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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 three 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

$$H_{\mathrm{TOT}} = H_S + \sum_k \left(H_B^{(k)} + H_I^{(k)} + H_C^{(k)}\right), \tag{1}$$

where

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

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 $m_b\omega_b^2$; ω_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 the time dependence of $C_b(t)$ when that is not a problem. The last term in the Hamiltonian Eq. (1) is the Caldeira-Leggett counter-term (a correction to the system Hamiltonian), $H_C(t) = \sum_b \frac{C_b^2(t)X^2}{2m_b\omega_b^2}$. The counter-term, the interaction term in Eq. (4) and the potential in Eq. (3) together form a sum of complete squares, $\sum_b \frac{1}{2} m_b \omega_b^2 (q_b - \frac{C_b X}{m_b \omega_b})^2$.

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 β_k. The total initial state of the system and the baths is thus

$$\rho_i^{\mathrm{TOT}} = \rho_{B_1}^{\mathrm{eq}}(\beta_1) \otimes \rho_{B_2}^{\mathrm{eq}}(\beta_2) \otimes \cdots \otimes |i\rangle\langle i|, \tag{5}$$

where $\rho_{B_k}^{\mathrm{eq}}(\beta_k)$ is the Gibbs state of bath k at inverse temperature β_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 β. For this they introduced the notation

$$P_{if} = \mathrm{Tr}_B \langle f| \big(U \rho_i^{\mathrm{TOT}} U^\dagger\big) |f\rangle. \tag{6}$$

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),

$$F_{if}(\nu_1,\nu_2,\ldots) = \prod_k \mathrm{Tr}_{B_k} \langle f| e^{i(\sum_k \nu_k H_{B_k})} \big(U \rho_i^{\mathrm{TOT}} U^\dagger\big) |f\rangle, \tag{7}$$

$$\begin{aligned} G_{if}(\nu_1,\nu_2,\ldots) = \prod_k \mathrm{Tr}_{B_k} \langle f| e^{i(\sum_k \nu_k H_{B_k})} \\ \times \big(U e^{-i(\sum_k \nu_k H_{B_k})} \rho_i^{\mathrm{TOT}} U^\dagger\big) |f\rangle, \end{aligned} \tag{8}$$

where $\nu_1,\nu_2,\ldots$ 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 ν 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 ν are large the functionals probe the distribution of large energy changes. The functional F_{if} will be referred to as the characteristic function. The functional G_{if} will be referred to as the full counting statistics (FCS). As we will see in the following sections, F_{if} and G_{if} 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_{if} is related to the generating function of the energy of the baths in the final state, as can be seen as follows. Consider one bath and the probability $p_B(E|i,f)$ of observing a bath energy E at the final time, after the final measurement on the system. The probability of observing *one* state of the bath $|\mathcal{E}\rangle$, is $\langle\mathcal{E}|\rho_B^{\mathrm{post}}|\mathcal{E}\rangle$, where ρ_B^{post} is the reduced density matrix of the bath, after measuring the system and finding final state $|f\rangle$. This quantity is

$$\rho_B^{\mathrm{post}} = \frac{1}{P_{if}} \langle f|\rho_{\mathrm{TOT}}|f\rangle, \tag{9}$$

where ρ_{TOT} is the total density operator of the system and the bath at the end of the process. We then have

$$p_B(E|if) = \sum_{\mathcal{E}} \frac{1}{P_{if}} \mathbf{1}_{E(\mathcal{E}),E} \langle \mathcal{E},f|\rho_{\mathrm{TOT}}|\mathcal{E},f\rangle, \tag{10}$$

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

$$\begin{aligned} \int e^{i\nu E} p_B(E|if) dE &= \sum_{\mathcal{E}} \frac{1}{P_{if}} e^{i\nu E(\mathcal{E})} \langle \mathcal{E},f|\rho_{\mathrm{TOT}}|\mathcal{E},f\rangle \\ &= \frac{1}{P_{if}} F_{if}(\nu), \end{aligned} \tag{11}$$

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

$G_{if}(\nu)$ 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, $|\mathcal{E}_i,i\rangle$. If the initial state of the bath is measured but not recorded the initial state is a statistical mixture where $|\mathcal{E}_i,i\rangle$ has Gibbs weight $Z_B^{-1}(\beta)\exp[-\beta E(\mathcal{E}_i)]$. Consider $p_B(\Delta E,f|\mathcal{E}_i,i)$, the conditional probability of observing a final state $|f\rangle$ of the system and bath energy change ΔE, conditioned on total initial state $|\mathcal{E}_i,i\rangle$. Consider further $\overline{p}_B(\Delta E,f|i) = \sum_{\mathcal{E}_i} p_B(\Delta E,f|\mathcal{E}_i,i) Z_B^{-1}(\beta)\exp[-\beta E(\mathcal{E}_i)]$, which is the average $p_B(\Delta E,f|\mathcal{E}_i,i)$ over the stistical mixture. Similar to above,

$$\begin{aligned} \overline{p}_B(\Delta E,f|i) = \sum_{\mathcal{E}_f,\mathcal{E}_i} Z_B^{-1}(\beta) e^{-\beta E(\mathcal{E}_i)} \mathbf{1}_{E(\mathcal{E}_f)-E(\mathcal{E}_i),\Delta E} \\ \times \langle \mathcal{E}_f,f|\rho_{\mathrm{TOT}}(\mathcal{E}_i,i)|\mathcal{E}_f,f\rangle, \end{aligned} \tag{12}$$

where $\rho_{\mathrm{TOT}}(\mathcal{E}_i,i)$ 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 $|\mathcal{E}_i,i\rangle$. Resolving the δ function one can write

$$\overline{p}_B(\Delta E,f|i) = \frac{1}{2\pi} \int e^{-i\nu\Delta E} G_{if}(\nu) d\nu, \tag{13}$$

where

$$G_{if}(\nu) = \sum_{\mathcal{E}_f,\mathcal{E}_i} Z_B^{-1}(\beta) e^{-\beta E(\mathcal{E}_i)} e^{i\nu[E(\mathcal{E}_f)-E(\mathcal{E}_i)]} \times \langle \mathcal{E}_f, f|\rho_{\mathrm{TOT}}(\mathcal{E}_i,i)|\mathcal{E}_f,f\rangle. \quad (14)$$

By linearity the Gibbs weight and the factor $e^{-i\nu E(\mathcal{E}_i)}$ can be taken inside the the big unitary transformation defining $\rho_{\mathrm{TOT}}(\mathcal{E}_i,i)$. The above is therefore alternatively

$$G_{if}(\nu) = \mathrm{Tr}_B\langle f|e^{i\nu H_B} U e^{-i\nu H_B} \rho_i^{\mathrm{TOT}} U^{\dagger}|f\rangle, \quad (15)$$

which is the same expression as Eq. (8), for brevity stated for one bath. $G_{if}(\nu)$, 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 F_{if} AND G_{if}

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_{if} for conditional probability of measuring the system in final state $|f\rangle$ given that it was initially in $|i\rangle$. Using the shorthand,

$$\int_{if}(\cdots) = \int dX_i dY_i dX_f dY_f \psi_i(X_i)\psi_i^*(Y_i)\psi_f^*(X_f) \times \psi_f(Y_f)(\cdots),$$

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

$$P_{if} = \int_{if} \mathcal{D}X\mathcal{D}Y e^{\frac{i}{\hbar}S_S[X]-\frac{i}{\hbar}S_S[Y]+\frac{i}{\hbar}S_i[X,Y]-\frac{1}{\hbar}S_r[X,Y]}, \quad (16)$$

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 $\hat{\rho}_f^{\mathrm{TOT}} = U\hat{\rho}_i^{\mathrm{TOT}}U^{-1}$, and then integrating out the bath variables. The effects of the bath are thus captured by the two kernels S_i and S_r 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_r from *one* oscillator with a time-dependent system-bath coupling is

$$S_i^b = \int^t\int^s (X-Y)(X'+Y')\frac{C_bC_b'}{2m_b\omega_b}\sin\omega_b(s-s')ds'ds, \quad (17)$$

$$S_r^b = \int^t\int^s (X-Y)(X'-Y')\frac{C_bC_b'}{2m_b\omega_b}\coth\left(\frac{\omega\hbar\beta}{2}\right) \times \cos\omega_b(s-s')ds'ds, \quad (18)$$

where primed (unprimed) quantities refer to time s' (s) and β is the inverse temperature of the bath to which this oscillator belongs. The quantities in S_i and S_r in Eq. (16) are the *sums* of S_i^b and S_r^b from Eqs. (17) and (18). The expression for S_r^b is symmetric in $s \leftrightarrow s'$ and this integral can therefore be extended over the whole square $t_i \leqslant s,s' \leqslant t$. 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 $t_i \leqslant s' \leqslant s \leqslant t$.

The path integral expressions for F_{if} and G_{if} can be written

$$F_{if} = \int_{if} \mathcal{D}X\mathcal{D}Y e^{\frac{i}{\hbar}S_S[X]-\frac{i}{\hbar}S_S[Y]} \prod_b \mathcal{F}_b^{(F)}(\nu), \quad (19)$$

$$G_{if} = \int_{if} \mathcal{D}X\mathcal{D}Y e^{\frac{i}{\hbar}S_S[X]-\frac{i}{\hbar}S_S[Y]} \prod_b \mathcal{F}_b^{(G)}(\nu), \quad (20)$$

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

$$\mathcal{F}_b^{(F)}(\nu) = \frac{\left(\frac{2\pi\hbar}{\omega m}\right)^2 e^{\frac{i}{2m\omega\hbar}\underline{u}\tilde{M}_F{}^{-1}\underline{u}+\frac{i}{\hbar}B}}{Z(\beta)N(i\beta\hbar)|N(t)|^2N(\hbar\nu)(\det\tilde{M}_F)^{\frac{1}{2}}}, \quad (21)$$

$$\mathcal{F}_b^{(G)}(\nu) = \frac{\left(\frac{2\pi\hbar}{\omega m}\right)^2 e^{\frac{i}{2m\omega\hbar}\underline{u}\tilde{M}_G{}^{-1}\underline{u}+\frac{i}{\hbar}B}}{Z(\beta)N(i\beta\hbar-\hbar\nu)|N(t)|^2N(\hbar\nu)(\det\tilde{M}_G)^{\frac{1}{2}}}. \quad (22)$$

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

It was shown in Ref. [29] that all the prefactors in Eq. (21) combine to $\sinh(\frac{\omega\hbar\beta}{2})\sinh^{-1}(\frac{\omega\hbar(\beta-i\nu)}{2})$. 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 $\underline{u}$, B, and $\tilde{M}$ and the results can be written as

$$\prod_b \mathcal{F}_b^{(F)}(\nu) = (\text{trivial})\cdot e^{\frac{i}{\hbar}S_i-\frac{1}{\hbar}S_r+\mathcal{J}^{(1)}(\nu)+\mathcal{J}^{(2)}(\nu)+\mathcal{J}^{(3)}(\nu)}, \quad (23)$$

$$\prod_b \mathcal{F}_b^{(G)}(\nu) = e^{\frac{i}{\hbar}S_i-\frac{1}{\hbar}S_r+\mathcal{J}^{(2)}(\nu)+\mathcal{J}^{(3)}(\nu)}, \quad (24)$$

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

$$\mathcal{J}^{(1)} = \frac{i}{2m\omega\hbar}\int^t\int^t (XX'+YY')CC'\cos\omega(s-s') \times \left(\frac{y-z}{\Delta} - \frac{i}{2}\coth\frac{\omega\hbar\beta}{2}\right), \quad (25)$$

$$\mathcal{J}^{(2)} = \frac{i}{2m\omega\hbar}\int^t\int^t (XY'-X'Y)CC'\sin\omega(s-s') \times \left(\frac{y'z'-yz}{\Delta} - \frac{1}{2}\right), \quad (26)$$

$$\mathcal{J}^{(3)} = \frac{i}{2m\omega\hbar}\int^t\int^t (XY' + X'Y)CC'\cos\omega(s-s') \times\left(\frac{z'-y'}{\Delta} + \frac{i}{2}\coth\frac{\omega\hbar\beta}{2}\right), \tag{27}$$

where the auxiliary variables z, z', y, y' and Δ are combinations of trigonometric and hyperbolic functions in ν and β given in Appendix A. The definitions of z, z' and Δ differ a bit between Case F (F_{if}) and Case G (G_{if}). However, for both cases $\mathcal{J}^{(1)}$, $\mathcal{J}^{(2)}$, and $\mathcal{J}^{(3)}$ all vanish at $\nu = 0$. For Case G (G_{if}) 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 $F_{if}(\nu_1,\nu_2,\ldots)$ and $G_{if}(\nu_1,\nu_2,\ldots)$ introduced in Eqs. (7) and (8). For the rest of this section I will assume that the system interacts with two baths, a cold ("left") bath at inverse temperature β_L, and a hot ("right") bath at inverse temperature β_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 to X_L, and then from X_L out into the cold bath. A similar setting was recently considered in Ref. [34].

Suppose one is mainly interest 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

$$\overline{p}_B(\Delta E|i) = \sum_f \overline{p}_B(\Delta E, f|i). \tag{28}$$

The corresponding generating functions is $G_i(\nu_1,\nu_2)$. We have

$$G_i(\nu_1,\nu_2) = \sum_f G_{if}(\nu_1,\nu_2). \tag{29}$$

The starting point is then

$$\begin{aligned}G_i(\nu_1,\nu_2) &= \mathrm{Tr}_{B_L,B_R,S}\big\{e^{i(\nu_1 H_{B_L}+\nu_2 H_{B_R})} \times\big[Ue^{-i(\nu_1 H_{B_L}+\nu_2 H_{B_R})}\rho_i^{\mathrm{TOT}}U^\dagger\big]\big\}\\ &= \int_i \mathcal{D}X\mathcal{D}Y e^{\frac{i}{\hbar}S_S[X]-\frac{i}{\hbar}S_S[Y]}\prod_{b\in L}\mathcal{F}_b^{(G)}(\nu_1) \times\prod_{b\in R}\mathcal{F}_b^{(G)}(\nu_2)\,\delta(X^f - Y^f),\end{aligned} \tag{30}$$

where the trace is over the system and both baths and $\delta(X^f - Y^f)$ is the path integral rendering of Tr_S. The subscript of the integral $\int_i$ indicates the remaining dependence on the initial state of the system. The two products in Eq. (30) are

$$\prod_{b\in L}\mathcal{F}_b^{(G)}(\nu_1) = e^{\frac{i}{\hbar}S_i[X_L,Y_L]-\frac{1}{\hbar}S_r[X_L,Y_L]+\mathcal{J}^{(2)}(\nu)[X_L,Y_L]+\mathcal{J}^{(3)}(\nu)[X_L,Y_L]}, \tag{31}$$

$$\prod_{b\in R}\mathcal{F}_b^{(G)}(\nu_2) = e^{\frac{i}{\hbar}S_i[X_R,Y_R]-\frac{1}{\hbar}S_r[X_R,Y_R]+\mathcal{J}^{(2)}(\nu)[X_R,Y_R]+\mathcal{J}^{(3)}(\nu)[X_R,Y_R]}, \tag{32}$$

and the functionals are given as sums of the terms in Eqs. (17), (18), and (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 ν_1 and ν_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

$$\begin{aligned}\dot{Q} = \lim_{t_f-t_i\to\infty}\frac{\partial_{i\nu_1}G_i|_{\nu=0}}{t_f-t_i} &= \int_{-\infty}^0 h^{(2)}(0,s)\langle(X_L(0)Y_L(s) - X_L(s)Y_L(0))\delta(X_L(0)-Y_L(0))\rangle ds\\ &+ \int_{-\infty}^0 h^{(3)}(0,s)\langle(X_L(0)Y_L(s)+X_L(s)Y_L(0)) \times\delta(X_L(0)-Y_L(0))\rangle ds,\end{aligned} \tag{33}$$

where the two kernels are the terms linear in ν_1 of $\mathcal{J}^{(2)}$ and $\mathcal{J}^{(3)}$ as given in Eq. (A21) and Eq. (A22).

$$h^{(2)}(s,s') = i\sum_b \frac{C_b^2}{2m_b}\coth\left(\frac{\beta\hbar\omega_b}{2}\right)\sin\omega_b(s-s'), \tag{34}$$

$$h^{(3)}(s,s') = \sum_b \frac{C_b^2}{2m_b}\cos\omega_b(s-s'). \tag{35}$$

Up to a factor β 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 $h^{(2)}(s,s') \approx -\frac{2i}{\beta_L \hbar}\eta\frac{d\delta(s-s')}{d(s-s')}$ and $h^{(3)}(s,s') \approx -\eta\frac{d^2\delta(s-s')}{d(s-s')^2}$ [30], where η is the friction coefficient. Integration by parts turns Eq. (33) into

$$\dot{Q} = \int dXdY\delta(X-Y)\frac{i\eta}{\hbar\beta}\langle\dot{X}Y - X\dot{Y}\rangle\overline{\rho}_L(X,Y) + \int dXdY\delta(X-Y)2\eta\langle\dot{X}\dot{Y}\rangle\overline{\rho}_L(X,Y), \tag{36}$$

where $\overline{\rho}_L(X,Y)$ 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:

$$\hat{O}_1 = -2\frac{\eta}{M}\frac{\partial}{\partial(X-Y)}(X-Y), \tag{37}$$

$$\hat{O}_2 = -2\eta\hbar^2\frac{\eta}{M^2}\frac{\partial^2}{\partial(X-Y)^2}, \tag{38}$$

and

$$\dot{Q} = \mathrm{Tr}[\hat{O}_1\overline{\rho}_S] + \mathrm{Tr}[\hat{O}_2\overline{\rho}_S]. \tag{39}$$

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 quantum way of writing the heat per unit time as in classical stochastic thermodynamics.

For a quantum system with discrete state space (some number of qubits), one would have to go back to Eq. (36) for an Ohmic bath. If the qubits interact only through one spin component, say through $\hat{\sigma}_z$, then the dynamics of the system has a path integral representation first introduced by Leggett and coworkers for the spin-boson problem [25]. This approach (with or without a bath) has been developed further in the statistical physics community to model quantum annealing protocols [37,38]. If, however, the qubits interact in a more general manner, as they would theoretically have to in general-purpose quantum computational device, then a more involved path integral representation would have to be used [39–41]. For a quantum system interacting with baths that are not Ohmic (non-Markovian state evolution), one would have to go back to Eq. (33).

V. CONCEPTUAL AND TECHNICAL PROBLEMS OF QUANTUM HEAT

In this paper I have defined quantum heat as the changes of bath energy when the baths are initially in thermal equilibrium and the system-bath interaction vanishes at the beginning and the end of a process. This translates to the quantum domain the strong-coupling classical definition of heat introduced in Ref. [30]. It could have been assumed that it would be simpler to take 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 fermonic 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 $e^{i\nu H_B + i\nu\lambda H_{SB}}$ at the final time and $e^{-i\nu H_B}$ at the initial time; λ is here an additional parameter. The interaction is with one bath at inverse temperature β, and leads to expressions of a similar structure to the ones given above for G_{if}. 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], 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 $e^{-i\nu(H_B+H_{SB})}$ at the final time and $e^{-i\nu(H_B+H_{SB})}$ 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_{if}. 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 $\langle H_B + H_{SB}\rangle_f - \langle H_+ + H_{SB}\rangle_i$ where both averages are over the system and the bath implies the same definition of quantum heat as used in Ref. [47].

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 system-bath interaction switched on/off at the beginning and the end of the process and was discussed in detail for a classical situation in Ref. [21]. The generating functions computed here directly generalize earlier results on the expected value (first moment) obtained in Refs. [29,30].

The most remarkable analytic properties of all these results are quite explicit formulas for the generating functions. These are quadratic functionals of the forward and backward paths in the Feynman-Vernon formalism, with kernels of a similar type as for the real and imaginary parts of the Feynman-Vernon action, i.e., combinations of trigonometric and hyperbolic functions of time differences, bath oscillator frequencies, bath temperatures, and the generating function parameters. The first and second derivatives of the generating functions at the origin have been evaluated (in Appendix A) and determine the expected value, variances, and cross-correlations of bath energy changes.

I have also in this paper pointed out that the extended Feynman-Vernon approach works equally well for systems interacting with more than one bath at different temperatures. It is therefore a principled way to define and estimate nonequilibrium quantum heat flows. As an example I have derived the quantum thermal power of a system connected to an Ohmic heat bath and showed that it agrees with average power in the classical limit.

The real potential advantage of the approach developed here would be that it could also in practice be applied to systems with discrete states. Superconducting qubits is the currently favored platform for quantum computing [48]; every computing element or "qubit" is then in fact a degree of freedom of a large (mesoscopic) object at very low temperature [49]. Understanding heat flow and other thermal properties of such objects is an active area of research [35], where a general theoretical framework so far has been lacking. In this context it is noteworthy that generating functions of the type considered here (with one bath) already were applied to the spin-boson problem in Ref. [32].

Finally, a thermal bath consisting of harmonic oscillators is a model of delocalized environmental modes such as phonons. Another class of solvable models are chains of harmonic oscillators with a prescribed state of heat flux, for recent use (and for a system with discrete state), see Ref. [50]. Physically this would model environmental modes that are localized, hence not phonons, and which can be described as coupled oscillators. The main degrees of freedom in a real material at very low temperature, such as defects and nuclear spins, are likely to be localized, but may be more accurately described as a spin bath [51]. Path integral representations of systems interacting with such spin baths were developed quite some time ago [52] and could potentially be extended to also describe heat flows between such baths.

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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 $\mathcal{J}^{(1)}$, $\mathcal{J}^{(2)}$, and $\mathcal{J}^{(3)}$ 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 $\underline{u}$, appropriate for when the coupling coefficient depends on time, is

$$\underline{u} = \begin{pmatrix} u = \frac{1}{\sin\omega t}\int^t \sin\omega(t-s)[C(s)X(s)]ds \\ v = \frac{1}{\sin\omega t}\int^t \sin\omega(t-s)[-C(s)Y(s)]ds \\ u' = \frac{1}{\sin\omega t}\int^t \sin\omega s[C(s)X(s)]ds \\ v' = \frac{1}{\sin\omega t}\int^t \sin\omega s[-C(s)Y(s)]ds \end{pmatrix}. \quad \text{(A1)}$$

The function B is similarly

$$B=-\frac{1}{m\omega\sin(\omega t)}\int^t\!\!\int^s \sin\omega(t-s)\sin\omega s' CXC'X'ds'ds +\frac{1}{m\omega\sin(\omega t)}\int^t\!\!\int^s \sin\omega(t-s)\sin\omega s' CYC'Y'ds'ds, \tag{A2}$$

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:

$$\tilde{M}=\begin{pmatrix} -x-z & z' & x' & 0\\ z' & x-z & 0 & x'\\ x' & 0 & -x+y & -y'\\ -x-z & z' & -y' & x+y \end{pmatrix}. \tag{A3}$$

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 $x=\cot(\omega t)$, $x'=\sin^{-1}(\omega t)$, $y=\cot(\omega\hbar\nu)$, $y'=\sin^{-1}(\omega\hbar\nu)$, $z=\cot(-i\omega\hbar\beta)=i\coth(\omega\hbar\beta)$ and $z'=\sin^{-1}(-i\omega\hbar\beta)=i\sinh^{-1}(\omega\hbar\beta)$.

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

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

$$z'^2-z^2=y'^2-y^2=x'^2-x^2=1. \tag{A4}$$

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

$$\tilde{M}^{-1}=\frac{1}{\Delta}\begin{pmatrix} y-z & y'-z' & D & -B\\ y'-z' & y-z & -C & A\\ D & -C & y-z & y'-z'\\ -B & A & y'-z' & y-z \end{pmatrix}, \tag{A5}$$

where new auxiliary variables are

$$A=\frac{1}{x'}(1+x(y-z)+yz-y'z'), \tag{A6}$$

$$B=\frac{1}{x'}(x(z'-y')+y'z-yz'), \tag{A7}$$

$$C=\frac{1}{x'}(x(z'-y')-y'z+yz'), \tag{A8}$$

$$D=\frac{1}{x'}(-1+x(y-z)-yz+y'z'), \tag{A9}$$

and

$$\Delta=AD-BC=2(y'z'-yz-1). \tag{A10}$$

The combination that enters the exponent in Eqs. (21) and (22) in the main text is thus

$$\underline{u}\tilde{M}^{-1}\underline{u}=\frac{1}{\Delta}((y-z)(u^2+v^2+u'^2+v'^2) +(y'-z')(2uv+2u'v')+2Duu' -2Buv'-2Cvu'+2Avv'), \tag{A11}$$

where u, v, u', and v' are given in Eq. (A1). Combining this with the term $\frac{i}{\hbar}B$ and using trigonometric identities the whole expression reduces to

$$\text{Expr.}=\frac{i}{\hbar}S_i-\frac{1}{\hbar}S_r+\mathcal{J}^{(1)}+\mathcal{J}^{(2)}+\mathcal{J}^{(3)}, \tag{A12}$$

where the Feynman-Vernon terms S_i and S_r are given in Eqs. (17) and (18). Restating for convenience here Eqs. (25)–(27) in the main text they are

$$\mathcal{J}^{(1)}=\frac{i}{2m\omega\hbar}\int^t\!\!\int^t (XX'+YY')CC'\cos\omega(s-s') \times\left(\frac{y-z}{\Delta}-\frac{i}{2}\coth\frac{\omega\hbar\beta}{2}\right), \tag{A13}$$

$$\mathcal{J}^{(2)}=\frac{i}{2m\omega\hbar}\int^t\!\!\int^t (XY'-X'Y)CC'\sin\omega(s-s') \times\left(\frac{y'z'-yz}{\Delta}-\frac{1}{2}\right), \tag{A14}$$

$$\mathcal{J}^{(3)}=\frac{i}{2m\omega\hbar}\int^t\!\!\int^t (XY'+X'Y)CC'\cos\omega(s-s') \times\left(\frac{z'-y'}{\Delta}+\frac{i}{2}\coth\frac{\omega\hbar\beta}{2}\right). \tag{A15}$$

The only difference in the expressions for cases **F** and **G** are the different interpretations of the auxiliary variables z, z', and Δ. We now proceed to simplify the coefficients in the kernels in the two cases.

1. Case F

We here have

$$\begin{aligned}\Delta=2(z'y'-yz-1)&=2i\sinh^{-1}(\omega\hbar\beta)\sin^{-1}(\omega\hbar\nu)[1-\cos(\omega\hbar\nu)\cosh(\omega\hbar\beta)+i\sin(\omega\hbar\nu)\sinh(\omega\hbar\beta)]\\ &=2i\sinh^{-1}(\omega\hbar\beta)\sin^{-1}(\omega\hbar\nu)\{1-\cos[\omega\hbar(\nu+i\beta)]\},\end{aligned} \tag{A16}$$

and the expressions simplify to

$$\begin{aligned}\frac{y-z}{\Delta}&=\frac{1}{2}\frac{\cos(\omega\hbar\nu)\sin(\omega\hbar(-i\beta))-\sin(\omega\hbar\nu)\cos[\omega\hbar(-i\beta)]}{1-\cos[\omega\hbar(\nu+i\beta)]}=\frac{1}{2}\cot\left[\frac{\omega\hbar(\nu+i\beta)}{2}\right],\\ \frac{y'z'-yz}{\Delta}&=\frac{1}{2}\frac{1-\cos(\omega\hbar\nu)\cos[\omega\hbar(-i\beta)]}{1-\cos[\omega\hbar(\nu+i\beta)]}=\frac{1}{2}+\frac{i}{4}\frac{\sin(\omega\hbar\nu)\sinh(\omega\hbar\beta)}{\sin^2\left(\frac{\omega\hbar(\nu+i\beta)}{2}\right)},\\ \frac{z'-y'}{\Delta}&=\frac{1}{2}\frac{\sin(\omega\hbar\nu)+i\sinh(\omega\hbar\beta)}{1-\cos[\omega\hbar(\nu+i\beta)]}=+\frac{1}{4}\frac{\sin(\omega\hbar\nu)+i\sinh(\omega\hbar\beta)}{\sin^2\left(\frac{\omega\hbar(\nu+i\beta)}{2}\right)}.\end{aligned}$$

All three functionals $\mathcal{J}^{(1)}$, $\mathcal{J}^{(2)}$, and $\mathcal{J}^{(2)}$ vanish at $\nu = 0$ as follows by insertion in the above. Their derivatives at $\nu = 0$ are

$$\frac{\partial \mathcal{J}^{(1)}}{\partial \nu}|_{\nu=0} = -\frac{i}{8m}\int^t\!\!\int^t (XX' + YY')CC' \cos\omega(s-s')\frac{1}{\sinh^2\left(\frac{\omega\hbar\beta}{2}\right)}, \tag{A17}$$

$$\frac{\partial \mathcal{J}^{(2)}}{\partial \nu}|_{\nu=0} = -\frac{1}{4m}\int^t\!\!\int^t (XY' - X'Y)CC' \sin\omega(s-s')\coth\left(\frac{\omega\hbar\beta}{2}\right), \tag{A18}$$

$$\frac{\partial \mathcal{J}^{(3)}}{\partial \nu}|_{\nu=0} = \frac{i}{8m}\int^t\!\!\int^t (XY' + X'Y)CC' \cos\omega(s-s')\left(\frac{1}{\sinh^2\left(\frac{\omega\hbar\beta}{2}\right)} + 2\right), \tag{A19}$$

The derivative of the second term $(y'z' - yz)/\Delta$ gives the term called $\mathcal{I}^{(2)}$ 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 $\nu = i\epsilon$ and a factor two from the definition of the double integrals.

2. Case G

We here have

$$\begin{aligned}\Delta = 2(z'y' - yz - 1) &= 2\sin^{-1}[\omega\hbar(\nu - i\beta)]\sin^{-1}(\omega\hbar\nu)\{1 - \cos(\omega\hbar\nu)\cos[\omega\hbar(\nu - i\beta)] - \sin(\omega\hbar\nu)\sin[\omega\hbar(\nu - i\beta)]\}\\ &= 2\sin^{-1}[\omega\hbar(\nu - i\beta)]\sin^{-1}(\omega\hbar\nu)[1 - \cosh(\omega\hbar\beta)],\end{aligned} \tag{A20}$$

and the expressions simplify a bit further to

$$\begin{aligned}\frac{y-z}{\Delta} &= \frac{1}{2}\frac{\cos(\omega\hbar\nu)\sin[\omega\hbar(\nu - i\beta)] - \sin(\omega\hbar\nu)\cos[\omega\hbar(\nu - i\beta)]}{1 - \cosh(\omega\hbar\beta)} = \frac{i}{2}\coth\left(\frac{\omega\hbar\beta}{2}\right),\\ \frac{y'z' - yz}{\Delta} &= \frac{1}{2}\frac{1 - \cos(\omega\hbar\nu)\cos[\omega\hbar(\nu - i\beta)]}{1 - \cosh(\omega\hbar\beta)} = \frac{1}{2} - \frac{1}{4}\frac{\sin\omega\hbar\nu\sin\omega\hbar(\nu - i\beta)}{\sinh^2\left(\frac{\omega\hbar\beta}{2}\right)},\\ \frac{z' - y'}{\Delta} &= \frac{1}{2}\frac{\sin(\omega\hbar\nu) - \sin[\omega\hbar(\nu - i\beta)]}{1 - \cosh(\omega\hbar\beta)} = -\frac{i}{2}\cos(\omega\hbar\nu)\coth\left(\frac{\omega\hbar\beta}{2}\right) + \frac{1}{2}\sin(\omega\hbar\nu).\end{aligned}$$

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

$$\frac{\partial \mathcal{J}^{(2)}}{\partial \nu}|_{\nu=0} = -\frac{1}{4m}\int^t\!\!\int^t (XY' - X'Y)CC' \sin\omega(s-s')\coth\left(\frac{\omega\hbar\beta}{2}\right), \tag{A21}$$

$$\frac{\partial \mathcal{J}^{(3)}}{\partial \nu}|_{\nu=0} = \frac{i}{4m}\int^t\!\!\int^t (XY' + X'Y)CC' \cos\omega(s-s'), \tag{A22}$$

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

$$\frac{\partial^2 \mathcal{J}^{(2)}}{\partial \nu^2}|_{\nu=0} = -\frac{i\omega\hbar}{4m}\int^t\!\!\int^t (XY' - X'Y)CC' \sin\omega(s-s')\left[1 + \coth^2\left(\frac{\omega\hbar\beta}{2}\right)\right], \tag{A23}$$

$$\frac{\partial^2 \mathcal{J}^{(3)}}{\partial \nu^2}|_{\nu=0} = \frac{\omega\hbar}{4m}\int^t\!\!\int^t (XY' + X'Y)CC' \cos\omega(s-s')\coth\left(\frac{\omega\hbar\beta}{2}\right). \tag{A24}$$

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 Ω and increases quadratically with frequency. The number of oscillators with frequencies in the interval $[\omega,\omega + d\omega]$ is $f(\omega)d\omega$ and

$$\begin{aligned} f(\omega) &= \tfrac{2}{\pi}\omega_c^{-3}\omega^2 & \omega < \Omega,\\ f(\omega) &= 0 & \omega > \Omega,\end{aligned} \tag{B1}$$

where ω_c is some characteristic frequency less than Ω. Alternatively, one can also consider an exponential cutoff $\exp(-\frac{\omega}{\Omega})$.

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

$$C_b = \sqrt{\omega_c^3 m_b \eta}. \tag{B2}$$

From this follows that

$$\frac{C_\omega^2 f(\omega)}{m_\omega} = \frac{2\sqrt{\eta(t)\eta(s)}}{\pi}\omega^2 \quad \omega < \Omega, \tag{B3}$$

where quantities pertaining to a bath oscillator having that angular velocity are indexed by ω.

Using that $\frac{1}{2\pi}\int \cos \omega t d\omega$ is a representation of $\delta(t)$, and assuming Ω very large (Ω^{-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) with friction coefficient η and noise strength $\sqrt{2k_BT\eta}$. Quantum-mechanically the situation also depends on bath temperature T, as discussed in Ref. [23]. If the thermal time $\hbar/k_BT$ 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 $\hbar/k_BT$ 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.

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