particle. Thus, reaching the stationary state and reaching the thermal equilibrium are equivalent for this case. However, for the harmonic oscillator, the stationary solution is not the thermal equilibrium, but rather, the two agree on the diagonal in the high temperature limit. High temperature limit is essential to the derivation of the master equation itself, thus, we can say that the stationary solution captures the thermal equilibrium as best as possible for the non-Lindblad Caldeira–Leggett master equation.

Our previous discussions suggest that the 'minimally invasive' term should not affect the physics significantly. We are not going to explicitly calculate the stationary solutions with this term, but our subsequent analysis will make it clear that the long time behaviour is identical to the non-Lindblad case.

3. Time evolution of the free particle system

3.1. Lindblad case

For our analysis, we employed the techniques given in the appendices of [26] and [27], where they are used for similar purposes. The main feature of our technique is the use of the Wigner function and the Gaussian ansatz. Details of the calculations can be found in appendix A.

The characteristic function associated with the Wigner function is defined as

$$\tilde{\rho}_t(k, x) = \mathrm{tr}\big(\rho_t\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(kq+xp)}\big) \tag{13}$$

with the inversion formulae in the momentum and position basis as

$$\begin{aligned} \langle p_1|\rho_t|p_2\rangle &= \frac{1}{2\pi\hbar}\int \mathrm{d}x\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}x(\frac{p_1+p_2}{2})}\tilde{\rho}_t(p_2 - p_1, x) \\ \langle q_1|\rho_t|q_2\rangle &= \frac{1}{2\pi\hbar}\int \mathrm{d}k\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}k(\frac{q_1+q_2}{2})}\tilde{\rho}_t(k, q_1 - q_2), \end{aligned} \tag{14}$$

respectively. For the Lindblad case, $V(q) = 0$, and a given initial data $\tilde{\rho}_0$, the exact time evolution of the Wigner function is given by

$$\tilde{\rho}_t(k, x) = \mathrm{e}^{-(\frac{k_BT}{2\hbar^2 m\gamma} + \frac{\gamma}{8mk_BT})k^2 t}\, \mathrm{e}^{\frac{mk_BT}{2\hbar^2}[k^2\frac{\Gamma_t^2+2\Gamma_t}{4m^2\gamma^2} - kx\frac{\Gamma_t^2}{m\gamma} - x^2(1-\mathrm{e}^{-4\gamma t})]}\,\tilde{\rho}_0\left(k, x\,\mathrm{e}^{-2\gamma t} + \frac{\Gamma_t k}{2m\gamma}\right). \tag{15}$$

In the long time limit, we expect to find that the density matrix will evolve to the stationary solution, which, as we have shown, is diagonal in the momentum representation. So, we solve the time evolution of the density matrix in this representation using (14) and reach

$$\begin{aligned} \langle p_1|\rho_t|p_2\rangle = R(t) + \sqrt{\frac{1}{2\pi mk_BT}}\frac{1}{\sqrt{1-\mathrm{e}^{-4\gamma t}}}\,\mathrm{e}^{-(\frac{k_BT}{2\hbar^2 m\gamma}+\frac{\gamma}{8mk_BT})(p_2-p_1)^2 t}\,\mathrm{e}^{\frac{(\Gamma_t^2+2\Gamma_t)k_BT}{8\hbar^2 m\gamma^2}(p_2-p_1)^2} \\ \times\, \mathrm{e}^{\frac{\hbar^2}{2(1-\mathrm{e}^{-4\gamma t})mk_BT}(\frac{i(p_1+p_2)}{2\hbar} + \frac{\Gamma_t^2 k_BT}{2\hbar^2\gamma}(p_2-p_1))^2}\,\tilde{\rho}_0\left(p_2 - p_1, \frac{\Gamma_t(p_2-p_1)}{2m\gamma}\right) \end{aligned} \tag{16}$$

where

$$R(t) = \frac{1}{2\pi\hbar}\,\mathrm{e}^{-\left(\frac{k_BT}{2\hbar^2 m\gamma}+\frac{\gamma}{8mk_BT}\right)(p_2-p_1)^2 t}\,\mathrm{e}^{\frac{(\Gamma_t^2+2\Gamma_t)k_BT}{8\hbar^2 m\gamma^2}(p_2-p_1)^2}$$
$$\times\int \mathrm{d}x\left\{\mathrm{e}^{-\frac{(1-\mathrm{e}^{-4\gamma t})mk_BT}{2\hbar^2}x^2-\left(\frac{i(p_1+p_2)}{2\hbar}+\frac{\Gamma_t^2 k_BT}{2\hbar^2\gamma}(p_2-p_1)\right)x}\right.$$
$$\left.\times\left[\tilde{\rho}_0\left(p_2-p_1, x\,\mathrm{e}^{-2\gamma t}+\frac{\Gamma_t(p_2-p_1)}{2m\gamma}\right)-\tilde{\rho}_0\left(p_2-p_1,\frac{\Gamma_t(p_2-p_1)}{2m\gamma}\right)\right]\right\}. \tag{17}$$

As long as $\tilde{\rho}_0(k,x)$ is bounded and well behaved around $\left(p_2-p_1,\frac{(p_2-p_1)}{2m\gamma}\right)$, $R(t)$ vanishes in the long time limit. Then, the main observation is that as $t\to\infty$, $\langle p_1|\rho_t|p_2\rangle$ vanishes except for the case $p_2-p_1=0$, due to the term $\exp\left[-\left(\frac{k_BT}{2\hbar^2 m\gamma}+\frac{\gamma}{8mk_BT}\right)(p_2-p_1)^2 t\right]$. Using the fact that $\tilde{\rho}_t(0,0)=\mathrm{tr}\rho_t=1$, we finally reach

$$\langle p_1|\rho_\infty|p_2\rangle = \begin{cases}\sqrt{\dfrac{1}{2\pi mk_BT}}\,\mathrm{e}^{-\frac{p_1^2}{2mk_BT}} & p_1=p_2\\ 0 & \text{otherwise}\end{cases} \tag{18}$$

which is the stationary solution of the master equation and the thermal equilibrium density matrix of a free particle (see section 2). Thus, the thermal equilibrium is indeed reached in the long time limit for the free particle in the Caldeira–Leggett model. Similar results were also reached in previous studies [6, 7].

All of the asymptotic behaviour of the density matrix can be read off from (16). Let us start by analysing the remainder term $R(t)$. For large times and for the values of x where the integrand is significantly different from 0, we can expand series $\tilde{\rho}_0$ through the leading term

$$\tilde{\rho}_0\left(p_2-p_1, x\,\mathrm{e}^{-2\gamma t}+\frac{\Gamma_t(p_2-p_1)}{2m\gamma}\right)$$
$$-\tilde{\rho}_0\left(p_2-p_1,\frac{\Gamma_t(p_2-p_1)}{2m\gamma}\right)\approx\left.\frac{\partial\tilde{\rho}_0(k,x)}{\partial x}\right|_{\left(p_2-p_1,\frac{(p_2-p_1)}{2m\gamma}\right)} x\,\mathrm{e}^{-2\gamma t}, \tag{19}$$

given that $\tilde{\rho}_0$ is well behaved around $x=(p_2-p_1)/2m\gamma$ and $\partial\tilde{\rho}_0(k,x)/\partial x$ does not vanish at the point $\left(p_2-p_1,\frac{(p_2-p_1)}{2m\gamma}\right)$. Under these conditions, $R(t)$ is given by

$$R(t\to\infty)\approx f(p_1,p_2)\,\mathrm{e}^{-\left(\frac{k_BT}{2\hbar^2 m\gamma}+\frac{\gamma}{8mk_BT}\right)(p_2-p_1)^2 t}\,\mathrm{e}^{-2\gamma t}, \tag{20}$$

where

$$f(p_1,p_2) = -\frac{\hbar^2}{\sqrt{2\pi(mk_BT)^3}}\left(\frac{\mathrm{i}(p_1+p_2)}{2\hbar}+\frac{k_BT}{2\hbar^2\gamma}(p_2-p_1)\right)\left.\frac{\partial\tilde{\rho}_0(k,x)}{\partial x}\right|_{\left(p_2-p_1,\frac{(p_2-p_1)}{2m\gamma}\right)}$$
$$\times\,\mathrm{e}^{\frac{\hbar^2}{2(1-\mathrm{e}^{-4\gamma t})mk_BT}\left(\frac{\mathrm{i}(p_1+p_2)}{2\hbar}+\frac{\Gamma_t^2 k_BT}{2\hbar^2\gamma}(p_2-p_1)\right)^2}\,\mathrm{e}^{\frac{3(p_2-p_1)^2 k_BT}{8\hbar^2 m\gamma^2}}. \tag{21}$$

This means, for the non-diagonal elements, $R(t)$ is dying much faster than the non-$R(t)$ term in (16), due to the extra exponential factor of $\mathrm{e}^{-2\gamma t}$, and is negligible. Then, the long time behaviour becomes

$$\langle p_1|\rho_{t\to\infty}|p_2\rangle = \sqrt{\frac{1}{2\pi mk_BT}}\,\mathrm{e}^{\frac{(p_2-p_1)^2 k_BT}{2\hbar^2 m\gamma^2}}\,\mathrm{e}^{-\frac{(p_1+p_2)^2}{8mk_BT}}\,\mathrm{e}^{\frac{i(p_2^2-p_1^2)}{4m\hbar\gamma}}\,\tilde{\rho}_0\left(p_2-p_1,\frac{p_2-p_1}{2m\gamma}\right)$$
$$\times\mathrm{e}^{-\left(\frac{k_BT}{2\hbar^2 m\gamma}+\frac{\gamma}{8mk_BT}\right)(p_2-p_1)^2 t}\qquad(p_1\neq p_2) \tag{22}$$

which is manifestly exponential. The time constant for relaxation is

$$\tau_{p_1,p_2} = \left(\frac{\gamma}{8mk_BT} + \frac{k_BT}{2\hbar^2 m\gamma}\right)^{-1} \frac{1}{(p_2-p_1)^2} = \frac{1}{1+\left(\frac{\hbar\gamma}{2k_BT}\right)^2} \frac{2\hbar^2 m\gamma}{k_BT(p_2-p_1)^2} \tag{23}$$

which leads to the following observations:

(1) In the momentum representation, relaxation to the thermal state becomes faster as one moves away from the diagonal in the density matrix.

(2) At a first look, relaxation is faster in both high and low temperature limits and is slowest at $T = \hbar\gamma/2k_B$, but remembering that $\hbar\gamma/k_BT \ll 1$ should hold for the validity of our master equation, only the high temperature limit is meaningful and the $\gamma/8mk_BT$ term can be neglected:

$$\tau_{p_1,p_2} \approx \frac{2m\hbar^2\gamma}{k_BT(p_2-p_1)^2} = \frac{2\hbar^2}{D(p_2-p_1)^2}. \tag{24}$$

Here, $D = k_BT/m\gamma$ is the diffusion constant, which can be readily demonstrated using (16)

$$\begin{aligned}\langle q^2\rangle &= \mathrm{tr}(q^2\rho_t) = \int \mathrm{d}p\langle p|q^2\rho_t|p\rangle = -\hbar^2\int \mathrm{d}p\left(\frac{\mathrm{d}^2}{\mathrm{d}q^2}\langle q|\rho_t|p\rangle\right)_{p=q}\\ &= -\hbar^2\int \mathrm{d}p\left(-2\left(\frac{k_BT}{2\hbar^2 m\gamma} + \frac{\gamma}{8mk_BT}\right)t\langle q|\rho_t|p\rangle + \text{time independent terms}\right)\\ &\approx \frac{k_BT}{m\gamma}t\,(t\to\infty),\end{aligned} \tag{25}$$

where we again used the fact that the trace of the reduced density matrix is unity. This reaffirms the previous results [6] and shows the connection between the decay constants and the diffusion coefficient.

For the diagonal elements, i.e. $p_1 = p_2$, there are two sources of correction to (18), one arising from $R(t)$ and the other from the corrections to the non-$R(t)$ term due to the finiteness of t. The latter is at the order $\mathrm{e}^{-4\gamma t}$, as can be seen from (16), so the leading correction comes from $R(t)$

$$\langle p|\rho_{t\to\infty}|p\rangle \approx \sqrt{\frac{1}{2\pi mk_BT}}\,\mathrm{e}^{-\frac{p^2}{2mk_BT}}\left(1 - \frac{\mathrm{i}\hbar p}{mk_BT}\left.\frac{\partial\tilde{\rho}_0(k,x)}{\partial x}\right|_{(0,0)}\mathrm{e}^{-2\gamma t}\right), \tag{26}$$

which shows that the relaxation time for the diagonal elements is $\tau_R \sim 1/\gamma$ as expected.

3.2. Non-Lindblad case and comparison

The originally derived master equation for the Caldeira–Leggett model, (3), was not in the Lindblad form, lacking the 'minimally invasive' term $-\frac{\gamma}{8mk_BT}[p,[p,\rho_t]]$. Not having this term leads to

$$\begin{aligned}\langle p_1|\rho_t|p_2\rangle = R(t) &+ \sqrt{\frac{1}{2\pi mk_BT}}\frac{1}{\sqrt{1-\mathrm{e}^{-4\gamma t}}}\,\mathrm{e}^{-\frac{k_BT}{2\hbar^2 m\gamma}(p_2-p_1)^2 t}\,\mathrm{e}^{\frac{(\Gamma_t^2+2\Gamma_t)k_BT}{8\hbar^2 m\gamma^2}(p_2-p_1)^2}\\ &\times \mathrm{e}^{\frac{\hbar^2}{2(1-\mathrm{e}^{-4\gamma t})mk_BT}\left(\frac{\mathrm{i}(p_1+p_2)}{2\hbar}+\frac{\Gamma_t^2 k_BT}{2\hbar^2\gamma}(p_2-p_1)\right)^2}\tilde{\rho}_0\left(p_2-p_1,\frac{\Gamma_t(p_2-p_1)}{2m\gamma}\right),\end{aligned} \tag{27}$$

whose origin can be seen in (A.3) (with $\omega = 0$), where the first equation reads $\dot{c}_1(t) = c_2(t)/m$ when we use the non-Lindblad master equation. This, in turn leads to the formally simple change that $\mathrm{e}^{-\frac{\gamma(p_2-p_1)^2}{8mk_B}t}$ term is not present in (16), thus (27) is reached.

This means

(1) Any initial density matrix still evolves into the form in (18) in the long time limit. So in the long time limit, the non-Lindblad and Lindblad equations give the same result, which is thermal equilibrium.

(2) Non-diagonal terms still vanish in the long time limit due to the $\mathrm{e}^{-\frac{k_B T}{2\hbar^2 m\gamma}(p_2-p_1)^2 t}$ term, but the decay is slower and the time constant is

$$\tau_{p_1,p_2} = \frac{2m\hbar^2\gamma}{k_B T(p_2-p_1)^2} \tag{28}$$

as opposed to (23). Nevertheless, remembering the condition $\hbar\gamma \ll k_B T$, we can see that the missing term in the non-Lindblad case is negligible, so the change in the time evolution for the non-diagonal terms is negligible.

(3) Since the $\mathrm{e}^{-\frac{\gamma(p_2-p_1)^2}{8mk_B}t}$ term was constant and equal to 1 for the diagonal matrix elements in the Lindblad form, not having this term does not have any effect. The time evolution of the diagonal elements of the density matrix is exactly the same as before.

In summary, for the free particle case, Lindblad and non-Lindblad master equations lead to the same density matrix in the long time limit, which is that of thermal equilibrium.

4. Time evolution of the simple harmonic oscillator system

4.1. Lindblad case

For a general potential

$$V(q) = \sum_m a_m q^m, \tag{29}$$

our current calculation methods are not very useful since they lead to nonlinear differential equations (see appendix A for more details on this shortcoming, see [8] for a discussion of general potentials). Still, it is possible to have an analytical solution for the exceptional, but important, case of the harmonic oscillator. For a system under the potential

$$V(q) = \tfrac{1}{2}m\omega^2 q^2, \tag{30}$$

we obtain (see appendix A)

$$\begin{aligned}\tilde{\rho}_t(k,x) &= \exp\left\{-\frac{mk_B T M_3(t)}{2\hbar^2}x^2\right\}\exp\left\{-\frac{k_B T}{2\hbar^2 m\omega^2}\left[M_1(t)k^2 + \frac{2m\omega^2}{\gamma}M_2(t)kx\right]\right\}\\ &\tilde{\rho}_0\left(\frac{\mathrm{e}^{-(\gamma-\mu)t}\Lambda_t}{2\mu}((\mu\coth\mu t+\gamma)k - m\omega^2 x), \frac{\mathrm{e}^{-(\gamma-\mu)t}\Lambda_t}{2\mu}\left((\mu\coth\mu t-\gamma)x + \frac{k}{m}\right)\right),\end{aligned} \tag{31}$$

where $\mu \equiv \sqrt{\gamma^2-\omega^2}$, $\Lambda_t \equiv 1-\mathrm{e}^{-2\mu t}$ and M_i are dimensionless functions with the asymptotic behaviours

$$\begin{aligned} M_1(t\to\infty) &= 1 + \left(\frac{\hbar\gamma}{2k_B T}\right)^2 + \left(\frac{\hbar\omega}{4k_B T}\right)^2 + \mathcal{O}(\mathrm{e}^{-\mathrm{Re}\{2\gamma-\mu\}t})\\ M_2(t\to\infty) &= -\frac{1}{8}\left(\frac{\hbar\gamma}{k_B T}\right)^2 + \mathcal{O}(\mathrm{e}^{-\mathrm{Re}\{2\gamma-\mu\}t})\\ M_3(t\to\infty) &= 1 + \left(\frac{\hbar\omega}{4k_B T}\right)^2 + \mathcal{O}(\mathrm{e}^{-\mathrm{Re}\{2\gamma-\mu\}t}).\end{aligned} \tag{32}$$

For the case of the harmonic oscillator, we will use the position representation where the thermal equilibrium density matrix is given by (11). Using the inversion formula (14), we reach the central result

$$\langle q_1|\rho_t|q_2\rangle = R_{\mathrm{HO}}(t) + \sqrt{\frac{m\omega^2}{2\pi k_B T M_1(t)}}\, \mathrm{e}^{-\frac{mk_BTM_3(t)}{2\hbar^2}(q_1-q_2)^2}\, \mathrm{e}^{\frac{\hbar^2 m\omega^2}{2k_BTM_1(t)}\left(\frac{\mathrm{i}(q_1+q_2)}{2\hbar}+\frac{k_BTM_2(t)(q_1-q_2)}{\hbar^2\gamma}\right)^2}, \tag{33}$$

with

$$R_{\mathrm{HO}}(t) = \frac{1}{2\pi\hbar}\, \mathrm{e}^{-\frac{mk_BTM_3(t)}{2\hbar^2}(q_1-q_2)^2} \int \mathrm{d}k\, \mathrm{e}^{-\frac{k_BTM_1(t)}{2\hbar^2 m\omega^2}k^2-\left(\frac{\mathrm{i}(q_1+q_2)}{2\hbar}+\frac{k_BTM_2(t)(q_1-q_2)}{\hbar^2\gamma}\right)k}(\tilde\rho_0(k',x')-1) \tag{34}$$

where

$$k' = \frac{\mathrm{e}^{-(\gamma-\mu)t}\Lambda_t}{2\mu}((\mu\coth\mu t+\gamma)k - m\omega^2(q_1-q_2))$$

$$x' = \frac{\mathrm{e}^{-(\gamma-\mu)t}\Lambda_t}{2\mu}\left((\mu\coth\mu t-\gamma)(q_1-q_2)+\frac{k}{m}\right).$$

Assuming that $\tilde\rho_0$ is well behaved around (0, 0), we again have a vanishing remainder term, $R_{\mathrm{HO}}(t\to\infty) = 0$. This means, in the infinite time limit

$$\begin{aligned}\langle q_1|\rho_\infty|q_2\rangle &= \left(\frac{m\omega^2}{2\pi k_BT}\right)^{1/2}\left[1+\left(\frac{\hbar\gamma}{2k_BT}\right)^2+\left(\frac{\hbar\omega}{4k_BT}\right)^2\right]^{-1/2} \mathrm{e}^{-\frac{m\omega^2}{8k_BT}[1+(\frac{\hbar\gamma}{2k_BT})^2+(\frac{\hbar\omega}{4k_BT})^2]^{-1}(q_1+q_2)^2}\\ &\quad\times \mathrm{e}^{-\frac{mk_BT}{2\hbar^2}[1+(\frac{\hbar\omega}{4k_BT})^2+(\frac{\hbar\omega}{4k_BT})^2(\frac{\hbar\gamma}{2k_BT})^2[1+(\frac{\hbar\gamma}{2k_BT})^2+(\frac{\hbar\omega}{4k_BT})^2]^{-1}](q_1-q_2)^2}\\ &\quad\times \mathrm{e}^{-\mathrm{i}\frac{m\omega^2}{16k_BT}(\frac{\hbar\gamma}{k_BT})[1+(\frac{\hbar\gamma}{2k_BT})^2+(\frac{\hbar\omega}{4k_BT})^2]^{-1}(q_1^2-q_2^2)}.\end{aligned} \tag{35}$$

This result does not exactly agree with the thermal equilibrium density matrix (11) or with the stationary solution to the non-Lindblad master equation (9). Nevertheless, conditions for the validity of the master equation imply that $\hbar\gamma/k_BT \ll 1$ and $\hbar\omega/k_BT \ll 1$. Also, $m\omega^2q^2 \sim \hbar\omega$ and

$$\mathrm{e}^{-\mathrm{i}\frac{m\omega^2}{16k_BT}(\frac{\hbar\gamma}{k_BT})(q_1^2-q_2^2)} \approx \mathrm{e}^{-\mathrm{i}(\frac{\hbar\omega}{16k_BT})(\frac{\hbar\gamma}{k_BT})} \approx 1 \tag{36}$$

for the typical length scales we encounter in the harmonic oscillator system. Putting all these conditions together:

$$\langle q_1|\rho_\infty|q_2\rangle \approx \sqrt{\frac{m\omega^2}{2\pi k_BT}}\, \mathrm{e}^{-\frac{m\omega^2}{8k_BT}(q_1+q_2)^2}\, \mathrm{e}^{-\frac{mk_BT}{2\hbar^2}(q_1-q_2)^2}. \tag{37}$$

So, the density matrix approaches the stationary solution (9) under the validity conditions of our master equation. Also, remember that the stationary solution agrees with the thermal equilibrium density matrix of the harmonic oscillator only on the diagonal and to the leading order in $\hbar\omega/k_BT$. Overall, these results agree with the previous findings in [6, 7].

Let us now analyse the corrections to the infinite time matrix elements. Assuming $\tilde\rho_0$ is well behaved around (0, 0) and defining $\partial\tilde\rho_0(k,x)/\partial k|_{(0,0)} \equiv D_k$ and $\partial\tilde\rho_0(k,x)/\partial x|_{(0,0)} \equiv D_x$, the remainder term has the long time behaviour

$$\begin{aligned}R_{\mathrm{HO}}(t) &\approx \mathrm{e}^{-(\gamma-\mu)t}\sqrt{\frac{m\omega^2}{2\pi k_BTM_1(t)}}\, \mathrm{e}^{-\frac{mk_BTM_3(t)}{2\hbar^2}(q_1-q_2)^2}\, \mathrm{e}^{\frac{\hbar^2m\omega^2}{2k_BTM_1(t)}\left(\frac{\mathrm{i}(q_1+q_2)}{2\hbar}+\frac{k_BTM_2(t)(q_1-q_2)}{\hbar^2\gamma}\right)^2}\\ &\quad\times((\mu\coth\mu t+\gamma)D_k+(D_x/m))\frac{\Lambda_t}{2\mu}\left(-\frac{\hbar m\omega^2\,(4\mathrm{i}k_BT(q_1+q_2)-\hbar\gamma(q_1-q_2))}{8k_B^2T^2}\right.\\ &\quad\left.+\frac{-m\omega^2D_k+(\mu\coth\mu t-\gamma)D_x}{(\mu\coth\mu t+\gamma)D_k+(D_x/m)}(q_1-q_2)\right)\end{aligned} \tag{38}$$

In the long time limit, again there are two sources of correction to the infinite time values of the matrix elements. The first is from R_{HO} which is exponentially small compared to the matrix element by $\mathrm{e}^{-\mathrm{Re}\{\gamma-\mu\}t}$, as seen in (38). The second correction comes from the corrections to the non-R_{HO} term due to the finiteness of t in (33), which mainly arises from $M_i(t) - M_i(\infty)$, and is at the order $\mathrm{e}^{-\mathrm{Re}\{2\gamma-\mu\}t}$ as seen in (32). Thus, after a sufficiently long time, the latter correction becomes negligible compared to the former unless R_{HO} vanishes, which is only possible for a special combination of the values of D_k and D_x. That is, the leading correction to (35) is (38), which dies out with a time constant of $1/\mathrm{Re}\{\gamma - \mu\}$. In summary

(1) If $\omega > \gamma, \mu$ is imaginary, and the relaxation time constant is $1/\mathrm{Re}\{\gamma - \mu\} = 1/\gamma$ as expected.

(2) If $\omega < \gamma, \mu$ is real and $\mu < \gamma$, so relaxation still occurs but at the slower rate of $\mathrm{e}^{-(\gamma-\sqrt{\gamma^2-\omega^2})t}$. The time constant behaves as $\sim\frac{\gamma}{\omega^2}$ as $\frac{\omega}{\gamma}$ approaches 0.

4.2. Non-Lindblad case and comparison

If we were to use the non-Lindblad master equation, than the only change would be that we would have no $-\frac{\gamma}{8mk_BT}k^2\tilde{\rho}_t(k, x)$ term in the master equation for the Wigner function (A.1), or equivalently, no $\gamma/8mk_BT$ term for $\dot{c}_1$ in (A.3), as in the case of the free particle. Effects of this can be easily traced by having $k_BT \to \infty$ and $\hbar \to \infty$ while keeping $\hbar^2/k_BT$ constant. This way, $\gamma/8mk_BT \to 0$, with all other coefficients in the differential equations remaining the same, giving us the non-Lindblad equation. Then

$$\frac{\hbar\omega}{k_BT} = \frac{\hbar^2}{k_BT}\frac{\omega}{\hbar} \to 0, \qquad \frac{\hbar\gamma}{k_BT} = \frac{\hbar^2}{k_BT}\frac{\gamma}{\hbar} \to 0, \tag{39}$$

that is, in this limit, terms of $\mathcal{O}(\hbar\gamma/k_BT)$ or $\mathcal{O}(\hbar\omega/k_BT)$ in the expressions for M_i, (32), vanish. Thus, without any approximations

$$\langle q_1|\rho_\infty|q_2\rangle = \sqrt{\frac{m\omega^2}{2\pi k_BT}}\,\mathrm{e}^{-\frac{m\omega^2}{8k_BT}(q_1+q_2)^2}\,\mathrm{e}^{-\frac{mk_BT}{2\hbar^2}(q_1-q_2)^2}. \tag{40}$$

This was expected, since the non-Lindblad master equation was anticipated to reach its stationary solution exactly, rather than approximately. This result was also reached in [11], where they also show that the density matrix is diagonal in the energy basis of the system harmonic oscillator, supporting the idea of the pointer states of Paz and Zurek [28].

For the non-Lindblad master equation, The leading correction to the thermal equilibrium density matrix at large times is the same as the Lindblad case and originates from $R_{\mathrm{HO}}(t)$. Thus it is $\mathcal{O}(\mathrm{e}^{-Re\{\gamma-\mu\}t})$.

To sum up, the Lindblad case infinite time density matrix is considerably more complex compared to the non-Lindblad case, if we compare the exact solutions. However, once the limits of the derivation of our master equations are taken into account, we can see that the two cases completely agree in the leading terms for which our equations are sensitive. Moreover, the time constants that control the approach to equilibrium are also the same for both cases. Hence, once again we see that the introduction of the 'minimally invasive' term to the master equation does not significantly affect the long time characteristics.

We should also note that we have not explicitly calculated the stationary solution of the harmonic oscillator for the Lindblad case, so we cannot definitively say that the stationary solution is reached in the infinite time limit for this case. However, all our findings strongly suggest that (35) is the stationary solution for the Lindblad master equation of the harmonic oscillator.

5. Conclusions

We have solved the complete time evolution of the Caldeira–Leggett model for the free particle and the harmonic oscillator, and shown that the reduced density matrix of the system approaches the exact thermal equilibrium for the free particle and an approximate thermal equilibrium for the harmonic oscillator in the long time limit, confirming the previous results in the field. The detailed study of the infinite time limit and the deviations from this at finite times showed that the Lindblad and non-Lindblad master equations do not differ in this aspect. This was the expected result since the main problem of the non-Lindblad equation, lacking positivity on short timescales, should not make a difference at the investigated limit.

We note that the methods we used, the characteristic function of the Wigner function and the Gaussian ansatz, can be utilized for more complex cases. We gave a treatment of the most general case in the appendices for the sake of generality.

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Appendix A. Green's function for the harmonic oscillator system

Here, we will give the details of the calculation that leads to (31). The case for the free particle and the non-Lindblad master equations are similar. Our treatment closely follows [26].

The master equation for a system under a quadratic potential $V(q) = \frac{1}{2}m\omega^2 q^2$ translates to the following differential equation for $\tilde{\rho}_t(k, x)$:

$$\frac{\partial}{\partial t}\tilde{\rho}_t(k, x) = \left(\frac{1}{m}k\frac{\partial}{\partial x} - m\omega^2 x\frac{\partial}{\partial k} - \frac{2\gamma m k_B T}{\hbar^2}x^2 - \frac{\gamma}{8mk_B T}k^2 - 2\gamma x\frac{\partial}{\partial x}\right)\tilde{\rho}_t(k, x). \quad \text{(A.1)}$$

The first key observation is that, under (A.1), initially Gaussian states remain Gaussian. If we make the ansatz

$$\tilde{\rho}_t(k, x) = \exp\{-c_1k^2 - c_2kx - c_3x^2 - \mathrm{i}c_4k - \mathrm{i}c_5x - c_6\}, \quad \text{(A.2)}$$

then the master equation, upon equating the coefficients of the independent terms, leads to a linear system of differential equations for $c_i(t)$,

$$\begin{aligned}
\dot{c}_1(t) &= \frac{c_2(t)}{m} + \frac{\gamma}{8mk_B T} \\
\dot{c}_2(t) &= \frac{2c_3(t)}{m} - 2\gamma c_2(t) - 2m\omega^2 c_1(t) \\
\dot{c}_3(t) &= \frac{2\gamma m k_B T}{\hbar^2} - 4\gamma c_3(t) - m\omega^2 c_2(t) \\
\dot{c}_4(t) &= \frac{c_5(t)}{m} \\
\dot{c}_5(t) &= -2\gamma c_5(t) - m\omega^2 c_4(t) \\
\dot{c}_6(t) &= 0.
\end{aligned} \quad \text{(A.3)}$$

Hence, we can calculate the exact time evolution of $\tilde{\rho}_t$ if the initial data is Gaussian.

The second key observation is that knowing the solution for given Gaussian initial data, we can solve the problem for any initial condition using the Green's function $\tilde{G}(k, x, t; k_0, x_0, 0)$

$$\tilde{\rho}_t(k, x) = \int \mathrm{d}k_0\, \mathrm{d}x_0 \tilde{G}(k, x, t; k_0, x_0, 0)\tilde{\rho}_0(k_0, x_0). \tag{A.4}$$

$\tilde{G}$ is defined as the solution to (A.1) that satisfies the initial condition

$$\lim_{t\to 0} \tilde{G}(k, x, t; k_0, x_0, 0) = \delta(k - k_0)\delta(x - x_0). \tag{A.5}$$

A Gaussian of the form

$$\tilde{\rho}_0^{k_0 x_0,\epsilon\eta}(k, x) = \frac{1}{\pi\sqrt{\epsilon\eta}}\, \mathrm{e}^{-\frac{1}{\epsilon}(k-k_0)^2}\, \mathrm{e}^{-\frac{1}{\eta}(x-x_0)^2} \tag{A.6}$$

has the limit

$$\tilde{\rho}_0^{k_0 x_0,\epsilon\eta}(k, x) \xrightarrow[\epsilon,\eta\to 0]{} \delta(k - k_0)\delta(x - x_0), \tag{A.7}$$

hence if we solve for the initial data of (A.6) using the equations for $c_i(t)$ and take the desired limit, we obtain the Green's function. The system of equations for $c_i(t)$ is quite cumbersome to solve by hand, unlike the case of the free particle in [26], hence we used Mathematica© to solve it and the final result is

$$\begin{aligned}\tilde{G}(k, x, t; k_0, x_0, 0) &= \delta\left(k_0 - \frac{\mathrm{e}^{-(\gamma-\mu)t}\Lambda_t}{2\mu}((\mu\coth\mu t + \gamma)k - m\omega^2 x)\right)\\ &\quad\times\delta\left(x_0 - \frac{\mathrm{e}^{-(\gamma-\mu)t}\Lambda_t}{2\mu}\left((\mu\coth\mu t - \gamma)x + \frac{k}{m}\right)\right)\\ &\quad\times\exp\left\{-\frac{k_B T}{2\hbar^2 m\omega^2}\left[M_1(t)k^2 + \frac{2m\omega^2}{\gamma}M_2(t)kx + m^2\omega^2 M_3(t)x^2\right]\right\},\end{aligned} \tag{A.8}$$

where $\mu \equiv \sqrt{\gamma^2 - \omega^2}$, $\Lambda_t \equiv 1 - \mathrm{e}^{-2\mu t}$. By integrating as in (A.4), we finally get

$$\begin{aligned}\tilde{\rho}_t^{k_0 x_0,\epsilon\eta}(k, x) &= \frac{1}{\pi\sqrt{\epsilon\eta}}\, \mathrm{e}^{-\frac{1}{\epsilon}[k_0 - \frac{\mathrm{e}^{-(\gamma-\mu)t}\Lambda_t}{2\mu}((\mu\coth\mu t+\gamma)k - m\omega^2 x)]^2}\\ &\quad\times\mathrm{e}^{-\frac{1}{\eta}[x_0 - \frac{\mathrm{e}^{-(\gamma-\mu)t}\Lambda_t}{2\mu}((\mu\coth\mu t-\gamma)x+\frac{k}{m})]^2}\\ &\quad\times\mathrm{e}^{-\frac{k_B T}{2\hbar^2 m\omega^2}[M_1(t)k^2+\frac{2m\omega^2}{\gamma}M_2(t)kx+m^2\omega^2 M_3(t)x^2]},\end{aligned} \tag{A.9}$$

where

$$\begin{aligned}M_1(t) &= -\frac{1}{\mu^2}[(\mathrm{e}^{-2\gamma t}\cosh 2\mu t - 1)\gamma^2 + \Gamma_t\omega^2 + \mathrm{e}^{-2\gamma t}\sinh 2\mu t\gamma\mu]\\ &\quad - \frac{\hbar^2}{16k_B^2 T^2\mu^2}[4(\mathrm{e}^{-2\gamma t}\cosh 2\mu t - 1)\gamma^4 - 3(\mathrm{e}^{-2\gamma t}\cosh 2\mu t - 1)\gamma^2\omega^2\\ &\quad + \Gamma_t\omega^4 + 4\,\mathrm{e}^{-2\gamma t}\sinh 2\mu t\gamma^3\mu - \mathrm{e}^{-2\gamma t}\sinh 2\mu t\,\gamma\omega^2\mu]\\ M_2(t) &= \frac{\gamma^2}{2\mu^2}\,\mathrm{e}^{-2(\gamma-\mu)t}\Lambda_t^2 + \frac{\hbar^2\gamma^2}{16k_B^2 T^2\mu^2}[2(\mathrm{e}^{-2\gamma t}\cosh 2\mu t - 1)\gamma^2\\ &\quad - (\mathrm{e}^{-2\gamma t} + \mathrm{e}^{-2\gamma t}\cosh 2\mu t - 2)\omega^2 + 2\,\mathrm{e}^{-2\gamma t}\sinh 2\mu t\,\gamma\mu]\\ M_3(t) &= \frac{1}{\mu^2}[-(\mathrm{e}^{-2\gamma t}\cosh 2\mu t - 1)\gamma^2 - \Gamma_t\omega^2 + \mathrm{e}^{-2\gamma t}\sinh 2\mu t\,\gamma\mu]\\ &\quad - \frac{\hbar^2\omega^2}{16k_B^2 T^2\mu^2}[(\mathrm{e}^{-2\gamma t}\cosh 2\mu t - 1)\gamma^2 + \Gamma_t\omega^2 + \mathrm{e}^{-2\gamma t}\sinh 2\mu t\,\gamma\mu].\end{aligned} \tag{A.10}$$

Taking the limits $\epsilon \to 0$ and $\eta \to 0$, we obtain (31).

Let us also explain why we employed the Wigner function. In the position representation, $\rho_t(q_1, q_2) = \langle q_1|\rho_t|q_2\rangle$, (4) is

$$\frac{\partial \rho_t(q_1, q_2)}{\partial t} = \left[\frac{\mathrm{i}\hbar}{2m}\left(\frac{\partial^2}{\partial q_1^2} - \frac{\partial^2}{\partial q_2^2}\right) - \frac{\mathrm{i}}{\hbar}(V(q_1) - V(q_2)) - \frac{2\gamma m k_B T}{\hbar^2}(q_1 - q_2)^2 + \frac{\hbar^2\gamma}{8mk_BT}\left(\frac{\partial}{\partial q_1} - \frac{\partial}{\partial q_2}\right)^2 - \gamma(q_1 - q_2)\left(\frac{\partial}{\partial q_1} - \frac{\partial}{\partial q_2}\right)\right]\rho_t(q_1, q_2) \quad \text{(A.11)}$$

Since this equation is second order in q_1, q_2 and their derivatives, we can propose a Gaussian ansatz, $\rho_t(q_1, q_2) = \exp\{-c_1q_1^2 - c_2q_1q_2 - c_3q_2^2 - \mathrm{i}c_4q_1 - \mathrm{i}c_5q_2 - c_6\}$, without using the characteristic function associated with the Wigner function. This will lead to a set of coupled differential equations which are nonlinear due to the double derivative terms, e.g.

$$\frac{\partial^2}{\partial q_1^2}\rho_t(q_1, q_2) = [(-2c_1q_1 - c_2q_2 - \mathrm{i}c_4)^2 - 2c_1]\rho_t(q_1, q_2). \quad \text{(A.12)}$$

Thus they will be much more cumbersome to solve compared to those we solve for the Wigner function.

In short, any equation of the form (A.11) that contains double derivatives leads to a nonlinear system of differential equations for c_i when we employ a Gaussian ansatz. This is the basic reason for using the characteristic function associated with the Wigner function to solve the evolution problem, where we solve a linear system of differential equations for c_i. See appendix C for more discussions.

Appendix B. The free particle as the limit of the harmonic oscillator

Note that the harmonic oscillator Hamiltonian gives the free particle Hamiltonian in the $\omega \to 0$ limit, so we expect the Green's function and the density matrix of the harmonic oscillator to converge to those of the free particle in this limit. Thus, one can obtain the results for the free particle by first solving the problem for the harmonic oscillator and then taking the said limit. In our strategy, we will rather use this correspondence as an independent check of our results. Using Taylor series, we can expand $M_i(t)$ around $\omega = 0$. After some lengthy calculations, one obtains

$$\begin{aligned} M_1(t) &= \frac{t\gamma(h^2\beta^2\gamma^2 + 4) - (3 - 4\,\mathrm{e}^{-2t\gamma} + \mathrm{e}^{-4t\gamma})}{4\gamma^2}\omega^2 + \mathcal{O}(\omega^4) \\ M_2(t) &= \frac{1}{2}\Gamma_t^2 + \mathcal{O}(\omega^2) \\ M_3(t) &= (1 - \mathrm{e}^{-4\gamma t}) + \mathcal{O}(\omega^2). \end{aligned} \quad \text{(B.1)}$$

Note also that $\mu \to \gamma$ in the vanishing ω limit. Then, it is trivial to recover (15) by inserting the above expressions into (A.9) and taking the $\omega \to 0$ limit.

Appendix C. The most general case for the Gaussian ansatz

In this appendix, we discuss the most general equation for which the Gaussian ansatz can be employed.

Gaussian ansatz is applicable to any equation of the form

$$\frac{\partial f_t(k,x)}{\partial t} = \left[A + Bk + Cx + D\frac{\partial}{\partial k} + E\frac{\partial}{\partial x} + Fk^2 + Gkx + Hx^2 + Lk\frac{\partial}{\partial k}\right.$$
$$\left. + Mk\frac{\partial}{\partial x} + Nx\frac{\partial}{\partial k} + Px\frac{\partial}{\partial x} + Q\frac{\partial^2}{\partial k^2} + R\frac{\partial^2}{\partial k\partial x} + S\frac{\partial^2}{\partial x^2}\right] f_t(k,x). \quad \text{(C.1)}$$

We argued in appendix A that we have to solve a nonlinear system of differential equations unless $Q, R, S = 0$. One special case we can avoid nonlinearity is when $F, G, H = 0$. In that case, we can Fourier transform f in both k and x, and since the Fourier transform converts differentiation into multiplication, we do not have second-order derivatives in the transformed equation. A single Fourier transformation can also be useful when $F, R, S = 0$ and $Q \neq 0$, or $H, Q, R = 0$ and $S \neq 0$. Roy and Venugopalan successfully use this approach in [11] to solve the time evolution of the harmonic oscillator density matrix for the non-Lindblad master equation, after certain change of coordinates in the position representation. However, if the 'minimally invasive' term is introduced (which they do not attempt to do), their method cannot avoid having a second-order derivative. For the rest of our discussion, we will set $Q, R, S = 0$ and use the shorthand notation

$$\frac{\partial f_t(k,x)}{\partial t} = \mathcal{D}(A, B, C, D, E, F, G, H, L, M, N, P) f_t(k,x). \quad \text{(C.2)}$$

When we propose a Gaussian ansatz of the form (A.2), we reach the following system of coupled linear equations:

$$\begin{pmatrix} \dot{c}_1(t) \\ \dot{c}_2(t) \\ \dot{c}_3(t) \\ \dot{c}_4(t) \\ \dot{c}_5(t) \\ \dot{c}_6(t) \end{pmatrix} = \begin{pmatrix} 2L & M & 0 & 0 & 0 & 0 \\ 2N & L+P & 2M & 0 & 0 & 0 \\ 0 & N & 2P & 0 & 0 & 0 \\ -2\mathrm{i}D & -\mathrm{i}E & 0 & L & M & 0 \\ 0 & -\mathrm{i}D & -2\mathrm{i}E & N & P & 0 \\ 0 & 0 & 0 & \mathrm{i}D & \mathrm{i}E & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \end{pmatrix} + \begin{pmatrix} -F \\ -G \\ -H \\ \mathrm{i}B \\ \mathrm{i}C \\ -A \end{pmatrix}. \quad \text{(C.3)}$$

This is a system of inhomogeneous ordinary linear differential equations which can be solved by basic methods, but the dimension of the matrix makes the solution intractable from a calculational point of view, even for mathematical software packages.

The first observation that makes the calculation considerably easier is that c_1, c_2, c_3 form an independent system of equations. This means, we can first solve for these three, then insert the solutions into the equations for c_4 and c_5 and solve the inhomogeneous equations for these two variables. We can finally insert c_4, c_5 into the equation for c_6 and find the solution by simple integration. This approach is tractable for Mathematica©, but the solutions are rather lengthy and give us little insight.

The crucial step that simplifies (C.3) is that by an affine transformation of the variables k, x in (C.1), we can set the coupling terms D, E, M, N to 0 for most cases, and have a diagonal matrix in (C.3). Let us define the variables l, y such that

$$k = l + ay \qquad x = bl + y, \quad \text{(C.4)}$$

which together with the scaling and swapping ($k \leftrightarrow x$) can account for all linear transformations. This leads to the equation

$$\frac{\partial f_t^{(ly)}(l,y)}{\partial t} = \mathcal{D}(A', B', C', D', E', F', G', H', L', M', N', P') f_t^{(ly)}(l,y) \quad \text{(C.5)}$$

with

$$M' = \frac{1}{1-ab}(-bL + M - b^2N + bP)$$
$$N' = \frac{1}{1-ab}(aL - a^2M + N - aP). \tag{C.6}$$

By choosing

$$a = \frac{(L-P) + \sqrt{(L-P)^2 + 4MN}}{2M}$$
$$b = \frac{-(L-P) - \sqrt{(L-P)^2 + 4MN}}{2N} \tag{C.7}$$

if M and N are both nonzero, and

$$a = 0 \qquad b = \frac{M}{L-P} \tag{C.8}$$

if $N = 0$ (the case of $M = 0$ is similar), we can set M' and N' to 0. The signs of the roots of the quadratics are chosen such that $ab \neq 1$, which ensures the linear independence of l and y. Note that this procedure cannot be used if $MN = 0$ and $L = P$.

Once we set $M', N' = 0$, given that L' and P' are nonzero, we can shift our variables as

$$m \equiv l + \frac{D'}{L'} \qquad z \equiv y + \frac{E'}{P'}, \tag{C.9}$$

which puts our equation into the form

$$\frac{\partial f_t^{(mz)}(m,z)}{\partial t} = \mathcal{D}(A'', B'', C'', 0, 0, F', G', H', L', 0, 0, P') f_t^{(mz)}(m,z). \tag{C.10}$$

This equation leads to six inhomogeneous ordinary differential equations which are not coupled and thus can be solved quite easily. One can further simplify the equations if $F' \neq 0$, by scaling $k \rightarrow \sqrt{F'}k$ to set the coefficient of the k^2 term to 1. By defining the function $\tilde{f}_t^{(mz)} = f_t^{(mz)} \mathrm{e}^{A''t}$, the constant term A'' can also be set to 0.

The special cases we did not discuss, e.g. $MN = 0$ and $P = L$, can also be handled using similar techniques. Above transformations do not work when certain coefficients vanish or are equal to each other in (C.1), e.g $N = 0$ and $P = L$. In these cases, solving (C.3) is already much easier before any affine transformation of the arguments of f. In short, using a Gaussian ansatz allows us to solve any equation in the form of (C.1) without much trouble, as long as no nonlinear terms arise.

References

[1] Caldeira A O and Leggett A J 1983 *Physica* A **121** 587–616
[2] Weiss U 1999 *Quantum Dissipative Systems* 2nd edn (Hackensack, NJ: World Scientific)
[3] Vacchini B 2001 *Phys. Rev.* E **63** 066115
[4] Petruccione F and Vacchini B 2005 *Phys. Rev.* E **71** 046134
[5] Schramm P and Grabert H 1987 *J. Stat. Phys.* **49** 767
[6] Grabert H, Schramm P and Ingold G-L 1988 *Phys. Rep.* **168** 115
[7] Halliwell J and Zoupas A 1995 *Phys. Rev.* D **52** 7294
[8] Presilla C, Onofrio R and Patriarca M 1997 *J. Phys. A: Math. Gen.* **30** 7385
[9] Isar A, Sandulescu A and Scheid W 1993 *J. Math. Phys.* **34** 3887–900
[10] Karrlein R and Grabert H 1997 *Phys. Rev.* E **55** 153–64
[11] Roy S M and Venugopalan A 1999 arXiv:quant-ph/9910004v1
[12] Spiller T P, Garraway B M and Percival I C 1993 *Phys. Lett.* A **179** 63
[13] Hakim V and Ambegaokar V 1985 *Phys. Rev.* A **32** 423

[14] Thorwart M, Reimann P and Hänggi P 2000 *Phys. Rev.* E **62** 5808
[15] Patriarca M 1996 *Nuovo Cimento* B **111** 61
[16] Haake F and Reibold R 1985 *Phys. Rev.* A **32** 2464
[17] Unruh W G and Zurek W H 1989 *Phys. Rev.* D **40** 1071
[18] Haake H 1991 *Phys. Rev.* A **44** 2314
[19] Ambegaokar V 1991 *Ber. Bunsenges. Phys. Chem.* **95** 400
[20] Lindblad G 1975 *Commun. Math. Phys.* **40** 147
[21] Lindblad G 1976 *Commun. Math. Phys.* **48** 119
[22] Diosi L 1993 *Europhys. Lett.* **22** 1
[23] Diosi L 1993 *Physica* A **199** 517
[24] Breuer H P and Petruccione F 2007 *The Theory of Open Quantum Systems* (Oxford: Oxford University Press)
[25] Landau L D and Lifshitz E M 1984 *Statistical Physics (Part 1)* (Oxford: Butterworth-Heinemann)
[26] Bassi A, Ippoliti E and Vacchini B 2005 *J. Phys. A: Math. Gen.* **38** 8017–38
[27] Joos E, Zeh H D, Kiefer C, Giulini D, Kupsch J and Stamatescu I-O 2003 *Decoherence and the Appearance of a Classical World in Quantum Theory* 2nd edn (Berlin: Springer)
[28] Paz J P and Zurek W H 1999 *Phys. Rev. Lett.* **82** 5181