On the von Neumann entropy of a bath linearly coupled to a driven quantum system

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Abstract
The change of the von Neumann entropy of a set of harmonic oscillators initially in thermal equilibrium and interacting linearly with an externally driven quantum system is computed by adapting the Feynman–Vernon influence functional formalism. This quantum entropy production has the form of the expectation value of three functionals of the forward and backward paths describing the system history in the Feynman–Vernon theory. In the classical limit of Kramers–Langevin dynamics (Caldeira–Leggett model) these functionals combine to three terms, where the first is the entropy production functional of stochastic thermodynamics, the classical work done by the system on the environment in units of $k_B T$, and the second and the third other functionals which have no analogue in stochastic thermodynamics.

1. Introduction
The goal of this article is to present a calculation of the change of the von Neumann entropy of a bath interacting with a quantum system between two measurements on the system. The system is described by a general non-relativistic Hamiltonian $H_S = \frac{p^2}{2M} + V(X, t)$ (no spin) with a time-dependent drive $V$, and the bath is modeled as a set of harmonic oscillators initially in thermal equilibrium, and linearly coupled to the system. The calculation is done by adapting the Feynman–Vernon approach [1].

The problem is of interest in two contexts. The first is stochastic thermodynamics [2–4], where the fundamental quantity is $\delta S_{\text{env}}$, the (classical) entropy production in the environment which is a functional of the system history. Mathematically, this quantity can be defined as the log-ratio of transition probabilities in a forward and a reversed process [5–7]. Physically, a heat bath is however an idealization of a large environment relaxing on a much faster time scale than the system of interest, and Clausius’ formula gives $\delta Q = T \delta S_{\text{env}}$ where $\delta Q$ is the energy (heat) transferred from the system to the bath. For standard physical kinetics without memory (master equations, diffusion equations) the two definition of $\delta S_{\text{env}}$ through $\delta Q$ or through the log-ratio agree [8–10], which directly implies the far-from-equilibrium fluctuation relations for physical quantities such as work [11–13].

Potential extensions of statistical thermodynamics and fluctuation relations to the quantum domain have been extensively investigated, and reviewed in [14, 15]. However, with the exception of the Jarzynski equality and Crooks’ fluctuation theorem in closed quantum systems [16], the results obtained to date lack the generality and simplicity of fluctuation relations in classical systems [17–21]. A core difficulty is that even properly defining quantum versions of heat, work and the entropy production in the environment is non-trivial since these are not standard quantum operators: according to the original proposal work in a closed quantum system depends on two measurements [16], while in a recent proposal involving only one measurement [22], a second system is needed to keep track of the work distribution. Hence the interest of studying what is arguably the most natural
extension of entropy production to the quantum domain, namely the change of the von Neumann entropy of the bath. To stress the connection to stochastic thermodynamics we will from here on denote this quantity $\Delta S_B$. The proposal to use a quantity equivalent to $\Delta S_B$ was introduced in [23], and more recently investigated in [24].

The second context where the calculations in this paper are of interest is quantum information theory where the von Neumann entropy is a measure of the amount of entanglement between a system and its environment [25, 26]. Using known inequalities we can then show that the absolute value of the change of von Neumann entropy of the bath is a lower bound of the entanglement created between a system and the bath on the one hand, and the rest of the world including the measurement apparatus on the other. As this discussion falls somewhat outside the main line of the argument of the paper it is presented separately in appendix C.

In the Feynman–Vernon method the bath is taken to consist of harmonic oscillators initially in thermal equilibrium and linearly coupled to the system, which allows for integrating out the bath. As a result $\Delta S_B$ can be written as the (quantum) expectation value of three functionals of the system history, similar but not identical to the real and imaginary actions $S_i$ and $S_f$ in the Feynman–Vernon theory. In the classical limit of a Brownian particle, where the system development is described by a Kramers–Langevin equation [27], these expectation values combine to three averages over the (classical) stochastic process, which will call $\Delta S_{\text{env}}$, $\Delta S_{\text{var}}$ and $\Delta S_B$. $\Delta S_{\text{env}}$ is the average over the process and over a finite time of $\Delta S_{\text{env}}$, the standard entropy production functional in stochastic thermodynamics. By Clausius’ formula and for Kramers–Langevin dynamics $\Delta S_{\text{env}}$ equals $\beta (\delta Q_{\text{friction}} + \delta Q_{\text{noise}})$ where $\delta Q_{\text{friction}}$ and $\delta Q_{\text{noise}}$ are the amounts of energy (heat) transmitted from the system to the bath by respectively the friction force and the random force. $\Delta S_{\text{var}}$ and $\Delta S_B$ are also averages over the same stochastic process, but which have no analogues in standard stochastic thermodynamics. In the case that the coupling strength between the bath and the system is constant $\Delta S_B$ only depends on the (classical) transition probability over a finite time interval, and is then not a proper functional, but more akin to a change of state. As will be discussed below, $\Delta S_B$ is also in other respects very different from what one expects for (classical) entropy production.

The paper is organized as follows: in section 2 we define $\Delta S_B$, equation (1), and show how to express it as a quantum expectation value, equations (3) and (4). In section 3 we introduce the Feynman–Vernon formalism and use it to give an expression for the expectation value, equation (12). In section 4 we evaluate this expression and in parallel give standard results of the Feynman–Vernon theory. The three functionals mentioned above then appear in equations (15) and (16). In section 5 we introduce the Caldeira–Leggett limit of the Feynman–Vernon model which leads to classical dynamics with noise and friction; the limit of the three functionals is given in equation (17). In section 6 we analyze the three functionals in this limit and separate out $\Delta S_B$, and in section 7 we group the remaining parts into $\Delta S_{\text{env}}$ and $\Delta S_{\text{var}}$. For completeness we also give, in section 6, a derivation of the Caldeira–Leggett result that the Wigner transform of the Feynman–Vernon propagator for the density matrix goes to the transition probability of the (classical) stochastic process. In section 8 we consider $\Delta S_B$ in the limit of weak coupling between the system and the bath, and in section 9 we sum up and discuss our results. In appendices A and B we discuss for completeness the time scales involved and higher-order corrections to the Caldeira–Leggett limit, and in appendix C we give the second context in which this work is relevant, as outlined above.

2. The first-order change of von Neumann entropy

We consider the setting where a quantum system is prepared in an initial pure state $|i\rangle$ at time $t_i$ and then attached to a bath with density operator $\rho^B_{\text{eq}}$ describing a state of thermal equilibrium. Over a time period $[t_i, t_f]$ the system and the bath develop while interacting such that the total state at time $t_f$ is $\rho^{\text{TOT}}_{t_f}$. At this point a measurement is made of an operator $O$ which depends on the system variables only, with outcome $\rho^B_{\text{eq}}$ corresponding to the pure state $|f\rangle\langle f|$ of the system. This happens with probability $P_f = \text{Tr}_B [\rho^{\text{TOT}}_{t_f} | f\rangle\langle f|]$. By the measurement postulate the total state after the measurement is $\rho^{\text{TOT}}_{t_f} = \frac{1}{P_f} | f\rangle\langle f| \otimes \rho^{\text{TOT}}_{t_f} | f\rangle\langle f|$, and we can therefore identify the density operator of the bath, after interacting with the system and after the measurement has been performed on the system, as $\rho^B_f = \frac{1}{P_f} | f\rangle\langle f|$. We assume $\delta \rho^B_f = \rho^B_f - \rho^B_{\text{eq}}$ to be small, and the first-order change of the bath entropy is then

$$\Delta S_B = \delta \left( \text{Tr}_B \left[ -\rho^B \log \rho^B \right] \right) = \text{Tr}_B \left[ -\delta \rho^B \log \rho^B_{\text{eq}} \right].$$

(1)
In a basis of energy eigenstates $|n⟩ = |n_1, n_2, \ldots⟩$ the density operator $\rho_B^{\text{eq}}$ is diagonal with elements

$$\langle n | \rho_B^{\text{eq}} | n⟩ = \prod_b e^{-\beta (E_b - F_b(\beta))}$$

where $E_b(n_b)$ is the energy of the $b$th degree of freedom of the bath in state $n_b$, and $F_b$ is its free energy at inverse temperature $\beta$. Therefore, we can write (1) as

$$\beta \sum_b \rho_b^{\text{eq}} = \beta \left[ \text{Tr}_B \left[ H_B^0 \rho_B^{\text{eq}} \right] - \text{Tr}_B \left[ H_B^0 \rho_B^{\text{eq}} \right] \right]$$

where $H_B$ is the Hamiltonian of the bath. Equation (2) has the form of Clausius’ formula. This is in contrast to the change of the von Neumann entropy of the system where there is no definite relation to a heat flow [28]. For computation it is more convenient to alternatively write (1) as

$$\delta \beta \rho_B^{\text{eq}} = -\beta \frac{d}{de} \log R_\beta(e) \bigg|_{e=0} - \beta \sum_b U_b(\beta),$$

where $U_b(\beta) = \frac{m_b}{2} \coth \left( \frac{m_b \beta h}{2} \right)$ is the internal energy of oscillator $b$, and

$$R_\beta(e) = \text{Tr}_B \left[ \langle f | \rho_B^{\text{tot}} | f \rangle e^{-e H_B} \right].$$

Note that $R_\beta(0) = P_\beta$. Equations (3) and (4) are the starting point of our analysis.

3. **The Feynman–Vernon method**

The Feynman–Vernon theory is a means to compute $P_\beta$ while we need to compute the slightly more complex quantity $R_\beta(0)$. Let us begin by noting that the time development of an open quantum system is described by a superoperator or quantum map $\Phi$ which maps density operators to density operators, and which can always be realized by adding another system or ancilla in state $\rho_a$, acting unitarily on the combined system and ancilla, and then tracing out the ancilla $\Phi \rho_a \rho \rho_a \oplus U^\dagger \rho$. The Feynman–Vernon approach consist in writing the two unitary operators $U$ and $U^\dagger$ as path integrals while taking the ancilla to be a bath of harmonic oscillators initially in thermal equilibrium, linearly coupled to the system. The total Hamiltonian describing the system and ancilla is thus

$$H = H_S(X, P, t) - X \sum_b C_b x_b + \sum_b \frac{P_b^2}{2 m_b} + \frac{m_b \omega_b^2}{2} x_b^2,$$

where $C_b$ is the strength of the interaction between the system and bath oscillator $b$. Integrating out the bath gives $\Phi$ in the coordinate representation as

$$\left[ \Phi \rho(t_i) \right] \left( X^f, Y^f \right) = \rho \left( X^f, Y^f, t_f \right)$$

$$= \int dX^i dY^i K \left( X^f, Y^f, t_f; X^i, Y^i, t_i \right) \rho \left( X^i, Y^i, t_i \right)$$

and the transition probability as

$$P_{if} = \int dX^i dY^i dX^f dY^f \psi_i \left( X^i \right) \psi_f^* \left( Y^i \right) K \left( X^f, Y^f, t_f; X^i, Y^i, t_i \right),$$

where $\psi_i$ and $\psi_f$ are the initial and final states in the coordinate representation and $K$ is the Feynman–Vernon propagator of the density operator of the system [1]. The first step in computing $K$ is the path integrals over the bath in $U \left( \rho \oplus \rho_a \right) U^\dagger$ with fixed initial and final position of each bath oscillator. The result of these path integrals is $K_b \left( q_f, q_i, t_f, t_i; X \right) K_b^* \left( q_f', q_i', t_f, t_i; Y \right)$ where the $K_b$’s are propagators of harmonic oscillators with linear terms in the action, $\int X \left( s \right) C_b x_b \left( s \right)$ for the forward path, and $\int Y \left( s \right) C_b y_b \left( s \right)$ for the backward path. The second step is to introduce a coordinate representation of the equilibrium density operator of the bath oscillator, proportional to the propagator in imaginary time. Integrating out the four positions $q_f, q_i, q_f'$ and $q_i'$ then gives the Feynman–Vernon influence functional $P_b \left[ \left( X \left( s \right), Y \left( s \right) \right) \right]$ as a four-dimensional integral.
where \( Z_b = \left( 2 \sinh \left( \frac{\alpha_b \epsilon}{2} \right) \right)^{-1} \) is the partition function of \( b \) at inverse temperature \( \beta \), and the delta function is the coordinate representation of the trace over the final state of \( b \). The Feynman–Vernon propagator can then be written as double path integral over the system variables only
\[
K = \int D X D Y e^{i \left( S_b(X) - S_b(Y) \right)} \prod_b F_b.
\]

A comparison between (4) on the one hand and (7) and (8) on the other shows that the only difference is the presence in (4) of a second heat kernel with time parameter \( \epsilon \). Writing this kernel in the coordinate representation means that to compute the first-order change of the von Neumann entropy of the bath we need
\[
R_\epsilon^{(e)} = \int dX' dY' dX' dY' \psi_f(X') \psi_f^*(X') \psi_f(Y) \psi_f^*(Y) = \int D X D Y e^{i \left( S_b(X) - S_b(Y) \right)} \prod_b F_b.
\]

Differentiating with respect to parameter \( \epsilon \) inside the path integral and then setting it to zero gives
\[
R_\epsilon^{(e)}(0) = \int dX' dY' dX' dY' \psi_f(X') \psi_f^*(X') \psi_f(Y) \psi_f^*(Y) = \int D X D Y e^{i \left( S_b(X) - S_b(Y) \right)} \prod_b \frac{d}{d \epsilon} \left( \sum_b \log F_b \right)_{\epsilon=0}.
\]

Comparing to (9) we see that \( R_\epsilon^{(e)}(0) \) is the matrix element between initial and final states of an expectation value, with respect to the Feynman–Vernon propagator, of the functional \( \frac{d}{d \epsilon} \left( \sum_b \log F_b \right)_{\epsilon=0} \), which is to be determined.

**4. Evaluating the entropy production functional**

The propagator of a harmonic oscillator is the exponential of terms constant, linear and quadratic in the initial and final position. Integrating out these initial and final positions means a four-dimensional Gaussian integral for each bath oscillator, and the modified influence functional is therefore
\[
F_b = \int dq \frac{1}{Z_b(\beta)} K_b \left( q_i, 0, q_j, 0, i \beta \hbar; 0 \right) \delta \left( q_f - q'_f \right)
\times K_b \left( q_f, t_f, q_i, t_i; X \right) K_b^* \left( q'_f, t_f, q_i, t_i; Y \right),
\]

where \( Z_b = \left( 2 \sinh \left( \frac{\alpha_b \epsilon}{2} \right) \right)^{-1} \) is the partition function of \( b \) at inverse temperature \( \beta \), and the delta function is the coordinate representation of the trace over the final state of \( b \). The Feynman–Vernon propagator can then be written as double path integral over the system variables only
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\]

Differentiating with respect to parameter \( \epsilon \) inside the path integral and then setting it to zero gives
\[
R_\epsilon^{(e)}(0) = \int dX' dY' dX' dY' \psi_f(X') \psi_f^*(X') \psi_f(Y) \psi_f^*(Y) = \int D X D Y e^{i \left( S_b(X) - S_b(Y) \right)} \prod_b \frac{d}{d \epsilon} \left( \sum_b \log F_b \right)_{\epsilon=0}.
\]

Comparing to (9) we see that \( R_\epsilon^{(e)}(0) \) is the matrix element between initial and final states of an expectation value, with respect to the Feynman–Vernon propagator, of the functional \( \frac{d}{d \epsilon} \left( \sum_b \log F_b \right)_{\epsilon=0} \), which is to be determined.
and the vector $y$ and the matrix $M(\epsilon)$, respectively given by

$$
\begin{pmatrix}
\frac{C}{\sin \omega t} \int_{t_f}^{t_i} ds \sin \omega (t_f - s) X(s) \\
\frac{-C}{\sin \omega t} \int_{t_f}^{t_i} ds \sin \omega (t_f - s) Y(s) \\
\frac{C}{\sin \omega t} \int_{t_f}^{t_i} ds \sin \omega s X(s) \\
\frac{-C}{\sin \omega t} \int_{t_f}^{t_i} ds \sin \omega s Y(s)
\end{pmatrix}
$$

and

$$
\begin{pmatrix}
\frac{1}{i} \cot \omega t + \coth \omega \beta \hbar \quad -\sinh^{-1} \omega \beta \hbar \\
-\sinh^{-1} \omega \beta \hbar & \frac{1}{i} \cot \omega t + \cosh \omega \beta \hbar \quad 0 \\
-\sinh^{-1} \omega \beta \hbar & i \cot \omega t + \coth \omega \beta \hbar \\
0 & -i \sinh^{-1} \omega \beta \hbar & \frac{1}{i} \cot \omega t + \coth \omega \beta \hbar
\end{pmatrix}.
$$

The pre-factors of the exponential in (13), including the square root of the determinant $(\det M(\epsilon))^{-\frac{1}{2}}$, combine to $\sinh\left(\frac{\omega \beta \hbar}{2}\right) \sinh^{-1}\left(\frac{\omega \beta \hbar}{2}(\beta + \epsilon)\right)$ which contributes to the derivative $\frac{d}{d\epsilon} F_{b,i=0}^+ \frac{\partial M}{\partial \epsilon}$ a term $\frac{\omega \hbar}{2} \coth \omega \beta \hbar$. In this term we recognize the internal energy of a harmonic oscillator at temperature $\beta^{-1}$, which therefore cancels with the term $U_0$ in (3). Writing $M_{\beta^{-1}}^+ (0)$ for $\frac{d}{d\epsilon} M(\epsilon)_{i=0}$, the quantity sought is thus

$$
\frac{\partial S_y}{\partial \epsilon} = \frac{1}{P_{yf}} \int dX'dY'dX'Y' dY' \psi_i(X') \psi_i^* (Y') \psi_f(X) \psi_f^* (Y) 
\times DXDY \exp\left[k_S^+ (X) - k_S (Y)\right] \prod_b \int_{-\beta}^{\beta} \frac{d\hbar \omega}{2m_b \omega \hbar} \left\{ u_b M_{\beta^{-1}}^+ (0) \right\} u_b.
$$

Equation (14) is the first result of this paper giving the entropy production in the bath between two measurements on the system as the expected value of a functional of the forward and backward system paths, divided by the transition probability. To proceed further we note that the product $\prod_b F_b$, which is $e^{\sum_b \left( \omega \omega \hbar \right)_{b} u_b M_{\beta^{-1}}^+ (0) \omega \omega \hbar}$, can be written as $e^{k_S^+ - k_S}$ defining the real and imaginary parts of the Feynman–Vernon influence action [1, 27]. These are quadratic functionals of the paths of the system

$$
S_i = \int_{t_i}^{t_f} \int_{t_i}^{t_f} (X - Y)(X' - Y') k_i(s - s') ds'ds', \\
S_r = \int_{t_i}^{t_f} \int_{t_i}^{t_f} (X - Y)(X' - Y') k_r(s - s') ds'ds',
$$

where we write $X$ and $Y$ for quantities at time $s$ and $X'$ and $Y'$ for quantities at the earlier time $s'$, and where the kernels are

$$
k_i(s - s') = \sum_b \frac{G_b^2}{2m_b \omega_b} \sin \omega_b (s - s'), \\
k_r(s - s') = \sum_b \frac{G_b^2}{2m_b \omega_b} \coth \left( \frac{\beta \hbar \omega_b}{2} \right) \cos \omega_b (s - s').
$$

The analysis leading to the explicit forms of $S_i$ and $S_r$ is based on repeated use of trigonometric identities and rewriting the double integrals. By similar steps the functional in (14) can be evaluated to $I^{(1)} [X, Y] + I^{(2)} [X, Y] + I^{(3)} [X, Y]$ where

$$
I^{(1)} = \int_{t_i}^{t_f} \int_{t_i}^{t_f} (X - Y)(X' - Y') h^{(1)}(s - s') ds'ds, \\
I^{(2)} = \int_{t_i}^{t_f} \int_{t_i}^{t_f} (XY' - XX') h^{(2)}(s - s') ds'ds, \\
I^{(3)} = \int_{t_i}^{t_f} \int_{t_i}^{t_f} (XY' + XX') h^{(3)}(s - s') ds'ds.
$$

(15)
with the kernels

\[
\begin{align*}
\mathcal{h}^{(1)} &= -\sum_b \beta C_b^2 \frac{\sinh^{-1} \left( \frac{\beta \hbar \eta b}{2} \right)}{4m_b} \cos \omega_b (s-s'), \\
\mathcal{h}^{(2)} &= i \sum_b \beta C_b^2 \frac{\operatorname{coth} \left( \frac{\beta \hbar \eta b}{2} \right)}{2m_b} \sin \omega_b (s-s'), \\
\mathcal{h}^{(3)} &= \sum_b \beta C_b^2 \frac{\cos \omega_b (s-s')}{2m_b}.
\end{align*}
\] 

Equations (15) and (16) is the second result of this paper. We note that while \( I^{(1)} \) equals \(-\frac{1}{\hbar} \beta \partial_{\beta} S_i \), \( I^{(2)} \) and \( I^{(3)} \) are new and non-causal terms, i.e. which do not fulfill general property 5 of influence functionals as discussed on pp 126–127 in [1]. We further note that \( I^{(1)} \) goes to zero in the low-temperature limit, while \( I^{(2)} \) and \( I^{(3)} \) diverge as \(-\frac{1}{k_B T}\).

5. The Caldeira–Leggett limit

The classical limit of the Feynman–Vernon theory was computed in [27]. The spectrum of the bath oscillators is then first assumed continuous with density \( f (\omega) \) such that \( f (\omega) C_{\omega}^2/\hbar m (\omega) \) equals \( \hbar \omega^2/2 \) up to some upper cut-off \( \Omega \). The parameter \( \eta \) has the dimension \( ML/T \) of a classical friction coefficient, and the first kernel in the Feynman–Vernon theory tends to \( k_i \approx -\eta \frac{d}{ds} \delta (s-s') \). The corresponding action \( S_i \) is a potential renormalization plus a term \(-\frac{1}{2} \int (X-Y)(X+Y) ds \). As a stochastic integral this finite part of \( S_i \) has to be interpreted in the post-point (anti-Itô) prescription since the time derivatives stem from the integral over \( s' \) up to \( s \). The other kernel Feynman–Vernon \( k_i \) has only small contributions for \(|\omega| > \frac{1}{\beta \hbar}\) and hence describes, if \( \Omega \) is large enough, a memory kernel of width \( \beta \hbar \), independently of \( \Omega \).

Similarly to \( k_i \), the \( h^{(3)} \) kernel in (16) tends to \(-\hbar \eta \frac{d^2}{ds} \delta (s-s')\) and the \( h^{(3)} \) term in (15) therefore tends to \( \hbar \eta \int \dot{X} \dot{Y} \). This has the physical meaning of \(-\hbar \eta \int \dot{v}^2 \) if \( \dot{X} \) and \( \dot{Y} \) can be approximated by a classical velocity \( v \). To a friction force \(-\eta v \) corresponds a reaction force \( \eta v \) from the system on the bath, and the work done by this force is \( \eta \int \dot{v}^2 \). The entropy production from \( I^{(3)} \) is therefore \( \beta \partial_{\beta} Q_{\text{friction}} \), where \( \delta Q_{\text{friction}} \) is the energy (heat) transferred from the system to the bath, as announced in introduction. When \( \beta \) is large (low temperature) the \( h^{(1)} \) kernel goes to zero and the \( h^{(2)} \) kernel tends to \( \hbar \eta \frac{d^2}{ds} \int \omega^2 \sin w (s-s') \). This integral is a representation of the principal value of \(-\frac{1}{\hbar} \), and the entropy production from \( I^{(2)} \) is therefore, up to boundary terms, in the low-temperature limit the functional \( \hbar \eta \int \dot{X} \dot{Y} \). If all times of interest in the system are longer than \( \beta \hbar \) then \( S_i \approx \frac{\hbar}{\beta \hbar} \int (X-Y)^2 ds \). The different time scales involved are briefly discussed in appendix A and possible higher-order corrections in appendix B. From here on we assume high temperature (small \( \beta \)); in this sense. The three terms in (15) then tend, up to boundary terms, to

\[
\begin{align*}
I^{(1)} &= -\frac{\eta}{\beta \hbar^2} \int^{t_f} (X-Y)^2 \, ds = -\frac{1}{\hbar} S_i, \\
I^{(2)} &= \frac{\eta}{\hbar} \int^{t_f} (\dot{X} \dot{Y} - X Y) \, ds, \\
I^{(3)} &= \beta \eta \int^{t_f} X Y \, ds.
\end{align*}
\]

The integral for \( I^{(2)} \) in (15) can be extended over the whole domain—i.e. \( \int^{t_f} \int^{t_f} (\cdots) ds' ds \)—and expanded around the diagonal \( (s = s') \). Contrary to the case of \( S_i \) there is therefore not any potential renormalization term from \( I^{(2)} \) in the Caldeira–Leggett limit. Furthermore, the limit of \( I^{(2)} \) given in (17) does not depend on the discretization scheme since the Itô contributions cancel. Therefore, we can alternatively write this term as
where

\[ \frac{2i}{\hbar} S_i^{(\text{mid})} = -i \hbar \int (X - Y)(X + Y) ds \]  \hspace{1cm} (19)

and

\[ \Delta S_b = \frac{i n}{\hbar} \int (XX - YY) ds \]  \hspace{1cm} (20)

and with the mid-point prescription for both terms. Consequently, we will interpret the term \( \Delta S_b \) as

\[ \frac{2i}{\hbar} \int \Delta \eta S_i^{(\text{mid})} (X, Y) ds \]  \hspace{1cm} (21)

If \( \eta \) would depend on time there would be corrections to (21) which will not be considered here.

6. Analysis of the classical limit

To further analyze the classical limit we use, as in [27], the Markov property of Feynman–Vernon propagator, in this limit. First it is convenient to introduce auxiliary variables

\[ \alpha = -\frac{Y}{X}, \quad \beta = \frac{q}{p} \]  \hspace{1cm} (22)

which we assume to be as for coherent states integrated against functions depending sufficiently weakly on phase space, i.e.

\[ \Phi^{(\alpha)}(\Delta \alpha) \approx \Phi^{(\alpha)}(\Delta \alpha) \]

and

\[ \Phi^{(\beta)}(\Delta \beta) \approx \Phi^{(\beta)}(\Delta \beta) \]

The quantum mechanical transition probability \( P_{ij} \) is then approximately

\[ P_{ij} \approx \frac{2i}{\hbar} \int \Delta \eta \Phi^{(\alpha)}(\Delta \alpha) \Phi^{(\beta)}(\Delta \beta) \]  \hspace{1cm} (23)

For a system with Hamiltonian

\[ H = \frac{p^2}{2M} + V(X) \]  \hspace{1cm} (24)

the short-time density matrix propagator, for \( \bar{K} \) and \( K \) is,

\[ \bar{K}_{i \Delta}(t) = \left( \frac{1}{2\pi \hbar \Delta s / M} \right)^{d/2} e^{-\frac{i \hbar \Delta q}{\Delta s / M} + \frac{1}{\Delta \alpha} \int \Delta q} \]

where \( \Delta q = q' - q \) and \( \Delta \alpha = \alpha' - \alpha \), the arguments on the left-hand side are understood and the contribution from \( S_i \) has been evaluated with the post-point prescription. The Chapman–Kolmogorov equation for \( K \) is, expanding in the increments

\[ \bar{K}(\cdot) = \int d\Delta q d\Delta \alpha K_{i \Delta}(t) \]

The integral over \( \Delta q \) of a term proportional to \( \Delta q^n \) in (26) gives, using (25),

\[ \left( \frac{1}{\Delta \alpha} \right)^n \delta^{(n)}(\Delta \alpha) \frac{\eta M}{\Delta s} \]

and when

\[ \frac{\eta M}{\Delta s} = \frac{\eta M}{\Delta s} - \frac{\eta M}{\Delta s} \]
integrated over $\Delta \alpha$ this gives zero unless $l = n$. Using $m = l = 0$, $m = 1$ and $l = 0$ and $m = l = 1$ equation (26) can hence be written

$$
\partial_t \tilde{K} = \left( -\frac{i}{\hbar} V' \left( \frac{\alpha - \alpha}{2} \right) + \frac{i}{\hbar} V \left( \frac{\alpha + \alpha}{2} \right) - \frac{n}{\beta \hbar^2} (\alpha)^2 \right) \tilde{K} - \frac{i}{\hbar} \partial_q^\alpha \tilde{K} - \frac{n}{\hbar} \alpha \partial_q \tilde{K}
$$

(27)

which is the quantum master equation derived in [27]. For the Wigner transform (27) gives

$$
\partial_t P = -\partial_p \left( \frac{P}{M} \right) + \frac{n}{\beta} \partial_{pp} P + \partial_q (V'(q) P) + \mathcal{O} (\hbar^2, V'').
$$

(28)

which is, up to terms of order $\hbar^2$, the Fokker–Planck equation of classical stochastic dynamics with friction coefficient $\eta$ [27]. We proceed to treat the three functionals in (17) in an analogous manner. Higher-order corrections to Fokker–Planck equation derived here (finite corrections) are briefly discussed in appendix B.

6.1. The $I^{(1)}$ contribution

At given initial and final positions of the system, $(q_i, \alpha_i)$ and $(q_f, \alpha_f)$, the path integrals in (14) give for the $I^{(1)}$ part

$$
\int \int ds \int dq \phi \phi (q_{j_f}, \alpha_f, q_i, \alpha_i, t_f, s) \left( -\frac{n}{\beta \hbar^2} \alpha^2 \right) \tilde{K} (q_i, \alpha_i, q_f, \alpha_f, s, t_i).
$$

Combining this with the integrals over initial and final positions and (23) and (24) we can write

$$
\int dq \phi \phi (q_{j_f}, \alpha_f, q_i, \alpha_i, t_f, s) \int \int dq \phi \phi (q_{j_f}, \alpha_f, q_i, \alpha_i, t_f, s) \left( -\frac{n}{\beta \hbar^2} \alpha^2 \right) \tilde{K} (q_i, \alpha_i, q_f, \alpha_f, s, t_i).
$$

The classical limit of the contribution of $\delta S Q$ from $I^{(1)}$ is therefore

$$
\int \int dq \phi \phi (q_i, \alpha_i, q_f, \alpha_f, s, t_i) \frac{n}{\beta} \partial_{pp} P (q_i, \alpha_i, q_f, \alpha_f, s, t_i).
$$

In section 7 below we show how this can be given an interpretation as an average $\delta S_{\text{net}}$ over the stochastic process.

6.2. The $\frac{2i}{\hbar} S^{(\text{mid})}$ contribution

For the $I^{(2)}$ contribution we have from the $\frac{2i}{\hbar} S^{(\text{mid})}$ part in equation (19)

$$
\int \int dq \phi \phi (q_{j_f}, \alpha_f, q_i, \alpha_i, t_f, s) \frac{2ni}{\hbar} \sum_{\Delta q} \Delta q \left( \alpha + \frac{\Delta \alpha}{2} \right) \tilde{K} (\Delta q, (q', \alpha', q, \alpha, s, t_i),
$$

where we have used the mid-point prescription, following the discussion around equation (20). Focusing first on the pre-point term (the term in the inner parenthesis proportional to $\alpha$), we use, similarly to (26), the short-time expression (25) and the expansion

$$
\tilde{K} (q_i, \alpha_i, q_f, \alpha_f, s, t_f, t_i) = \sum_{nm} \frac{(\Delta q)^m (\Delta \alpha)^n}{n!m!} \partial_{\alpha}^n \delta_{\alpha}^m \tilde{K} (q_i, \alpha_i, q_f, \alpha_f, s, t_f, t_i).
$$

(30)

The integral over $\Delta q$ gives $\frac{1}{\hbar} \int ds \int dq \phi \phi (q_{j_f}, \alpha_f, q_i, \alpha_i, t_f, s) \frac{2ni}{\hbar} \sum_{\Delta q} \Delta q \left( \alpha + \frac{\Delta \alpha}{2} \right) \tilde{K} (\Delta q, (q', \alpha', q, \alpha, s, t_i),
$$

The only contribution of order $\Delta s$ is $n = 0$ and $m = l = 1$ which gives

$$
\frac{2ni}{\hbar} \int \int dq \phi \phi (q_i, \alpha_i, q_f, \alpha_f, s, t_i) \partial_{\alpha} \tilde{K} (q_i, \alpha_i, q_f, \alpha_f, s, t_i).
$$

(31)
Combining this with the integrals over initial and final positions as above we have

\[
\int dq_i dp_i dq_j dp_j \int ds \int dq \alpha_i \left( \int dp e^{\frac{i\alpha}{\hbar}P(q, p, t_i)} \right)
\]

\[
\frac{1}{(2\pi\hbar)^{2d}} \int dp e^{\frac{i\alpha}{\hbar}P(q, p, t_i)}
\]

The factor \(\alpha\) can be interpreted as \(-\frac{\hbar}{i}\partial_p\) acting on \(e^{\frac{i\alpha}{\hbar}}\) and the derivative moved then to the last \(P\), while the derivative \(\partial_{\alpha}\) brings down \(e^{\frac{i\alpha}{\hbar}}\) multiplying the first \(P\). Combining these terms gives

\[
\left(\frac{1}{2\pi\hbar}\right)^d \int dq_i dp_i dq_j dp_j \int ds \int dq dp \partial_p \left( q_j, p_j, q_i, p_i, t_i \right) \frac{2\hbar}{M} \partial_{\alpha} P(q, p, t_i, t_f).
\]

The classical contribution from the first term in \(\frac{2\hbar}{M} S_i^{(mid)}\) to \(\delta S_q\) is therefore

\[
\int ds dq dp \left( q_f, p_f, q_i, p_i \right) \frac{2\hbar}{M} \partial_{\alpha} P(q, p, t_i, t_f).
\]

The second term in (19) (term in inner parenthesis proportional to \(\Delta \alpha\)) is on the other hand

\[
\int ds \int dq dq' \partial_{\alpha} K(q_j, \alpha_j, q', \alpha', t_f, s) \left( \frac{\hbar}{\delta S_q} \right)
\]

\[
\times (\Delta \alpha \Delta q) K_{\alpha}(q', \alpha', q, \alpha, \cdot) \Delta S(q, \alpha, q, \alpha, s, t_i).
\]

The only contribution of order \(\Delta s\) is then \(n = m = 0\) and \(l = 1\) which gives

\[
\int ds \int dq dq' \partial_{\alpha} K(q_j, \alpha_j, q, \alpha, t_f, s) \left( \frac{\hbar}{\delta S_q} \right)
\]

\[
K(q_j, \alpha_j, q, \alpha, s, t_i) = -\left( t_f - t_i \right) \frac{\hbar}{M} \Delta S(q, \alpha_j, q, \alpha, s, t_i).
\]

This leads to the very simple classical contribution:

\[
-\frac{\hbar}{M} (t_f - t_i).
\]

By one integration by parts (32) and (33) can be combined to

\[
\int ds dq dp \left( q, p, \cdot \right) \left( \frac{2\hbar}{M} \partial_p \frac{\hbar}{\delta S_q} \right) P(q_f, p_f, q_i, p_i, t_i).
\]

We will show in section 7 that (34) together are nothing but \(P\delta Q_{\text{noise}}\), where \(\delta Q_{\text{noise}}\) is the energy (heat) transferred from the system to the bath by the random force.

6.3. The \(\Delta S_q\) contribution

To compute the classical limit of this term we consider directly the Wigner transform \(P\) of the Feynman–Vernon propagator over the whole time interval and interpret \(\frac{1}{\hbar}\partial_{\alpha}\) multiplying \(K\) as \(-\partial_p\), acting on \(P\), and similarly \(\frac{1}{\hbar}\partial_{\alpha}P\) as \(\partial_{\alpha}P\). This gives

\[
-\frac{\hbar}{M} \left( \partial_{\alpha}P + \partial_{\alpha}P \right) P(q_f, p_f, q_i, p_i, t_f, t_i).
\]

As (35) is not a proper functional, it is different from a classical entropy production term, and in this sense more akin to a change in state function. In addition, it depends explicitly on initial and final position for which there is no analogy in stochastic thermodynamics. We will return to a discussion of (35) in section 8 below.
6.4. The $I^{(3)}$ contribution

For the $I^{(3)}$ part we finally have

$$
\int ds \int dq dq' ds' K(q_f, \alpha_f, q', \alpha', \cdot) \left( \frac{\beta q}{(\Delta s)^2} \right) 
$$

The integral over $\Delta q$ of the term in $(\Delta q)^2$ in the inner parenthesis can be evaluated as

$$
\left( \frac{1}{M^2} \right)^{n+2} \delta^{(n+2)}(\Delta \alpha - \eta M \alpha' \Delta s) \text{ which selects } n = 0 \text{ and } m = l = 2. \text{ The combination of pre-factors multiplying } \delta_{\eta M \Delta q} \text{ is then } \beta q \left( \frac{\eta M}{2} \right)^2 \alpha^2. \text{ This is the same contribution as from } I^{(1)}, \text{ up to the dimensionless factor } -\left( \frac{\beta \eta}{2 M} \right)^2. \text{ Since } \beta \eta \text{ is the decorrelation time of the bath and } \eta/M \text{ is the (mesoscopic) Langevin relaxation time of the system this factor must be very small in the set-up considered here, and can therefore be ignored.}
$$

7. Interpretations as stochastic functionals

The purpose of this section is to interpret all the terms derived above except $\Delta S_b$ as expectation values with respect to the (classical) Kramers–Langevin process. We begin with the term from $I^{(3)}$ in (36), and express it symbolically as

$$
\int ds \int dq dp (q, p, \bar{q}, \bar{p}, s, t_i) \beta q \left( \frac{p}{M} \right)^2 \int ds' \int dq dq' ds' K(q_f, \alpha_f, q', \alpha', \cdot) \left( \frac{\beta q}{(\Delta s)^2} \right).
$$

As already remarked above, this quantity is $\beta \eta Q_{\text{friction}}$.

The remaining term $-\frac{1}{4} (\Delta \alpha)^2$ in the inner parenthesis above selects $l = n = 0$ and $m = 2$ giving

$$
\beta q \left( \frac{\eta M}{2} \right)^2 \alpha^2. \text{ This is the same contribution as from } I^{(1)}, \text{ up to the dimensionless factor } -\left( \frac{\beta \eta}{2 M} \right)^2. \text{ Since } \beta \eta \text{ is the decorrelation time of the bath and } \eta/M \text{ is the (mesoscopic) Langevin relaxation time of the system this factor must be very small in the set-up considered here, and can therefore be ignored.}
$$
Using alternatively $F_{\text{noise}} = \dot{p} - F + \eta \frac{p}{M}$, we should hence compute

$$\int_{q_i, p_i}^{q_f, p_f} D(\text{path}) \text{Prob}(\text{path}) \left[ \int -\beta \frac{p}{M} \left( \dot{p} - F ds + \eta \frac{p}{M} \right) \right].$$

We do this by discretizing the time in steps $t_i = t_0, t_1, \ldots, t_N = t_f$ and using the propagator of the Kramers–Langevin equation

$$\sum_{n=1}^{N} \int dq_n dp_n dq_{n-1} dp_{n-1} \int -\frac{p_n + p_{n-1}}{2M} \beta \left( p_n - p_{n-1} - F ds + \eta \frac{p_n + p_{n-1}}{2M} \right)\frac{\text{Prob}(\text{path})}{P(q_{n-1}, p_{n-1}, q_f, p_f)}.$$

The short-time propagator is

$$P_\Delta (\cdot) = \delta \left( q' - q - \frac{p' + p}{2M} \Delta s \right) f (\cdot)$$

and we therefore have

$$\dot{p} \left( p' - p - F \Delta s + \eta \frac{p' + p}{2M} \Delta s \right) P_\Delta = -2\eta \Delta s \delta (\cdot) \partial_p f.$$

Integration by parts gives three terms where the derivative $\partial_p$ is moved respectively to $\delta (\cdot), \frac{p' + p}{2M}$ or $P(q_f, p_f, q', p')$. The first term will be overall quadratic in $\Delta s$, and the other two can be compared to (34).

Hence we have indeed that (34) is equal to $\overline{Q_{\text{noise}}}$. Combining (38) and (41) we have $\overline{\delta s_{\text{env}}}$, the average of the entropy production in stochastic thermodynamics, as announced in the introduction.

The term from $T(1)$ in (29) can also be given a probabilistic interpretation, albeit not a standard one in stochastic thermodynamics. We start by observing that the increments of a standard Wiener process are Gaussian distributed and that for an unconstrained average $E \left[ (d \zeta)^2 \right] = ds$ with no term of order $(ds)^2$. If however we average over the paths of the stochastic process that start at $(q_i, p_i)$ and end at $(q_f, p_f)$ we can have

$$\int_{q_i, p_i}^{q_f, p_f} D(\text{path}) \text{Prob}(\text{path}) \left( \frac{2k_B T\eta}{(ds)^2} \delta \right) = ds + b \left[ q_i, p_i, s | q_i, p_i, q_f, p_f \right] (ds)^2$$

with a non-trivial coefficient $b$. We relate the expression in (29) to such a term by observing, in analogy to (41), that

$$\int_{q_i, p_i}^{q_f, p_f} D(\text{path}) \text{Prob}(\text{path}) \left( \frac{2k_B T\eta}{2M} \right) P_\Delta = \delta (\cdot) \left( 2k_B T\eta (\Delta s)^2 \partial_p^2 f + \Delta s f \right).$$

By two integrations by parts we therefore find that (29) is also an average over the stochastic process

$$\overline{\delta s_{\text{st}}} = \int_{t_i}^{t_f} \left( ds \frac{b}{2} q_i, p_i, s | q_i, p_i, q_f, p_f \right),$$

where $b$ is defined by the ansatz in (41). Formally we could also write (43) as

$$\overline{\delta s_{\text{var}}} = \int_{t_i}^{t_f} \left( ds \frac{1}{2} \text{Finite} \left[ F_{\text{noise}}^2 \right] \right) \text{ (Formal)},$$

where we mean the finite remainder after a term diverging as $(ds)^{-1}$ has been subtracted from the random force squared.

8. Asymptotic analysis of $\Delta S_b$

The most surprising term that have come from the above analysis is the $\Delta S_b$ given in (35), primarily because of its dependence on initial and final position. We will here consider this term in the limit of weak coupling. As this is essentially a classical problem we will adopt the dimension-less units introduced below in appendix A where
the Kramers–Langevin equation reads
\[ \dot{p} = f - \gamma p + \sqrt{2\gamma} \zeta, \quad \dot{q} = p, \] (44)
where \(\zeta\) is standard white noise and where
\[ \Delta S_b = -\gamma \left( q_i \partial_{p_i} + q_j \partial_{p_j} \right) \log P, \] (45)
where \(P\) is the transition probability of (44).

We will consider the case when \(t\), the duration of the process, is of order one in (44) \((t \sim t_{osc}, \gamma \to 0)\), the characteristic time of the system, in the original dimensional variables, and \(\gamma\) tending to zero. Let \((q_f^*, p_f^*)\) be the final position and momentum at time \(t\) of the deterministic system defined by (44), starting from \((q_i, p_i)\). If \(\Delta q_f = q_f - q_f^*\) and \(\Delta p_f = p_f - p_f^*\) are the deviations of the actual final positions from the classical path in is reasonable to assume \(P(q_f, p_f, q_i, p_i)\) to be a Gaussian distribution, i.e.
\[ P(\cdot) \sim e^{-\frac{1}{2} \xi^2}, \] (46)
where
\[ \Sigma = \frac{1}{2} \left( \Delta p_f, \Delta q_f \right) C^{-1} \left( \Delta p_f, \Delta q_f \right)^T \] (47)
and where \(C\) is the correlation matrix of the deviations in units of \(\gamma t\). Under these assumptions we have the two contributions to \(\Delta S_b\) as
\[ \frac{1}{t} q_f \partial_{p_f} \Sigma = \frac{1}{t} q_i \left( C_{ii}^{-1} \Delta p_f + C_{ij}^{-1} \Delta q_f \right), \] (48)
\[ \frac{1}{t} q_i \partial_{p_i} \Sigma = \frac{1}{t} q_i \left( \frac{\partial p_f}{\partial p_i}, -\frac{\partial q_f}{\partial p_i} \right) C^{-1} \left( \Delta p_f, \Delta q_f \right)^T. \] (49)

As functions of \((q_i, p_i, q_f, p_f)\) these terms do not go to zero with \(\gamma\), unless \((\Delta p_f, \Delta q_f)\) vanish, which is when \((q_f, p_f)\) is on the deterministic path starting from \((q_i, p_i)\). On the other hand, \((\Delta p_f, \Delta q_f)\) is typically of order \(\sqrt{\gamma t}\), and the probability that \(\Delta S_b\) is of order one is hence exponentially small in \(\gamma^{-1}\).

9. Discussion

In this contribution we have computed the entropy production in a bath coupled to a driven quantum system defined as the change of the von Neumann entropy of the bath. Except for the (central) assumption that the bath is comprised of a set of harmonic oscillators initially in thermal equilibrium and interacting linearly with the system, the analysis starting from (3) is general. A main result is that this entropy production can be written as a (quantum) expectation value of three functionals given in equations (15) and (16). The limit when the bath spectrum is continuous and temperature is low is briefly discussed in section 5.

The classical limit of these functionals is however puzzling. While we do recover \(\delta S_{env}^{class}\), the average over a classical Kramers–Langevin process and for a finite time of the standard entropy functional \(\delta S_{env}\), we also find two other functionals which we have here called \(\delta S_{env}^{class}\) and \(\Delta S_b\). As we have shown above, in the limit of weak time–constant coupling \(\Delta S_b\) does not vanish except when the initial and final points are on the same classical path—an unsatisfactory result from a physical point of view. A possible way out is that in this limit, and the assumptions made, the system is (almost) conservative and follows (nearly) the classical equations of motion. Deviations from the classical path leading to non-zero \(\Delta S_b\) are very rare and mean that the random force \(F_{noise}\) from the bath has a considerable effect on the system, even if this force has a very small amplitude. The degrees of freedom of the bath must then exercise some kind of coordinated action which is atypical of a thermal state, and the starting assumption made in equation (1), that it suffices to consider a first-order change of the density operator of the bath away from thermal equilibrium, is at least questionable. More work will be needed to find out if this is a viable explanation.

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Appendix A. Time scales

In this appendix we discuss for completeness what means the assumption that $\hbar \beta$ is much smaller than all times scales of interest in the system. Our starting point is that the short-time expression of the Feynman–Vernon propagator (25) should then be valid for $\Delta s = \hbar \beta$. This is so for any constant potential $V$ hence a restriction from the system can only come from spatial variations of $V$. We use that the increments that matter are those for which $(\Delta X)^2 \sim \frac{\hbar^2 \beta}{M}$ and $(\Delta Y)^2 \sim \frac{\hbar^2 \beta}{M}$, and assume that $V = EU(q/\ell')$ where $E$ is a characteristic energy scale, $\ell'$ is a characteristic length, and $U$ is a dimension-less function of order unity. The variation of the potential term in the action—with respect to constant potential—over a time $\hbar \beta$ is then

$$\delta \left( \frac{1}{\hbar} \int_{t_0}^{t_0 + \hbar \beta} V(q_s') \, ds' \right) \approx (\hbar \beta) \cdot \frac{\hbar^2 \beta}{M} \cdot \left( \frac{\hbar^2 \beta}{M} \right)^2. $$

The condition that (A1) is much less than one means

$$\hbar \beta \ll (\beta E)^{1/2} \cdot \frac{M}{\sqrt{E}}. $$

The second term on the right-hand side is a characteristic time of the system $t_{osc}$ which can alternatively be found as the period of an oscillation, assuming that the potential somewhere has a quadratic minimum such that $V \sim \frac{1}{2} E (q - q^*)^2$. The first term on the right-hand side is dimension-less, and by the standard assumption of stochastic thermodynamics that thermal and mechanic energy are comparable it can be taken of order unity.

We hence have three characteristic times: $\hbar \beta$, which is a property of the bath, $t_{osc}$, which is a property of the system, and the Langevin relaxation time $M/\eta$, which is a property of the interaction between the system and the bath, and by assumption $\hbar \beta \ll t_{osc}$ and $\hbar \beta \ll M/\eta$. Introducing the dimension-less ratio $\gamma = \frac{\eta_{osc}}{M}$, the new dimension-less variables $t \rightarrow \frac{t - t_0}{t_{osc}}$, $q \rightarrow q/\ell'$, $p \rightarrow pt_{osc}/M\ell'$, and writing the force $F = \frac{1}{\beta \ell'} f(\xi)$ where $f(\xi) = -U'(\xi)$, we have the Kramers–Langevin equation as given in (44) in the main text.

Appendix B. Higher-order corrections to the Caldeira–Leggett theory

In this appendix we compare the the first correction to the Fokker–Planck equation (28) which stems from the third-order derivative of the potential, to a higher-order correction to the Caldeira–Leggett theory. It is easily seen that the third-order term is $-\frac{\hbar^2}{24} \partial_{ppp}(V^{(3)} P)$. The Wigner function would hence to this order obey a partial differential equation, albeit not a Fokker–Planck equation, and we will see that this is true for the higher-order correction to the Caldeira–Leggett theory as well.

The starting point in computing the higher-order correction is to expand the coth function in the Feynman–Vernon action $S$, to next order i.e. coth$(\frac{\hbar \beta}{2}) = \frac{1}{\beta \hbar \beta} + \frac{1}{3} \beta \hbar \beta + \ldots$. This gives a first-order correction

$$\sum_b \frac{C_{5b}}{12\hbar \beta} \cos \omega_n (s - s') \to \text{the kernel } k_r. A \text{ term in this kernel independent of frequency will in the limit tend to the second derivative of a delta function (as we have seen above for } I^{(5)} \text{) which hence gives a first-order correction } -\frac{\hbar \beta}{6} \int \alpha^2 ds \to S_r. \text{ This is a kinetic term, which hence gives a correction to the Feynman–Vernon short-time propagator } e^{-\frac{\hbar \beta}{6} (\Delta s^2)}, \text{ smaller than the main kinetic term by the dimension-less ratio } \frac{\beta \hbar}{M/\eta}. \text{ We assume this ratio small and expand the correction to the kinetic term as } 1 - \frac{\hbar \beta}{6\Delta s} (\Delta s)^2 + \ldots \text{ and carry out the integration over } \Delta q \text{ as in (26). The presence of an additional term } (\Delta s)^2, \text{ which can be expanded as } (\Delta s - \frac{\eta}{M} \Delta s)^2 + \ldots \text{ allows for a second-order term } (\Delta q)^2 \text{ in the expansion in (26), which then results in an additional term } \frac{\hbar}{6 M} \frac{\beta \hbar \beta}{M} \delta_{qq} \hbar K \text{ in (27). That leads a Wigner transform obeying (28) plus a term } \frac{\hbar}{6 M} \frac{\beta \hbar \beta}{M} \delta_{qq} \hbar P \text{ which has the meaning of a diffusion acting directly on position.}

To differentiate the two terms derived in this section, which are both quadratic in $\hbar$, we use the dimension-less variables introduced in appendix A above and write the generalization of (28) as
\[
\partial_t P = -\partial_x (pP) - \partial_y ((f - \gamma p) P) + \gamma \partial_{pp} P \\
+ \left( \frac{\hbar}{\eta_{\text{loc}}} \right)^2 \left[ \frac{1}{24} \partial_{ppp} (f^{(2)} P) + \frac{\xi}{6} \partial_{ppp} P \right] + \text{h.o.t},
\]
where \( \gamma = \eta_{\text{loc}}/M \) is the ratio of the characteristic time of the system and the Langevin relaxation time. In principle the higher-order correction to the Caldeira–Leggett theory is hence more important than expanding the potential \( V \) if either \( \gamma \) is much larger than unity, or if \( f^{(2)} \approx 0 \). The first case however corresponds to the over-damped limit classically described by spatial diffusion with diffusion coefficient \( \gamma \gamma^{-1} \), which is much larger than the spatial diffusion term derived here unless \( M/\eta \sim \hbar \), while one of the assumptions made above was that \( M/\eta \gg \hbar \). Therefore it is only consistent to retain only the higher-order correction if the potential is approximately harmonic, as then in fact \( f^{(2)} \approx 0 \).

**Appendix C. Change of von Neumann entropy as a measure of entanglement**

In quantum information theory the von Neumann entropy is both a measure of the lack of information about a quantum state, and also, when the total state is pure, of the amount of entanglement between a system and its environment [25, 26]. Other invariant measures of entanglement are complicated to compute and only explicitly known in some cases [30, 31]. In this appendix we interpret the change of von Neumann entropy of the bath in this context.

We start by representing a mixed initial state of the bath as an entangled state with a super-bath or ancilla

\[
|\Phi^{B,A}\rangle = \sum_i a_i \left( |\phi_i^B\rangle \right) \otimes \left| \phi_i^A\rangle \right),
\]

where \( |\phi_i^B\rangle \) and \( |\phi_i^A\rangle \) are states of the bath and the ancilla, and \( a_i \) are positive constants satisfying \( \sum_i a_i^2 = 1 \). The ancilla in (C1) is a theoretical device which serves to represent the initial mixed state of the bath as a pure state in a larger space. The ancilla is assumed not to interact with the bath or the system (or with anything else) after the start of the process, and the only property we need of (C1) is that as \( |\Phi^{B,A}\rangle \) is pure, from which follows that the von Neumann entropies of the two reduced density operators \( \rho_B^f \) and \( \rho_A^f \) are equal.

Now the bath interacts with the system during a process until the system is measured, while the ancilla is disconnected. The dynamics of the ancilla, described by its reduced density operator, is thus that of a closed quantum system, and the von Neumann entropy of its final state remains equal to \( S(\rho_B^f) \). Nevertheless, the ancilla remains entangled with the bath, and as the bath interacts with the system it becomes entangled with the system also.

According to standard quantum mechanics the combined state of the system and the bath after the measurement is a separated mixed state \( \rho_B^f \otimes \left| f \right\rangle \left\langle f \right| \) where \( \left| f \right\rangle \left\langle f \right| \) is the (pure) state of the system and \( \rho_B^f \) is the (mixed) state of the bath, as introduced in section 2 in the main text. In quantum information theory one can alternatively consider the system and the bath to interact with an ideal measurement apparatus and to end up in a combined entangled state [25, 26, 32]. Including the ancilla in such a description the combined total state can then be written

\[
|\Phi^{B,A,S,M}\rangle = \sum_i c_i \left( |\phi_i^{BA}\rangle \right) \otimes \left| \phi_i^M\rangle \right) \otimes \left| f \right\rangle,
\]

where \( |\phi_i^{BA}\rangle \) are states in the product Hilbert space of the bath and the ancilla, \( |\phi_i^M\rangle \) are states of the measurement apparatus, and the \( c_i \) are new positive constants. Since \( |\Phi^{B,A,S,M}\rangle \) and \( |f\rangle \) are pure the von Neumann entropies of \( \rho_{B,A}^{BA} \) and \( \rho_{A,S}^{BA} \) are the same. Neither of these is known, but by the Araki–Lieb theorem \( S(\rho_{B,A}^{BA}) \) is lower bounded by \( S(\rho_B^f) - S(\rho_A^f) \) and by above \( S(\rho_A^f) = S(\rho_B^f) \). The absolute value of the change of the von Neumann entropy of the bath is therefore a lower bound on the amount of entanglement generated during the measurement between on one hand the apparatus, and the other the system and the bath.

**References**

[1] Feynman R P and Vernon F 1963 *Ann. Phys.* 24 118
[2] Sevick E, Prabhakar R, Williams S R and Searles D J 2008 *Annu. Rev. Phys. Chem.* 59 603
[3] Jarzynski C 2011 *Annu. Rev. Condens. Matter Phys.* 2 329
[4] Seifert U 2012 *Rep. Prog. Phys.* 75 1
[5] Maas C 1999 *J. Stat. Phys.* 95 367
[6] Chatrrie R and Gawędzki K 2007 *Commun. Math. Phys.* 282 469–518
[7] Gawędzki K 2012 *Fluctuation relations in stochastic thermodynamics* (arXiv:1308.1518)
[8] Jarzynski C 1997 *Phys. Rev. E* 56 5018
[9] Kurchan J 1998 *J. Phys. A: Math. Gen.* 31 3719
[10] Lebowitz J L and Spohn H 1999 J. Stat. Phys. 95 333
[11] Evans DJ and Searles DJ 1994 Phys. Rev. E 50 1645
[12] Gallavotti G and Cohen EG D 1995 Phys. Rev. Lett. 94 2694
[13] Jarzynski C 1997 Phys. Rev. Lett. 78 2690
[14] Esposito M, Harbola U and Mukamel S 2009 Rev. Mod. Phys. 81 1665
[15] Campisi M, Hanggi P and Talkner P 2011 Rev. Mod. Phys. 83 771
[16] Kurchan J (arXiv:cond-mat/0007360)
[17] Rastegin A E and Życzkowski K 2014 Phys. Rev. E 89 012127
[18] Leggio R, Napoli A, Messina A and Breuer H-P 2013 Phys. Rev. A 88 042111
[19] Hekking F and Pekola J 2013 Phys. Rev. Lett. 111 093602
[20] Horowitz J M and Parrondo J M 2013 New J. Phys. 15 085028
[21] Chétrite R and Mallick K 2012 J. Stat. Phys. 148 480–501
[22] Roncaglia A J, Cerisola F and Paz JP 2014 Phys. Rev. Lett. 113 250601
[23] Esposito M, Lindenberg K and den Broeck CV 2010 New J. Phys. 12 013013
[24] Pucci L, Esposito M and Peliti L 2013 J. Stat. Mech. 2013 P04005
[25] Bengtsson I and Życzkowski K 2006 Geometry of Quantum States (Cambridge: Cambridge University Press) (http://www.rintonpress.com/journals/qic-1-1/eofz.pdf)
[26] Breuer H-P and Petruccione F 2002 The Theory of Open Quantum Systems (Oxford: Oxford University Press)
[27] Caldeira A and Leggett A 1983 Physica A 121 587
[28] Allahverdyan A E and Nieuwenhuizen T M 2001 Phys. Rev. E 64 056117
[29] Chruściński D and Sarbicki G 2014 J. Phys. A: Math. Theor. 47 483001
[30] Wootters W K 2001 Quantum Inf. Comput. I 27–44
[31] Amico L, Fazio R, Osterloh A and Vedral V 2008 Rev. Mod. Phys. 80 517
[32] Allahverdyan A E, Balian R and Nieuwenhuizen T M 2013 Phys. Rep. 00 1