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Characteristic functions of quantum heat with baths at different temperatures

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This paper is about quantum heat defined as the change in energy of a bath during a process. The presentation takes into account recent developments in classical strong-coupling thermodynamics and addresses a version of quantum heat that satisfies quantum-classical correspondence. The characteristic function and the full counting statistics of quantum heat are shown to be formally similar. The paper further shows that the method can be extended to more than one bath, e.g., two baths at different temperatures, which opens up the prospect of studying correlations and heat flow. The paper extends earlier results on the expected quantum heat in the setting of one bath [E. Aurell and R. Eichhorn, New J. Phys. 17, 065007 (2015); E. Aurell, Entropy 19, 595 (2017)].

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I. INTRODUCTION

The study of fluctuating work and heat in open quantum systems is an active interface between nonequilibrium statistical physics and quantum information. As statistical physics the starting point is classical stochastic thermodynamics [1–4] extended toward the quantum domain [5–12]. In quantum information the term Quantum Thermodynamics has become standard [13]; the approach is then full quantum descriptions of nonequilibrium statistical physics of small systems often formulated as resource theories [14,15].

Fluctuation relations in classical stochastic thermodynamics follow from ratios of path probabilities in forward and reverse processes. This is so both for standard models of kinetic theory, where it has been known for almost two decades [16–18], as well as at strong coupling [19–21]. In statistical physics a main problem of quantum thermodynamics is therefore that a quantum path is not an observable and so cannot be used as a conceptual building block of the theory. As quantum information the main problem is, on the other hand, that work and heat are not standard quantum operators in a Hilbert space or in a space of density matrices. Indeed, in thermodynamics these quantities are not exact differentials and are therefore properties of processes with a history and not state functions.

One approach to quantum thermodynamics has its origin in the work of Feynman and Vernon [22]. An open quantum system is then explicitly modeled as a system of interest interacting with a bath, and the bath variables are integrated out. For a bath of harmonic oscillators initially in thermal equilibrium this procedure can be carried out exactly and was used by Leggett and coworkers to investigate quantum Brownian motion, quantum tunneling, and the spin-boson problem in several seminal papers in the 1980s [23–25]. This theory, covered in several reviews and monographs, cf. Refs. [26–28], can be extended to also treat quantum heat as investigated recently by several groups [29–33].

The first goal of the present paper is to extend the results obtained for the expected value (first moment) in Refs. [29,30] to full generating functions of quantum heat. Analogous results have been obtained already in Refs. [32,33], up to differences in the physical set-up, which will be discussed in the following. The second goal is to show that all the procedures in the paper can be carried out for a system interacting with two or more baths at different temperatures. As far as I am aware this observation is new. The Feynman-Vernon approach thus opens a way to investigate the generating functions of quantum heat in a genuine nonequilibrium setting of heat flow between different reservoirs. As an example I derive an expression for quantum thermal power, the expected bath energy change per unit time in the long-time limit.

The organization of the paper is as follows. Section II states the problem studied, and the calculation for one bath oscillator is described in Sec. III. Related technical details are given in Appendix A. The setting of two or more baths at different temperatures and quantum thermal power are discussed in Sec. IV. Various conceptual and technical problems related to quantum heat are discussed in Sec. V. Section VI sums up the paper and gives additional remarks. Appendix A summarizes for completeness properties of Ohmic baths, with pointers to more detailed presentations in the literature.

II. GENERATING FUNCTIONS OF QUANTUM HEAT

This section builds extensively on Refs. [29,30]. The setting is that of one quantum system (“the system”) linearly coupled to a large number of harmonic oscillators (“the baths”). The total Hamiltonian of the bath and the system is

$$H_{\text{TOT}} = H_S + \sum_k \left( H_B^{(k)} + H_I^{(k)} + H_C^{(k)} \right),$$

where

$$H_S = \frac{P^2}{2M} + V(X,t)$$

is the system Hamiltonian (typically explicitly time dependent) and $k$ labels the baths. All parts of the Hamiltonian are for simplicity of expression stated classically. When the distinction

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between the baths is not necessary the index \( k \) will be dropped. The bath Hamiltonians (for each bath) are thus

\[
H_b = \sum_b \frac{p_b^2}{2m_b} + \frac{1}{2} m_b \omega_b^2 q_b^2, \tag{3}
\]

where the mass and spring constant of oscillator \( b \) are \( m_b \) and \( m_b \omega_b^2 \), \( \omega_b \) is the natural frequency in units rad/s, and \( q_b \) and \( p_b \) are, respectively, the oscillator’s coordinate and momentum. The interaction Hamiltonian is

\[
H_I(t) = - \sum_b C_b(t) q_b X, \tag{4}
\]

where the \( C_b(t) \) are functions of time which start out at zero, rise up to a constant value at the beginning of a process, and then go back to zero before the end of the process. Such time-dependent system-bath coupling or other more radical changes are needed to have a consistent classical theory of mesoscopic heat at strong coupling, as recently discussed in Ref. [21]; see references therein for other approaches. In this paper we will for the most part leave these considerations aside and drop references therein for other approaches. The last term in the Hamiltonian Eq. (1) is the Caldeira-Leggett counter-term (a correction to the system Hamiltonian),

\[
H_C(t) = \sum_b G^{(2)}_{\beta} X, \tag{12}
\]

The interaction term in Eq. (4) and the potential in Eq. (3) together form a sum of complete squares, \( \sum_b \frac{1}{2} m_b \omega_b^2 (q_b - \frac{\omega_b X}{m_b})^2 \).

Let now \( |i\rangle \) and \( |f\rangle \) be two states of the system, and let the system initially start in pure state \( |i\rangle \langle i| \). The oscillators in bath \( k \) are initially in equilibrium at some inverse temperature \( \beta_k \). The total initial state of the system and the baths is thus

\[
\rho_i^{\text{TOT}} = \rho_B^i(\beta_i) \otimes \rho_i^\text{eq}(\beta_2) \otimes \cdots \otimes |i\rangle \langle i|, \tag{5}
\]

where \( \rho_B^i(\beta_i) \) is the Gibbs state of bath \( k \) at inverse temperature \( \beta_k \). Feynman and Vernon in a famous paper [22] considered the probability of observing the system in final state \( |f\rangle \) given that it started out in state \( |i\rangle \) when it is interacting with one bath at inverse temperature \( \beta \). For this they introduced the notation

\[
P_{ij} = \text{Tr}_B (f | (U_{\beta_i}^{\text{TOT}} U^i) | f). \tag{6}
\]

The formula extends in a trivial way when the system interacts with more than one bath, as I will also comment upon later. The goal of this paper is to compute the functionals (functionals of the system, functions of the parameters in the arguments),

\[
F_{ij}(v_1,v_2,\ldots) = \prod_k \text{Tr}_B (f | e^{(\sum \nu \lambda H_{\nu b})} (U_{\nu b}^{\text{TOT}} U^i) | f), \tag{7}
\]

\[
G_{ij}(v_1,v_2,\ldots) = \prod_k \text{Tr}_B (f | e^{(\sum \nu \lambda H_{\nu b})} \times (U_{\nu b}^{\text{TOT}} U^i) | f), \tag{8}
\]

where \( v_1,v_2,\ldots \) are parameters that probe the energy of each bath. When the parameters are small this is a way to generate moments (averages, variances, cross-correlations, etc.) between energy changes in one or several baths. The derivative with respect to just one \( v \) at the origin (zero value of all of them) brings out the expected energy change of that bath; for a system connected to one bath the resulting functionals were computed in Refs. [29,30]. When one or several \( v \) are large the functionals probe the distribution of large energy changes. The functional \( F_{ij} \) will be referred to as the characteristic function. The functional \( G_{ij} \) will be referred to as the full counting statistics (FCS). As we will see in the following sections, \( F_{ij} \) and \( G_{ij} \) are structurally very similar, though not identical. In fact, they only differ by the same kind of terms already found for their expected values in, respectively, Refs. [29,30].

\[
F_{ij} \text{ is related to the generating function of the energy of the \( i \) bath \text{ in the final state, as can be seen as follows. Consider one bath and the probability } p_B(E|i,f) \text{ of observing a bath energy } E \text{ at the final time, after the final measurement on the system. The probability of observing one state of the bath } |E\rangle, \text{ is } \langle E | \rho_B^{\text{post}} | E \rangle, \text{ where } \rho_B^{\text{post}} \text{ is the reduced density matrix of the bath, after measuring the system and finding final state } |f\rangle \text{. This quantity is}
\]

\[
\rho_B^{\text{post}} = \frac{1}{P_{ij}} (f | \rho_{\text{TOT}} | f), \tag{9}
\]

where \( \rho_{\text{TOT}} \) is the total density operator of the system and the bath at the end of the process. We then have

\[
p_B(E|i,f) = \sum_{E} \frac{1}{P_{ij}} 1_{E(\mathcal{E},f)} \langle \mathcal{E},f | \rho_{\text{TOT}} | \mathcal{E},f \rangle, \tag{10}
\]

where \( E(\mathcal{E}) \) is the energy of bath state \( |\mathcal{E}\rangle \). Integrating both sides one has

\[
\int e^{i\nu E} p_B(E|i,f) dE = \sum_{E} \frac{1}{P_{ij}} e^{i\nu E} \langle \mathcal{E},f | \rho_{\text{TOT}} | \mathcal{E},f \rangle = \frac{1}{P_{ij}} F_{ij}(v), \tag{11}
\]

\( F_{ij}(v) \) is therefore up to the factor \( P_{ij} \) the generating function of the bath energy in the final state.

\( G_{ij}(v) \) can on the other hand be related to a bath energy change in a two-measurement protocol. If the initial state of the bath is both measured and recorded the initial state of the system and the bath is a pure state, \( |\mathcal{E},i\rangle \). If the initial state of the bath is measured but not recorded the initial state is a statistical mixture where \( |\mathcal{E},i\rangle \) has Gibbs weight \( Z_B^{-1}(\beta) \exp \{ -\beta E(\mathcal{E}) \} \). Consider \( p_B(\Delta E,i) \mathcal{E},i\rangle \), the conditional probability of observing a final state \( |f\rangle \) of the system and bath energy change \( \Delta E \), conditioned on total initial state \( \mathcal{E},i\rangle \). Consider further \( \mathcal{P}_B(\Delta E,|f\rangle,i) = \sum_{\mathcal{E},i} p_B(\Delta E,i) (|\mathcal{E},i\rangle Z_B^{-1}(\beta) \exp \{ -\beta E(\mathcal{E}) \}), \) which is the average \( p_B(\Delta E,|f\rangle,i) \) over the statistical mixture. Similar to above, \( \mathcal{P}_B(\Delta E,|f\rangle,i) \) is the total density operator of the system and the bath at the end of the process when the system and the bath started in the pure state \( |\mathcal{E},i\rangle \). Resolving the \( \delta \) function one can write

\[
\mathcal{P}_B(\Delta E,|f\rangle,i) = \frac{1}{2\pi} \int e^{-i\nu \Delta E} G_{ij}(v) dv, \tag{13}
\]
where

\[
G_{ij}(v) = \sum_{E_i, E_j} Z^{-1}(\beta) e^{-\beta E_j \xi_i} \psi_{E_i}(v) \psi_{E_j}(v)
\]

\[
\times \langle E_{i}, f | \rho_{\text{TOT}}(E_{i}, t) | E_{f}, f \rangle.
\]

By linearity the Gibbs weight and the factor \( e^{-i v E(t)} \) can be taken inside the big unitary transformation defining \( \rho_{\text{TOT}}(E_{i}, t) \). The above is therefore alternatively

\[
G_{ij}(v) = \text{Tr}_B (|f \rangle e^{i v H B} U e^{-i v H B} \hat{\rho}_{\text{TOT}} U |f \rangle),
\]

which is the same expression as Eq. (8), for brevity stated for one bath. \( G_{ij}(v) \), referred to a full counting statistics, is hence the generating function of the energy change in the bath, averaged over an initial equilibrium distribution of the bath.

III. THE PATH INTEGRAL EXPRESSIONS FOR THE FUNCTIONALS \( \mathcal{F}_{ij} \) AND \( G_{ij} \)

Path integrals for harmonic oscillators can be done exactly since they are Gaussian. As the initial state of the bath oscillators is factorized (they are independent) and since they do not interact with one another, the path integral of each bath oscillator can be done separately.

To keep the central message (and results) visible notional simplifications will be introduced as needed. The first such notation simplification, introduced by Feynman and Vernon [22], is to write \( P_{ij} \) for conditional probability of measuring the system in final state \(|f \rangle \) given that it was initially in \(|i \rangle \). Using the shorthand,

\[
\int_{if} \cdots = \int dX_i dY_i dX_f dY_f \psi_i(X_i) \psi_f(X_f) \psi_i(Y_i) \psi_f(Y_f)
\]

where \( \psi_i \) and \( \psi_f \) are the wave functions of the states \(|i \rangle \) and \(|f \rangle \). I write the transition probability in Eq. (6) as

\[
P_{ij} = \int_{if} \mathcal{D}X_i \mathcal{D}X_f \mathcal{D}Y_i \mathcal{D}Y_f e^{i S_i[X_i] - i S_j[X_f]} e^{i S_j[Y_i] - i S_i[Y_f]} e^{i S_f[X_f] - i S_i[X_i]},
\]

where the two path integrals are over, respectively, the forward path \( X(t) \) from \( X_i \) to \( X_f \) and the backward path \( Y(t) \) from \( Y_i \) to \( Y_f \). These two path integrals emanate from a representation of the total unitary \( U \) and its inverse \( U^{-1} \) in the time development of the total density operator of the bath and the system \( \hat{\rho}^\text{TOT} = U \hat{\rho}^\text{TOT} U^{-1} \), and then integrating out the bath variables. The effects of the bath are thus captured by the two kernels \( S_i \) and \( S_i \) in Eq. (16), which couple the forward and backward paths, and which are referred to as the real and the imaginary part of the Feynman-Vernon action. The contribution to \( S_i \) and \( S_i \) from one oscillator with a time-dependent system-bath coupling is

\[
S_i^B = \int_{-\infty}^{\infty} \langle X - Y | X' + Y' \rangle C_B \psi_i(X) \sin \omega_B (s - s') ds' ds,
\]

\[
S_i^B = \int_{-\infty}^{\infty} \langle X - Y | X' + Y' \rangle C_B \psi_i(X) \cos \omega_B (s - s') ds' ds,
\]

where primed (unprimed) quantities refer to time \( s' \) (and \( s' \) is the inverse temperature of the bath to which this oscillator belongs. The quantities in \( S_i \) and \( S_i \) in Eq. (16) are the sums of \( S_i^B \) and \( S_i^B \) from Eqs. (17) and (18). The expression for \( S_i^B \) is symmetric in \( s \leftrightarrow s' \) and this integral can therefore be extended over the whole square \( t_i \leq s, s' \leq t \). The expression for \( S_i^B \) is on the other hand not symmetric in \( s \leftrightarrow s' \) so this integral has to be taken over the triangular domain \( t_i \leq s' \leq s \leq t \).

The path integral expressions for \( \mathcal{F}_{ij} \) and \( G_{ij} \) can be written

\[
\mathcal{F}_{ij} = \int_{if} \mathcal{D}X_i \mathcal{D}X_f \mathcal{D}Y_i \mathcal{D}Y_f e^{i S_i[X_i] - i S_j[X_f]} \sum_b \mathcal{F}_{b}^{(F)}(v),
\]

\[
G_{ij} = \int_{if} \mathcal{D}X_i \mathcal{D}X_f \mathcal{D}Y_i \mathcal{D}Y_f e^{i S_i[X_i] - i S_j[X_f]} \sum_{b} \mathcal{F}_{b}^{(G)}(v),
\]

where the products are over the bath oscillators \( b \). The results of the corresponding integrations over each bath oscillator are as in Ref. [29], Eq. (13). I will write them as

\[
\mathcal{F}_{b}^{(F)}(v) = \frac{(2 \pi \omega)^2 e^{i \nu H_i B} e^{i \nu H B}}{Z(B) N(\beta \hbar B) N(t)^2 N(\hbar v) \det \mathcal{M}_F},
\]

\[
\mathcal{F}_{b}^{(G)}(v) = \frac{(2 \pi \omega)^2 e^{i \nu H_i B} e^{i \nu H B}}{Z(B) N(\beta \hbar B - \hbar v) N(t)^2 N(\hbar v) \det \mathcal{M}_G},
\]

All quantities in above refer to one bath oscillator, the index \( b \) understood in angular frequency \( \omega \), mass \( m \), etc. The quantities \( N(t) = \sqrt{2 \pi \hbar \sin(\omega t)} \) in the denominators are the normalization factors of the harmonic oscillators with the corresponding timelike arguments. The vector \( u \) and the function \( B \) arise from the propagators of the harmonic oscillators and are listed in Appendix A; they do not depend on \( v \). The matrices \( \mathcal{M}_F \) and \( \mathcal{M}_G \) collect terms from the harmonic oscillator propagators, the initial equilibrium state of the bath, and \( e^{-i v H_B} \) and \( e^{-i v H_B} \); they depend on \( v \) and are also listed in Appendix A.

It was shown in Ref. [29] that all the prefactors in Eq. (21) combine to \( \sinh(\omega_B \beta) \sin^{-1}(\omega_B \beta - i \nu) \). Using the same line of argument it is seen that all the prefactors in Eq. (22) combine to give one. The whole nontrivial part hence stems from \( u, B \), and \( \mathcal{M} \) and the results can be written as

\[
\prod_b \mathcal{F}_{b}^{(F)}(v) = (\text{trivial}) \cdot e^{\nu S_i - \nu S_i + \nu J^{(1)}(v) + \nu J^{(2)}(v) + \nu J^{(1)}(v)},
\]

\[
\prod_b \mathcal{F}_{b}^{(G)}(v) = e^{\nu S_i - \nu S_i + \nu J^{(1)}(v) + \nu J^{(2)}(v) + \nu J^{(1)}(v)},
\]

where the Feynman-Vernon terms \( S_i \) and \( S_i \) are given in Eqs. (17) and (18). The three new functionals, which are all symmetric in \( s \leftrightarrow s' \), are

\[
J^{(1)} = \frac{i}{2m \omega_B} \int_{s}^{s'} (X' + \gamma Y') C C' \cos \omega(s - s') \times \frac{y - z}{\Delta} - \frac{i}{2} \coth \frac{\omega_B}{2},
\]

\[
J^{(2)} = \frac{i}{2m \omega_B} \int_{s}^{s'} (X' + \gamma Y') C C' \sin \omega(s - s') \times \frac{y' z' - y z}{\Delta} - \frac{1}{2},
\]
\[ \mathcal{J}^{(3)} = \frac{i}{2m_0 h} \int_t^{t'} (XY' + XY) C^* \cos \omega(s - s') \times \left( \frac{z' - y'}{\Delta} + \frac{i}{2} \coth \frac{\omega h \beta}{2} \right), \] (27)

where the auxiliary variables \( z, z', y, y' \) and \( \Delta \) are combinations of trigonometric and hyperbolic functions in \( \nu \) and \( \beta \) given in Appendix A. The definitions of \( z, z' \) and \( \Delta \) differ a bit between Case F \( (F_{ij}) \) and Case G \( (G_{ij}) \). However, for both cases \( \mathcal{J}^{(1)}, \mathcal{J}^{(2)}, \) and \( \mathcal{J}^{(3)} \) all vanish at \( v = 0 \). For Case G \( (G_{ij}) \) the functional \( \mathcal{J}^{(1)} \) as defined by Eq. (25) is identically zero, so that the only remaining pieces are \( \mathcal{J}^{(2)} \) and \( \mathcal{J}^{(3)} \), in agreement with the expression given in Eq. (24).

IV. QUANTUM HEAT FLOWS AND QUANTUM THERMAL POWER

The first point of this section is that if a system interacts with two or more harmonic oscillator heat baths that do not interact directly with one another, the corresponding Feynman-Vernon actions simply add. The reason is the same as used to derive the Feynman-Vernon action from one bath by adding the contributions from each oscillator separately.

The second point is that the same property holds for the generating functions \( F_{ij}(v_1, v_2, \ldots) \) and \( G_{ij}(v_1, v_2, \ldots) \) introduced in Eqs. (7) and (8). For the rest of this section I will assume that the system interacts with two baths, a cold \("\text{left}\) bath at inverse temperature \( \beta_L \), and a hot \("\text{right}\) bath at inverse temperature \( \beta_R \) \( (\beta_R < \beta_L) \). It is natural to expect that if the system has some structure all parts of the system do not interact with two baths in the same way. Previously it was not necessary to make this distinction, but here it is convenient to think of one system coordinate \( X_L \), which interacts linearly with the cold bath, and one system coordinate \( X_R \), which interacts linearly with the hot bath, and all the other system coordinates grouped into \( X_C \). Classically one then expects heat to flow from right to left from the hot bath to \( X_R \), then from \( X_R \), through the system \( X_C \), and then from \( X_C \) out into the cold bath. A similar setting was recently considered in Ref. [34].

Suppose one is mainly interested in the long-time limit of the expected energy change in a bath per unit time, which defines quantum thermal power in steady state. The energy change should to leading order scale linearly in the time, with a prefactor that will not depend on the initial or the final state of the system. It therefore makes sense to consider the average of the energy change(s) in the bath(s) over the final state of the system (also at finite time), which is

\[ \bar{\rho}_b(\Delta E|i) = \sum_f \bar{\rho}_b(\Delta E, f|i). \] (28)

The corresponding generating functions is \( G_i(v_1, v_2) \). We have

\[ G_i(v_1, v_2) = \sum_f G_{i,f}(v_1, v_2). \] (29)

The starting point is then

\[ G_i(v_1, v_2) = \text{Tr}_{B_i B_R S_i} \left[ e^{i(v_1 H_{B_i} + v_2 H_{B_R})} \times \left[ U e^{-i(v_1 H_{B_i} + v_2 H_{B_R}) \frac{\rho_i^\text{TOT} U^*}} \right] \right] \]

where the trace is over the system and both baths and \( \delta(X_f - Y_f) \) is the path integral rendering of Trs. The subscript of the integral \( f \) indicates the remaining dependence on the initial state of the system. The two products in Eq. (30) are

\[ \prod_{b \in L} F_{b}^{(G)}(v_1) \]

\[ = e^{\frac{i}{2} S_i[X_i, Y_i] + \frac{i}{2} S_i[Y_i, Y_i] + \delta(Y_i - Y_i) + \delta(Y_i)}/\Delta_1 \]

\[ \prod_{b \in R} F_{b}^{(G)}(v_2) \]

\[ = e^{\frac{i}{2} S_i[X_i, Y_i] + \frac{i}{2} S_i[Y_i, Y_i] + \delta(X_i)}/\Delta_1 \]

and the functionals are given as sums of the terms in Eqs. (17), (18), (25)–(27). Averages, correlations, and cross-correlations of the energy changes in the two baths can be evaluated as derivatives of \( G_i \) with respect to \( v_1 \) and \( v_2 \).

Quantum thermal machine are quantum systems that transform heat to useful work. Quantum analogues of Carnot, Otto, and diesel engines as well as quantum refrigerators have been proposed and partly experimentally realized [35,36] and were reviewed in Ref. [13]. The amount of heat flowing through the working fluid of a quantum thermal machine per unit of time limits how much work the machine can do per unit of time, i.e., the power. The simplest quantity that can be considered by the above analysis is quantum thermal power defined as the energy change in the one of the baths per unit time, in the limit when the process is in steady state.

To be concrete, let the bath be the cold bath. One can expect the dependence on the initial state \( |i\rangle \) of the system to drop out, and one can write

\[ \dot{Q} = \lim_{v \to -\infty} \frac{\delta}{\delta v_i} G_i|_{v=0} \int_{t_i}^{0} h^{(2)}(0, s)((X_L(0)Y_L(s) - X_L(s)Y_L(0)))ds + \int_{-\infty}^{0} h^{(3)}(0, s)((X_L(0)Y_L(s) + X_L(s)Y_L(0)))ds \]

where the two kernels are the terms linear in \( \mathcal{J}^{(2)} \) and \( \mathcal{J}^{(3)} \) as given in Eq. (A21) and Eq. (A22).

\[ h^{(2)}(s, s') = i \sum_b C_b^2 \frac{\coth (\frac{\beta h \omega_b}{2})}{2m_b} \sin \omega_b(s - s'), \]

\[ h^{(3)}(s, s') = \sum_b C_b^2 \frac{\coth (\frac{\beta h \omega_b}{2})}{2m_b} \sin \omega_b(s - s'). \] (35)

Up to a factor \( \beta \) the above is the same as Eq. (16) in Ref. [29]. As we consider a long-time limit the time-dependence of \( C_b \) in the equivalent expressions in Eqs. (A21) and (A22) can be ignored. The expectation values in Eq. (33) are over a steady-state reduced description of “left” part of the system only.
An interesting special case is when the bath is Ohmic and the temperature (in this case, of the cold bath) is sufficiently high (Caldeira-Leggett limit). For completeness definitions and basic properties of Ohmic baths are briefly summarized in Appendix B. The two kernels can then be approximated as $\hat{h}^{(2)}(s,s') \approx -\frac{2}{\pi x^2} \frac{d^2}{ds^2} - \frac{2}{\pi x^2} \frac{d}{ds}$ [30], where $\eta$ is the friction coefficient. Integration by parts turns Eq. (33) into

$$\dot{Q} = \int dX dY \hat{b}(X-Y) \frac{i\eta}{\hbar} \langle \hat{X} \hat{Y} - \hat{Y} \hat{X} \rangle \bar{\rho}_L(X,Y)$$

$$+ \int dX dY \hat{b}(X-Y) 2\eta \langle \hat{X} \hat{Y} \rangle \bar{\rho}_L(X,Y),$$

(36)

where $\bar{\rho}_L(X,Y)$ is the stationary reduced density matrix of the left part of the system in the coordinate representation.

When the system has continuous state space the averages in Eq. (36) and over the system development in the Caldeira-Leggett limit and were evaluated in Ref. [29], Secs. 6.2 and 6.4. The result can be expressed by two operators:

$$\dot{O}_1 = -2 \eta \frac{\partial}{\partial (X-Y)} (X-Y),$$

(37)

$$\dot{O}_2 = -2\eta \frac{\partial^2}{\partial (X-Y)^2},$$

(38)

and

$$\dot{Q} = \text{Tr}[\dot{O}_1 \bar{\rho}_S] + \text{Tr}[\dot{O}_2 \bar{\rho}_S].$$

(39)

The Caldeira-Leggett limit is essentially a classical limit because the Wigner transform of the density matrix obeys classical Fokker-Planck equation. The above is hence just a simple to approximate the system-bath interaction constant and to somehow estimate quantum heat from the bath Hamiltonian and interaction Hamiltonian at the initial and final time. The section discusses why such an approach is not straightforward.

A first indication of a problem is that if one would simply take quantum heat as change of bath energy and the system-bath interaction constant in time there appears in the classical limit (Caldeira-Leggett model) boundary contributions, discussed at length in Ref. [29]. In such an approach there is hence not a complete quantum-classical correspondence for heat even on the level of expectation values.

A second indication comes from the recent development of strong-coupling stochastic thermodynamics [19,42]. Even classically it is only when the system-bath interaction energy is negligible that one can at the same time take it constant and define heat as change in bath energy. If the system-bath interaction energy is comparable to changes in system energy or bath energy then a fraction should be counted as heat, and a fraction as change of system energy. Certain choices of these fractions, where also part of the bath energy is counted as internal energy of the system, have been found to be consistent, albeit at the price that the resulting heat has to determined by thermodynamic integration. The latter has led to a vigorous polemic [43], which I have recently discussed elsewhere [21]. The main problem in the present (quantum) context is that even when the proposals in Refs. [19,42] can be accepted classically, they lead to quite involved definitions in the quantum domain; compare Eq. (28) in Ref. [19]. The alternative procedure of a time-dependent system-bath interaction avoids this problem on both the classical and the quantum level, at the price of a new term in the work; see Ref. [30].

It can be concluded that quantum heat is in some sense always a strong-coupling phenomenon, and problems with various naïve versions of heat in open quantum systems indeed central issues in quantum thermodynamics. The earliest indication may have been Ref. [44], where it was shown that the quantum dynamics of a single oscillator coupled to a heat bath of harmonic oscillators depends sensitively on the exact initial conditions, and in particular if the bath is brought into contact immediately before or immediately after the system is measured initially. A second problem was identified in Refs. [45,46], where it was shown that different definitions of specific heat of a quantum particle interacting strongly with a bosonic heat bath yield different results. A further step was taken in Ref. [12], where it was shown that for a system interacting with a fermionic bath one cannot consistently include any fixed nonzero fraction of the system-bath interaction in the heat. This excludes, for instance, the choice of including all system-bath interaction, as proposed in Ref. [47]. However, including no part of the system-bath interaction in the heat means to treat it as if weakly coupled, which brings the issue that third law is no longer satisfied [12].

Note that the choice in Refs. [19,42] includes (classically) a definite but not a fixed fraction of the system-bath interaction energy in the heat.

Earlier work technically most similar to the determination of the generating function of heat in this paper are Refs. [31–33]. Those papers mostly appeared before the recent developments of (classical) strong-coupling stochastic thermodynamics, and were hence developed independently of that context. In Ref. [32] was computed a generating function formed from inserting the operators $e^{i \Theta H_S + iv \Theta H_B}$ at
the final time and \( e^{-i\lambda H_0} \) at the initial time; \( \lambda \) is here an additional parameter. The interaction is with one bath at inverse temperature \( \beta \), and leads to expressions of a similar structure to the ones given above for \( G_{ij} \). The expectation value formed by differentiating this generating function with respect to \( i \nu \) at \( \nu = 0 \) is \( \langle H_B + \lambda H_{SB} \rangle_f - \langle H_B \rangle_i \), where \( \langle \cdots \rangle_i \) means averaging with respect to the initial state of the bath (independent of the system) and \( \langle \cdots \rangle_f \) means averaging with respect to the final state of the system and the bath. By the discussion above this choice does not correspond classically to any of the proposals currently considered viable for strong-coupling heat in stochastic thermodynamics, the only exception being \( \lambda = 0 \) and weak coupling. One may note that the boundary contribution in the classical limit from Ref. [29] does not appear in the formulation in Ref. [32]. The generating functions computed here are quadratic functionals of the forward and backward paths in moment obtained in Refs. [29, 30].

VI. DISCUSSION

I have in this paper computed the generating functions of the distributions of the final energy in a bosonic bath (or baths) and the change of bath energy as functionals of a system interacting with the bath (or baths). From a technical point of view analogous results were obtained Refs. [32, 33] but in slightly different settings which do fit the recently developed (classical) stochastic thermodynamics at strong coupling [19, 42].

The version of strong-coupling used in this paper is based on the classical limit from Ref. [29], at least not at the initial time, due to an additional assumption that the initial state of the system is diagonal. In Ref. [33] (v1 as available on arXiv, Supplemental Material Sec. III) a similar calculation is carried out from the operators \( e^{-i\nu H_B+\nu H_a} \) at the final time and \( e^{-i\lambda H_B+\lambda H_a} \) at the initial time, with the bath and system initially in joint equilibrium. This leads again to expressions of a similar structure to the ones given above for \( G_{ij} \). The choice of an initial joint equilibrium state of the system and the bath is the same as in Refs. [45, 46]. Classically it can be seen as special case of of the choice in [19, 42] when the initial state of the system is an equilibrium at mean force, for a comparison see Ref. [21]. The corresponding expectation value is \( \langle H_B + H_{cb} \rangle_f - \langle H_B \rangle_i \), where both averages are over the system and the bath implies the same definition of quantum heat as used in Ref. [47].

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APPENDIX A: INVERTING THE MATRICES AND DETERMINING THE FUNCTIONALS

This Appendix contains the derivation of Eqs. \((23) - (27)\) in the main text, and then the closed-form expressions of the kernels \( f^{(1)} \), \( f^{(2)} \), and \( f^{(3)} \) for cases F and G. Conventions are as in Ref. [29] except that a factor \( i \) for convenience has been included in the definitions of the matrices \( \tilde{M} \). The vector \( u \) appropriate for when the coupling coefficient depends on \( t \), is

\[
\begin{align*}
\frac{u}{v} &= \frac{1}{\sin(\alpha)} \int \sin \omega(t-s)(C(s)X(s))ds \\
\frac{u'}{v'} &= \frac{1}{\sin(\alpha)} \int \sin \omega(C(s)X(s))ds \\
\end{align*}
\]

(A1)
The function $B$ is similarly

$$B = -\frac{1}{m_0 \sin(\omega t)} \int^{t'}_t \sin \omega (t - s) \sin \omega 'CXC'X'd's'ds$$

$$+ \frac{1}{m_0 \sin(\omega t)} \int^{t'}_t \sin \omega (t - s) \sin \omega 'CYC'Y'd's'ds,$$

(A2)

where the primed (unprimed) quantities refer to time $s'$ ($s$).

The matrix $\tilde{M}$ can be written in the same way for the two cases by introducing auxiliary variables:

$$\tilde{M} = \begin{pmatrix} -x - z & z' & 0 \\ z' & x - z & x' \\ x' & y' & -x + y - y' \\ -x - z & z' & -y' & x + y \end{pmatrix}.$$

(A3)

These auxiliary variables are the same as in Eqs. (25)–(27) in the main text and are defined as follows:

**Case F:** In this case $x = \cot(\omega t)$, $x' = \sin^{-1}(\omega t)$, $y = \cot(\omega \hbar v)$, $y' = \sin^{-1}(\omega \hbar v)$, $z = \cot(-i \omega \hbar \beta) = i \coth(\omega \hbar \beta)$ and $z' = \sin^{-1}(-i \omega \hbar \beta) = i \sin^{-1}(\omega \hbar \beta)$.

**Case G:** In this case $x$, $x'$, $y$, and $y'$ are the same as in case F while $z = \cot[\omega \hbar (v - i \beta)]$ and $z' = \sin^{-1}[\omega \hbar (v - i \beta)]$.

**Algebraic relations:** In both cases the auxiliary variables satisfy obvious relations, namely

$$z'^2 - z^2 = y'^2 - y^2 = x'^2 - x^2 = 1.$$  

(A4)

Using Eq. (A4) repeatedly it is straightforward to determine the matrix inverse as

$$\tilde{M}^{-1} = \frac{1}{\Delta} \begin{pmatrix} y - z & y - z' & D & -B \\ y' - z & y' - z' & y - z & -C \\ D & -C & y - z & y' - z' \\ -B & A & y' - z' & y - z \end{pmatrix},$$  

(A5)

where new auxiliary variables are

$$A = \frac{1}{X'}(1 + x(y - z) + yz - y'z'),$$

(A6)

$$B = \frac{1}{X'}(x(z' - y') + y'z - y'z'),$$

(A7)

$$C = \frac{1}{X'}(x(z' - y') - y'z + y'z').$$

(A8)

1. **Case F**

We here have

$$\Delta = 2(z'y' - yz - 1) = 2i \sinh^{-1}(\omega \hbar \beta) \sin^{-1}(\omega \hbar v)[1 - \cos(\omega \hbar v) \cosh(\omega \hbar \beta) + i \sin(\omega \hbar v) \sinh(\omega \hbar \beta)]$$

$$= 2i \sinh^{-1}(\omega \hbar \beta) \sin^{-1}(\omega \hbar v)[1 - \cos(\omega \hbar (v + i \beta))],$$

(A16)

and the expressions simplify to

$$\frac{y - z}{\Delta} = \frac{1}{2} \frac{\cos(\omega \hbar v) \sin[\omega \hbar (v + i \beta)] - \sin(\omega \hbar v) \cos[\omega \hbar (v + i \beta)]}{1 - \cos(\omega \hbar (v + i \beta))} = \frac{1}{2} \coth \left[ \frac{\omega \hbar (v + i \beta)}{2} \right],$$

$$\frac{y'z' - yz}{\Delta} = \frac{1}{2} \frac{1 - \cos(\omega \hbar v) \cos(\omega \hbar (v - i \beta))}{1 - \cos(\omega \hbar (v + i \beta))} = \frac{1}{2} + i \frac{\sin(\omega \hbar v) \sinh(\omega \hbar \beta)}{4 \sin^2 \left( \frac{(\omega \hbar (v + i \beta)}{2} \right)},$$

$$\frac{z' - y'}{\Delta} = \frac{1}{2} \frac{\sin(\omega \hbar v) + i \sinh(\omega \hbar \beta)}{1 - \cos(\omega \hbar (v + i \beta))} = \frac{1}{4} \frac{\sinh \left( \frac{(\omega \hbar (v + i \beta)}{2} \right)}{\sin^2 \left( \frac{(\omega \hbar (v + i \beta)}{2} \right)}.$$
All three functionals \( \mathcal{J}^{(1)}, \mathcal{J}^{(2)}, \) and \( \mathcal{J}^{(3)} \) vanish at \( v = 0 \) as follows by insertion in the above. Their derivatives at \( v = 0 \) are

\[
\frac{\partial \mathcal{J}^{(1)}}{\partial v} |_{v=0} = -i \frac{1}{8m} \int_{t'}^{t} (XX' + YY') \cos \omega (s - s') \frac{1}{\sinh \left( \frac{\omega h}{2} \right)}, \]

(A17)

\[
\frac{\partial \mathcal{J}^{(2)}}{\partial v} |_{v=0} = -\frac{1}{4m} \int_{t'}^{t} (XY' - X'Y) \sinh \omega (s - s') \coth \left( \frac{\omega h \beta}{2} \right), \]

(A18)

\[
\frac{\partial \mathcal{J}^{(3)}}{\partial v} |_{v=0} = i \frac{1}{8m} \int_{t'}^{t} (XY' + X'Y) \cos \omega (s - s') \left( \frac{1}{\sinh \left( \frac{\omega h \beta}{2} \right)} + 2 \right), \]

(A19)

The derivative of the second term \( (y'z' - yz)/\Delta \) gives the term called \( \mathcal{J}^{(2)} \) in Refs. [29,30], while the derivatives of \( (y - z)/\Delta \) and \( (z' - y')/\Delta \) combine to give the terms called \( \mathcal{I}^{(1)} \) and \( \mathcal{I}^{(3)} \) in Ref. [29], with the identification \( v = i \epsilon \) and a factor two from the definition of the double integrals.

2. Case G

We here have

\[
\Delta = 2(z'y' - yz - 1) = 2 \sin^{-1} [\omega h (v - i \beta)] \sin^{-1} [\omega h v] [1 - \cos (\omega h v) \cos [\omega h (v - i \beta)] - \sin (\omega h v) \sin [\omega h (v - i \beta)]]
\]

\[
= 2 \sin^{-1} [\omega h (v - i \beta)] \sin^{-1} [\omega h v] [1 - \cos (\omega h \beta)], \quad (A20)
\]

and the expressions simplify a bit further to

\[
\frac{y - z}{\Delta} = \frac{1}{2} \frac{\cos (\omega h v) \sin [\omega h (v - i \beta)] - \sin (\omega h v) \cos [\omega h (v - i \beta)]}{1 - \cosh (\omega h \beta)} = i \frac{1}{2} \coth \left( \frac{\omega h \beta}{2} \right).
\]

\[
\frac{y'z' - yz}{\Delta} = \frac{1}{2} \frac{1 - \cos (\omega h v) \cos [\omega h (v - i \beta)]}{1 - \cosh (\omega h \beta)} = 1 - \frac{1}{4} \frac{\sin \omega h v \sin [\omega h (v - i \beta)]}{\sinh^2 \left( \frac{\omega h \beta}{2} \right)},
\]

\[
\frac{z' - y'}{\Delta} = \frac{1}{2} \frac{\sin (\omega h v) - \sin [\omega h (v - i \beta)]}{1 - \cosh (\omega h \beta)} = -i \frac{1}{2} \cos (\omega h v) \coth \left( \frac{\omega h \beta}{2} \right) + \frac{1}{2} \sin (\omega h v).
\]

The functional \( \mathcal{J}^{(1)} \) here vanishes completely, while the functionals \( \mathcal{J}^{(2)} \) and \( \mathcal{J}^{(3)} \) vanish at \( v = 0 \). Their derivatives at \( v = 0 \) are

\[
\frac{\partial \mathcal{J}^{(2)}}{\partial v} |_{v=0} = -\frac{1}{4m} \int_{t'}^{t} (XY' - X'Y) \sinh \omega (s - s') \coth \left( \frac{\omega h \beta}{2} \right), \quad (A21)
\]

\[
\frac{\partial \mathcal{J}^{(3)}}{\partial v} |_{v=0} = i \frac{1}{4m} \int_{t'}^{t} (XY' + X'Y) \cos \omega (s - s') \left[ 1 + \coth^2 \left( \frac{\omega h \beta}{2} \right) \right], \quad (A22)
\]

which are the same as \( \mathcal{I}^{(2)} \) and \( \mathcal{I}^{(3)} \) in Ref. [30], with the identification \( v = i \epsilon \) and a factor two from the definition of the double integrals. The second derivatives at \( v = 0 \), which determine the variance of the change in bath energy, are

\[
\frac{\partial^2 \mathcal{J}^{(2)}}{\partial v^2} |_{v=0} = -\frac{i \omega h}{4m} \int_{t'}^{t} (XY' - X'Y) \sinh \omega (s - s') \left[ 1 + \coth^2 \left( \frac{\omega h \beta}{2} \right) \right], \quad (A23)
\]

\[
\frac{\partial^2 \mathcal{J}^{(3)}}{\partial v^2} |_{v=0} = \frac{\omega h}{4m} \int_{t'}^{t} (XY' + X'Y) \cos \omega (s - s') \left( \frac{\omega h \beta}{2} \right), \quad (A24)
\]

### APPENDIX B: THE OHMIC BATH

For completeness I describe here properties of the Ohmic bath, as such environments have been referred to at least since the work of Caldeira and Leggett [23]. For classical systems one of the first presentations was by Zwanzig [53]. The material can also be found in monographs such as, e.g., Refs. [27,28]. The Ohmic bath with a time-dependent system-bath coupling is described in more detail in Ref. [30].

The starting point is the spectrum of the bath oscillators is continuous up to an upper cutoff \( \omega \) and increases quadratically with frequency. The number of oscillators with frequencies in the interval \([\omega, \omega + d\omega]\) is \( f(\omega)d\omega \) and

\[
f(\omega) = \begin{cases} \frac{3}{2} \omega_c^{-3} \omega^2 & \omega < \Omega, \\ 0 & \omega > \Omega, \end{cases}
\]

(B1)

where \( \omega_c \) is some characteristic frequency less than \( \Omega \). Alternatively, one can also consider an exponential cutoff \( \exp(-\omega/\Omega) \).

The interaction strength is given by a constant \( \eta \) with dimension (mass/time), such that

\[
C_b = \sqrt{\omega_c^3 m_b \eta}.
\]

(B2)
From this follows that
\[ \frac{C_{\omega, f}(\omega)}{m_\omega} = \frac{2\sqrt{\eta(t)\eta(s)}}{\pi} \omega^2 \omega < \Omega, \] (B3)
where quantities pertaining to a bath oscillator having that angular velocity are indexed by \( \omega \).

Using that \( \frac{1}{2} \int \cos \omega t \omega d\omega \) is a representation of \( \delta(t) \), and assuming \( \Omega \) very large (\( \Omega^{-1} \) much shorter than any relevant time scale of the system), the classical dynamics of this system is that of under-damped diffusion (Kramers-Langevin equation), while if \( h/k_B T \) is also shorter than any relevant timescale of the system (high enough temperature), then coherences (off-diagonal terms in the density matrix) are so small that the system behaves essentially classically and also obeys Kramers-Langevin equation, while if \( h/k_B T \) is not so small there are memory effects. A short discussion of the different timescales involved can be found in Ref. [29], Appendices A and B.