Clausius inequality beyond the weak-coupling limit: The quantum Brownian oscillator

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We consider a quantum linear oscillator coupled at an arbitrary strength to a bath at an arbitrary temperature. We find an exact closed expression for the oscillator density operator. This state is noncanonical but can be shown to be equivalent to that of an *uncoupled* linear oscillator at an effective temperature $T_{\text{eff}}^{\star}$ with an effective mass and an effective spring constant. We derive an effective Clausius inequality $\delta Q_{\text{eff}}^{\star} \le T_{\text{eff}}^{\star} dS$, where $\delta Q_{\text{eff}}^{\star}$ is the heat exchanged between the effective (weakly coupled) oscillator and the bath, and S represents a thermal entropy of the effective oscillator, being identical to the von-Neumann entropy of the coupled oscillator. Using this inequality (for a cyclic process in terms of a variation of the coupling strength) we confirm the validity of the second law. For a fixed coupling strength this inequality can also be tested for a process in terms of a variation of either the oscillator mass or its spring constant. Then it is never violated. The properly defined Clausius inequality is thus more robust than assumed previously.

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I. INTRODUCTION

Thermodynamics of small quantum objects coupled to quantum environments in the low-temperature regime has attracted considerable interest as the need for a better theoretical understanding increases in response to novel experimental manipulation of such systems. In particular, the finite coupling strength between system and environment gives rise to some quantum subtleties and so can no longer be neglected (calling for methods addressed by "quantum thermodynamics" [1–3]) whereas ordinary quantum statistical mechanics is intrinsically based on a vanishingly small coupling between them.

At the heart of quantum thermodynamics, the foundational question as to the validity of the second law of thermodynamics comes up. In fact, with its challenge the applicability of thermodynamics is at stake. So far, the validity of this basic law has extensively been examined in the scheme of a quantum harmonic oscillator linearly coupled to an independent-oscillator model of a heat bath (quantum Brownian oscillator) in equilibrium at a low temperature T. It has been argued here that there is a violation of the Clausius inequality representing the second law [4,5] in such a way that $\delta Q \nleq T dS$ at $T \to 0$ with respect to a variation of a Hamiltonian parameter of the coupled oscillator, namely, either its mass or spring constant. In the above relation, δQ is the heat and dS is the entropy change.

However, following the second law in its Kelvin-Planck form, which states that it is impossible to devise a machine (i.e., a heat engine) which, operating in a cycle, produces no effect other than the extraction of heat from a thermal energy reservoir and the performance of an equal amount of work [6], it has been demonstrated that an apparent excess energy in the coupled oscillator at zero temperature ($T=0$) is less than the minimum value of the work (equivalent to the Helmholtz free energy at a constant temperature) to couple the free oscillator to a bath so that the second law is not violated down to zero temperature [7,8].

This result has been generalized to a cyclic process of coupling and decoupling between the oscillator and a bath at an arbitrary temperature by obtaining the positive valuedness of the minimum work needed for the coupling minus the maximum useful work obtainable from the oscillator in the decoupling (the second law with respect to a variation of the coupling strength) [9]. This positive valuedness is actually at its maximum at zero temperature and asymptotically vanishes with increasing temperature, whereas the classical counterpart would identically vanish at an arbitrary temperature (even for a nonvanishing coupling). It was further claimed here that this quantum behavior is associated with the system-bath entanglement induced by the finite coupling strength between them (clearly, the coupled total system (i.e., the coupled oscillator plus bath) is in a thermal state with (partial) entanglement whereas the decoupled total system is simply in a separable state). It has, indeed, been found that at zero temperature the energy fluctuation in the coupled oscillator can provide entanglement information [10,11]. This claim was supported by the numerical analysis of the system-bath negativity as an exact entanglement measure [12] that the negativity behavior versus temperature is in accordance with the above quantum behavior of the second law up to the existence of the critical temperature above which the negativity vanishes.

It has also been shown [12] that the Clausius inequality (in terms of the equilibrium temperature of the *total* coupled system and the von-Neumann entropy of the coupled oscillator) is actually violated with respect to a variation of the mass of the coupled oscillator (not a variation of the coupling strength); the behavior of this violation versus the temperature is essentially different from that of the system-bath negativity so that it has been concluded that the system-bath entanglement is not responsible for the violation of the Clausius inequality. However, as the reduced equilibrium density operator of the coupled oscillator is not in form of the canonical thermal state $\hat{\rho}_\beta \propto e^{-\beta \hat{H}_s}$, there is not a well-defined

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local temperature of the coupled oscillator (especially in the low-temperature limit) so that applying the equilibrium temperature of the *total* coupled system for the violation of the Clausius inequality for the subsystem (actually with respect to a variation of a *local* parameter of the coupled oscillator, namely, either its mass or spring constant) is not justified. Further, this violation was actually based on the numerical findings [12] that the heat $\delta\mathcal{Q}$ exchanged with a bath in a reversible variation of the local parameter is always strictly greater than TdS, which, however, does not satisfy the equality condition of a well-defined Clausius inequality for the reversible process.

On the other hand, introducing some generalized entropic measure and using its maximum condition [13] it has been shown that the Clausius inequality obtained in some operational form is valid under such a generalization [14]. However, this approach is not directly applicable for the quantum Brownian oscillator since the reduced density operator of the coupled oscillator in equilibrium [cf. Eqs. (17) and (18)] is not in form of the stationary state obtained from the maximum condition of this generalization.

In this paper we intend to resolve the above controversial issue by introducing an effective Clausius inequality with no violation, well defined in the scheme of quantum Brownian oscillator. To do so, we begin with considering the reduced density operator of the coupled oscillator.

II. REDUCED DENSITY OPERATOR OF THE COUPLED OSCILLATOR

The quantum Brownian motion in consideration is described by the model Hamiltonian

$$\hat{H} = \hat{H}_s + \hat{H}_b + \hat{H}_{sb}, \tag{1}$$

where

$$\hat{H}_s = \frac{\hat{p}^2}{2M} + \frac{k_0}{2}\hat{q}^2; \quad \hat{H}_b = \sum_{j=1}^{N}\left(\frac{\hat{p}_j^2}{2m_j} + \frac{k_j}{2}\hat{x}_j^2\right),$$

$$\hat{H}_{sb} = -\hat{q}\sum_{j=1}^{N} c_j\hat{x}_j + \hat{q}^2\sum_{j=1}^{N}\frac{c_j^2}{2k_j}, \tag{2}$$

and the spring constants are $k_0 = M\omega_0^2$ and $k_j = m_j\omega_j^2$. From the hermiticity of Hamiltonian, the coupling constants c_j are obviously real valued. The total system is assumed to be in the canonical thermal equilibrium state $\hat{\rho}_\beta = e^{-\beta\hat{H}}/Z_\beta$ where $\beta = 1/(k_B T)$, and Z_β is the partition function. From the fluctuation-dissipation theorem [15,16], it is known [17] that

$$\langle\hat{q}^2\rangle_\beta = \frac{\hbar}{\pi}\int_0^\infty d\omega \coth\left(\frac{\beta\hbar\omega}{2}\right)\mathrm{Im}\{\widetilde{\chi}(\omega + i0^+)\} \tag{3}$$

$$\langle\hat{p}^2\rangle_\beta = \frac{M^2\hbar}{\pi}\int_0^\infty d\omega\omega^2 \coth\left(\frac{\beta\hbar\omega}{2}\right)\mathrm{Im}\{\widetilde{\chi}(\omega + i0^+)\} \tag{4}$$

in terms of the susceptibility

$$\widetilde{\chi}(\omega) = -\frac{1}{M}\frac{\prod_{j=1}^{N}(\omega^2 - \omega_j^2)}{\prod_{k=0}^{N}(\omega^2 - \varpi_k^2)}, \tag{5}$$

where $\{\varpi_k\}$ are the normal-mode frequencies of the total system $\hat{H}$. For an uncoupled oscillator, Im $\widetilde{\chi}(\omega+i0^+)$ obviously reduces to $\frac{\pi}{2M\omega_0}\delta(\omega-\omega_0)$ and thus $\langle\hat{q}^2\rangle_\beta = \frac{\hbar}{2M\omega_0}\coth\frac{\beta\hbar\omega_0}{2}$ and $\langle p^2\rangle_\beta = \frac{M\hbar\omega_0}{2}\coth\frac{\beta\hbar\omega_0}{2}$. For the well-known Drude model (with a cutoff frequency ω_d and a damping parameter γ_o), which is a prototype for physically realistic damping, we have [9]

$$\langle\hat{q}^2\rangle_\beta^{(d)} = \frac{1}{M}\sum_{l=1}^{3}\lambda_d^{(l)}\left\{\frac{1}{\beta\underline{\omega_l}} + \frac{\hbar}{\pi}\psi\left(\frac{\beta\hbar\underline{\omega_l}}{2\pi}\right)\right\} \tag{6}$$

$$\langle\hat{p}^2\rangle_\beta^{(d)} = -M\sum_{l=1}^{3}\lambda_d^{(l)}\underline{\omega_l}^2\left\{\frac{1}{\beta\underline{\omega_l}} + \frac{\hbar}{\pi}\psi\left(\frac{\beta\hbar\underline{\omega_l}}{2\pi}\right)\right\} \tag{7}$$

in terms of the digamma function $\psi(y) = d\ln\Gamma(y)/dy$ [18], where $\underline{\omega_1} = \Omega$, $\underline{\omega_2} = z_1$, $\underline{\omega_3} = z_2$, and the coefficients

$$\lambda_d^{(1)} = \frac{z_1 + z_2}{(\Omega - z_1)(z_2 - \Omega)}; \quad \lambda_d^{(2)} = \frac{\Omega + z_2}{(z_1 - \Omega)(z_2 - z_1)};$$

$$\lambda_d^{(3)} = \frac{\Omega + z_1}{(z_2 - \Omega)(z_1 - z_2)}. \tag{8}$$

Here we have adopted, in place of $(\omega_0, \omega_d, \gamma_o)$, the parameters $(\mathbf{w}_0, \Omega, \gamma)$ through the relations [7]

$$\omega_0^2 \coloneqq \mathbf{w}_0^2\frac{\Omega}{\Omega + \gamma}; \quad \omega_d \coloneqq \Omega + \gamma; \quad \gamma_o \coloneqq \gamma\frac{\Omega(\Omega + \gamma) + \mathbf{w}_0^2}{(\Omega + \gamma)^2}, \tag{9}$$

and then $z_1 = \gamma/2 + i\mathbf{w}_1$ and $z_2 = \gamma/2 - i\mathbf{w}_1$ with $\mathbf{w}_1 = \sqrt{(\mathbf{w}_0)^2 - (\gamma/2)^2}$.

The equilibrium density operator of the coupled oscillator is known as [16,19]

$$\langle q|\hat{\rho}_s|q'\rangle = \frac{1}{\sqrt{2\pi\langle\hat{q}^2\rangle_\beta}}\exp\left(-\frac{(q+q')^2}{8\langle\hat{q}^2\rangle_\beta} - \frac{\langle\hat{p}^2\rangle_\beta(q-q')^2}{2\hbar^2}\right). \tag{10}$$

For an uncoupled oscillator this easily reduces to a well-known expression [20]

$$\langle q|\hat{\rho}_\beta|q'\rangle = \sqrt{\frac{c^2}{\pi}\tanh\frac{\beta\hbar\omega_0}{2}}\exp\left(-\frac{c^2}{4}\left\{(q+q')^2\tanh\left(\frac{\beta\hbar\omega_0}{2}\right) + (q-q')^2\coth\left(\frac{\beta\hbar\omega_0}{2}\right)\right\}\right) \tag{11}$$

where the parameter

$$c = \sqrt{\frac{M\omega_0}{\hbar}}. \tag{12}$$

Let us now derive a closed form of the matrix elements

$$\rho_{nm} := \langle n|\hat{\rho}_s|m\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dq dq' \, \psi_n^*(q)\langle q|\hat{\rho}_s|q'\rangle\psi_m(q') \tag{13}$$

in the basis composed of the eigenstates $\{|n\rangle, |m\rangle\}$ of an uncoupled oscillator to confirm its deviation from a (diagonal) form of the canonical thermal state $\hat{\rho}_\beta$. After making lengthy calculations, every single step of which is provided in a detail in Appendix A, we arrive at the closed expressions

$$\rho_{2k,2l+1} = \rho_{2k+1,2l} = 0, \tag{14a}$$

$$\rho_{2k,2l} = \frac{(-\Upsilon_\beta)^{k+l}}{c\sqrt{2\pi\langle\hat{q}^2\rangle_\beta A_\beta}}\sqrt{\frac{\Gamma\left(k+\frac{1}{2}\right)}{k!}\frac{\Gamma\left(l+\frac{1}{2}\right)}{l!}} \times {}_2F_1\left(-k,-l;\frac{1}{2};\frac{1}{\Delta_\beta}\right) \tag{14b}$$

$$\rho_{2k+1,2l+1} = \frac{2\Lambda_\beta(-\Upsilon_\beta)^{k+l}}{c\sqrt{2\pi\langle\hat{q}^2\rangle_\beta A_\beta}}\sqrt{\frac{\Gamma\left(k+\frac{3}{2}\right)}{k!}\frac{\Gamma\left(l+\frac{3}{2}\right)}{l!}} \times {}_2F_1\left(-k,-l;\frac{3}{2};\frac{1}{\Delta_\beta}\right) \tag{14c}$$

in terms of the hypergeometric function ${}_2F_1(a,b;c;z)$ [18]. Here, the four dimensionless quantities

$$A_\beta = \frac{\left(c^2+\frac{2\langle\hat{p}^2\rangle_\beta}{\hbar^2}\right)\left(c^2+\frac{1}{2\langle\hat{q}^2\rangle_\beta}\right)}{4c^4}; \quad \Upsilon_\beta = \frac{\frac{\langle\hat{p}^2\rangle_\beta}{\hbar^2\langle\hat{q}^2\rangle_\beta}-c^4}{4c^4A_\beta};$$

$$\Lambda_\beta = \frac{\frac{\langle\hat{p}^2\rangle_\beta}{\hbar^2}-\frac{1}{4\langle\hat{q}^2\rangle_\beta}}{2c^2A_\beta}; \quad \Delta_\beta = \left(\frac{\Upsilon_\beta}{\Lambda_\beta}\right)^2. \tag{15}$$

As shown, the reduced density matrix $(\hat{\rho}_s)_{nm}$ is symmetric with respect to (n,m). Subsequently we also find (cf. Appendix A) that for $k \geq l$,

$$\rho_{2k,2l} = \frac{(-\Upsilon_\beta)^{k-l}(\Lambda_\beta)^{2l}(1-\Delta_\beta)^l}{c\sqrt{2\langle\hat{q}^2\rangle_\beta A_\beta}} \times \sqrt{\frac{\Gamma\left(k+\frac{1}{2}\right)}{\Gamma\left(l+\frac{1}{2}\right)}\frac{k!}{l!}\frac{\Gamma(2l+1)}{\Gamma(k+l+1)}} P_{2l}^{(k-l,k-l)}\left(\frac{1}{\sqrt{1-\Delta_\beta}}\right), \tag{16a}$$

$$\rho_{2k+1,2l+1} = \frac{(-\Upsilon_\beta)^{k-l}(\Lambda_\beta)^{2l+1}(1-\Delta_\beta)^{l+1/2}}{c\sqrt{2\langle\hat{q}^2\rangle_\beta A_\beta}} \times \sqrt{\frac{\Gamma\left(k+\frac{3}{2}\right)}{\Gamma\left(l+\frac{3}{2}\right)}\frac{k!}{l!}\frac{\Gamma(2l+2)}{\Gamma(k+l+2)}} \times P_{2l+1}^{(k-l,k-l)}\left(\frac{1}{\sqrt{1-\Delta_\beta}}\right), \tag{16b}$$

in terms of the Jacobi polynomial [18] and for $k<l$ the matrix elements $\rho_{2k,2l}$ and $\rho_{2k+1,2l+1}$ correspond, respectively, to Eqs. (16a) and (16b) with exchange of k and l. These are easily united into such a single expression that for either (n even$\geq m$ even) or (n odd$\geq m$ odd),

$$(\hat{\rho}_s)_{nm} = \frac{(-\Upsilon_\beta)^{n-m/2}(\Lambda_\beta)^{m+1/2}(\sqrt{1-\Delta_\beta})^m}{\sqrt{\frac{\langle\hat{q}^2\rangle_\beta\langle\hat{p}^2\rangle_\beta}{\hbar^2}-\frac{1}{4}}} \times \sqrt{\frac{\Gamma\left(\left[\frac{n+1}{2}\right]+\frac{1}{2}\right)\left[\frac{n}{2}\right]!}{\Gamma\left(\left[\frac{m+1}{2}\right]+\frac{1}{2}\right)\left[\frac{m}{2}\right]!}\frac{\Gamma(m+1)}{\Gamma\left(\frac{n+m}{2}+1\right)}} \times P_m^{(n-m/2,n-m/2)}\left(\frac{1}{\sqrt{1-\Delta_\beta}}\right), \tag{17}$$

and for either (n even$<m$ even) or (n odd$<m$ odd) the matrix elements $(\hat{\rho}_s)_{nm}$ are obviously given by Eq. (17) with exchange of m and n, where $[y]$ represents the greatest integer less than or equal to y. On the other hand, from Eq. (14a),

$$(\hat{\rho}_s)_{nm} = 0 \tag{18}$$

where either (n even,m odd) or (n odd,m even). As seen, the reduced density matrix $(\hat{\rho}_s)_{nm}$ is, in general, not in diagonal form of the canonical thermal state $e^{-\beta\hbar\omega_0(n+1/2)}/Z_\beta$ being valid for an uncoupled oscillator, where $\Lambda_\beta \to e^{-\beta\hbar\omega_0}$ and $\Delta_\beta \to 0$. This confirms that there is not a well-defined *local* temperature when one keeps starring at the oscillator $\hat{H}_s$, hence ignoring that it (strongly) couples to a bath (cf. Sec. III, in which, on the other hand, a well-defined effective local temperature is introduced). We note here, however, that by using $\hat{q}=\sqrt{\frac{\hbar}{2m\omega_0}}(\hat{a}+\hat{a}^\dagger)$, $\hat{p}=i\sqrt{\frac{m\hbar\omega_0}{2}}(\hat{a}^\dagger-\hat{a})$, and the matrix elements [Eq. (18)] with $\hat{a}|n\rangle=\sqrt{n}|n-1\rangle$ and $\hat{a}^\dagger|n\rangle=\sqrt{n+1}|n+1\rangle$, as is the case for an uncoupled oscillator,

$$\langle\hat{q}\rangle_\beta = \mathrm{Tr}_s(\hat{q}\hat{\rho}_s) = \sqrt{\frac{\hbar}{2m\omega_0}}\sum_{n=0}^{\infty}(\sqrt{n}\rho_{n,n-1}+\sqrt{n+1}\rho_{n,n+1}) = 0 \tag{19}$$

and likewise $\langle\hat{p}\rangle_\beta=0$. Actually, it can straightforwardly be verified that $\langle\hat{q}^l\rangle_\beta=\langle\hat{p}^l\rangle_\beta=0$ with l odd.

Let us consider the probability of finding the nth eigenstate from the coupled oscillator in $\hat{\rho}_s$, which reads as

$$p_n = (\hat{\rho}_s)_{nn} = \frac{(\Lambda_\beta)^{n+1/2}(\sqrt{1-\Delta_\beta})^n}{\sqrt{\frac{\langle\hat{q}^2\rangle_\beta\langle\hat{p}^2\rangle_\beta}{\hbar^2} - \frac{1}{4}}} P_n\left(\frac{1}{\sqrt{1-\Delta_\beta}}\right) \tag{20}$$

in terms of the Legendre polynomial [18]

$$P_n(z) = P_n^{(0,0)}(z) = \frac{1}{2^n}\sum_{k=0}^{[n/2]}(-1)^k\binom{n}{k}\binom{2n-2k}{n}z^{n-2k}. \tag{21}$$

Here the normalization $\Sigma_n p_n = 1$ easily appears with the aid of Eq. (15) and the relation [18]

$$\sum_{n=0}^{\infty} P_n(z) h^n = \frac{1}{\sqrt{1-2zh+h^2}}, \tag{22}$$

where $z = \frac{1}{\sqrt{1-\Delta_\beta}}$ and $h = \Lambda_\beta\sqrt{1-\Delta_\beta}$. Then the internal energy of the coupled oscillator is

$$U_s = \langle \hat{H}_s\rangle_\beta = \sum_n p_n E_n = \frac{\langle\hat{p}^2\rangle_\beta}{2M} + \frac{M\omega_0^2}{2}\langle\hat{q}^2\rangle_\beta. \tag{23}$$

A comment deserves here. In [10] and then [21], each of diagonal elements W_n was obtained in terms of the Legendre polynomial P_n like in Eq. (20). On the other hand, the closed expression for off-diagonal elements $(\hat{\rho}_s)_{nm}$ in Eqs. (17) and (18) has not been known, while by means of the numerical integration of Eq. (13) the off-diagonal elements $|(\hat{\rho}_s)_{nm}|$ have been obtained for $m,n \le 10$ in [21]. We will next consider the eigenvalues and eigenstates of the reduced density operator $\hat{\rho}_s$.

III. EIGENVALUE PROBLEM FOR THE OSCILLATOR DENSITY OPERATOR

The eigenvalue problem to be solved reads as

$$\mathrm{EV}_n := \int_{-\infty}^{\infty} dq' \langle q|\hat{\rho}_s|q'\rangle \phi_n(q') \overset{!}{=} p_n\phi_n(q) \tag{24}$$

where the matrix element $\langle q|\hat{\rho}_s|q'\rangle$ is given in (10), and the eigenvalue p_n is the probability of finding the nth eigenstate of the *coupled* oscillator. Following the idea used in [22], we put an ansatz

$$\phi_n(q') = \sqrt{\frac{\tilde{c}}{2^n n!\sqrt{\pi}}} e^{-(\tilde{c}^2/2)q'^2} H_n(\tilde{c}q') \tag{25}$$

[cf. Eq. (A1)] into the integral in Eq. (24), which will yield

$$\mathrm{EV}_n = \sqrt{\frac{\tilde{c}}{2^n n!\sqrt{\pi}}}\frac{1}{\sqrt{\pi}\tilde{v}} \times \exp\left(-\left\{\frac{\tilde{c}^2}{2} + \left(\frac{\langle\hat{p}^2\rangle_\beta}{\hbar^2\langle\hat{q}^2\rangle_\beta} - \tilde{c}^4\right)\frac{\langle\hat{q}^2\rangle_\beta}{2\tilde{v}^2}\right\}q^2\right)(I). \tag{26}$$

Here $\tilde{v} = \sqrt{\frac{1}{4} + \tilde{c}^2\langle\hat{q}^2\rangle_\beta + v^2}$ with $v = \frac{1}{\hbar}\sqrt{\langle\hat{q}^2\rangle_\beta\langle\hat{p}^2\rangle_\beta}$, and

$$(\mathrm{I}) := \int_{-\infty}^{\infty} d\tilde{q}' e^{-(\tilde{q}'-y)^2} H_n(s\tilde{q}') \tag{27}$$

where the dimensionless quantities

$$\tilde{q}' = \frac{\tilde{v}}{\sqrt{2\langle\hat{q}^2\rangle_\beta}}q'; \quad y = \frac{\sqrt{\langle\hat{p}^2\rangle_\beta}}{\sqrt{2}\hbar\tilde{v}}\left(v - \frac{1}{4v}\right)q; \quad s = \frac{\tilde{c}}{\tilde{v}}\sqrt{2\langle\hat{q}^2\rangle_\beta}. \tag{28}$$

The integral in Eq. (27) can be evaluated in closed form of [23]

$$(\mathrm{I}) = \sqrt{\pi}(1-s^2)^{n/2} H_n\left(\frac{sy}{\sqrt{1-s^2}}\right). \tag{29}$$

For $\phi_n(q)$ to be an eigenstate of the operator $\hat{\rho}_s$, from Eqs. (24)–(26) with Eq. (29) we need to require the argument of the Hermite polynomial, $\frac{sy}{\sqrt{1-s^2}} = (v^2 - \frac{1}{4})(\tilde{v}\sqrt{\tilde{v}^2 - 2\tilde{c}^2\langle\hat{q}^2\rangle_\beta})^{-1}\tilde{c}q$ to equal $\tilde{c}q$, which immediately gives

$$\tilde{c} = \left(\frac{\langle\hat{p}^2\rangle_\beta}{\hbar^2\langle\hat{q}^2\rangle_\beta}\right)^{1/4} \tag{30}$$

and subsequently the probability for the nth eigenstate $\phi_n(q)$ as

$$p_n = \frac{1}{v+\frac{1}{2}}\left(\frac{v-\frac{1}{2}}{v+\frac{1}{2}}\right)^n. \tag{31}$$

As a result, we obtained the eigenvalues p_n and the eigenstates $\phi_n(q)$ in closed form.

From comparison between Eqs. (12) and (30), we introduce an effective mass M_{eff} and an effective frequency ω_{eff}, which satisfy the relationship

$$M_{\mathrm{eff}}\omega_{\mathrm{eff}} = \sqrt{\langle\hat{p}^2\rangle_\beta/\langle\hat{q}^2\rangle_\beta}. \tag{32}$$

For an uncoupled oscillator, this obviously reduces to $\langle\hat{p}^2\rangle_\beta/\langle\hat{q}^2\rangle_\beta = (M\omega_0)^2$. For a later purpose, it is useful to note that either M_{eff} or ω_{eff} is not yet determined. The probability in Eq. (31) can then be rewritten as $p_n = (1-\xi_\beta)(\xi_\beta)^n$ in terms of $\xi_\beta = (v-\frac{1}{2})/(v+\frac{1}{2}) = e^{-\beta_{\mathrm{eff}}\hbar\omega_{\mathrm{eff}}}$ with an effective temperature

$$\beta_{\mathrm{eff}} = -\frac{\ln\xi_\beta}{\hbar\omega_{\mathrm{eff}}}, \tag{33}$$

and subsequently as

$$p_n = \frac{1}{Z_{\mathrm{eff}}}e^{-\beta_{\mathrm{eff}}\hbar\omega_{\mathrm{eff}}(n+1/2)} \tag{34}$$

in terms of an effective partition function $Z_{\mathrm{eff}} = \Sigma_n e^{-\beta_{\mathrm{eff}}\hbar\omega_{\mathrm{eff}}(n+1/2)} = \{\mathrm{csch}(\beta_{\mathrm{eff}}\hbar\omega_{\mathrm{eff}}/2)\}/2$. Therefore the density operator $\hat{\rho}_s$ of the coupled oscillator is equivalent to that $(\hat{\rho}_{\mathrm{eff}})$ of an *uncoupled* linear oscillator

$$\hat{H}_{\text{eff}} = \frac{\hat{p}^2}{2M_{\text{eff}}} + \frac{k_{\text{eff}}}{2}\hat{q}^2 \tag{35}$$

at temperature $T_{\text{eff}}=1/(k_B\beta_{\text{eff}})$ such that $\hat{\rho}_s=e^{-\beta_{\text{eff}}\hat{H}_{\text{eff}}}/Z_{\text{eff}}$. Here the spring constant $k_{\text{eff}}=M_{\text{eff}}\omega_{\text{eff}}^2$. Needless to say, the temperature $T_{\text{eff}}\to T$ if the coupling constants $c_j\to 0$ in Eq. (2). With the aid of Eqs. (32) and (33) we can easily confirm that

$$\langle\hat{q}^2\rangle_\beta = \frac{\hbar}{2M_{\text{eff}}\omega_{\text{eff}}}\coth\left(\frac{\beta_{\text{eff}}\hbar\omega_{\text{eff}}}{2}\right);$$

$$\langle\hat{p}^2\rangle_\beta = \frac{M_{\text{eff}}\hbar\omega_{\text{eff}}}{2}\coth\left(\frac{\beta_{\text{eff}}\hbar\omega_{\text{eff}}}{2}\right), \tag{36}$$

which can subsequently be used for the internal energy

$$U_{\text{eff}} = \langle\hat{H}_{\text{eff}}\rangle_\beta = \frac{\hbar\omega_{\text{eff}}}{2}\coth\frac{\beta_{\text{eff}}\hbar\omega_{\text{eff}}}{2} = \omega_{\text{eff}}\sqrt{\langle\hat{p}^2\rangle_\beta\langle\hat{q}^2\rangle_\beta} \tag{37}$$

(note again, though, that since ω_{eff} is not yet determined, $U_{\text{eff}}\neq U_s$). Further, choosing the effective frequency

$$\omega_{\text{eff}}^\star = \frac{1}{2M}\sqrt{\frac{\langle\hat{p}^2\rangle_\beta}{\langle\hat{q}^2\rangle_\beta}} + \frac{M\omega_0^2}{2}\sqrt{\frac{\langle\hat{q}^2\rangle_\beta}{\langle\hat{p}^2\rangle_\beta}} \tag{38}$$

from Eq. (32), we then have $U_{\text{eff}}^\star=U_s$. Accordingly, $M_{\text{eff}}^\star=\langle\hat{p}^2\rangle_\beta/U_s$ and

$$k_{\text{eff}}^\star = \frac{1}{2}\left(k_0 + \frac{\langle\hat{p}^2\rangle_\beta}{M\langle\hat{q}^2\rangle_\beta}\right). \tag{39}$$

Here k_0 is the spring constant of the uncoupled oscillator $\hat{H}_s$. All effective parameters are now uniquely determined in terms of the starred quantities, namely, $M_{\text{eff}}^\star$, $k_{\text{eff}}^\star$, the effective temperature $T_{\text{eff}}^\star=-\hbar\omega_{\text{eff}}^\star/(k_B \ln \xi_\beta)$, and the internal energy $U_{\text{eff}}^\star=\langle\hat{H}_{\text{eff}}^\star\rangle_\beta$ $(=U_s)$ where $\hat{H}_{\text{eff}}^\star=\hat{p}^2/(2M_{\text{eff}}^\star)+(k_{\text{eff}}^\star/2)\hat{q}^2$ (cf. note, on the other hand, that clearly $\hat{\rho}_s=\hat{\rho}_{\text{eff}}=\hat{\rho}_{\text{eff}}^\star$). With the aid of Eq. (6) and (7), Fig. 1 demonstrates that $k_{\text{eff}}^\star\geq k_0$, which leads to $M_{\text{eff}}^\star\geq M$ from $M_{\text{eff}}^\star k_{\text{eff}}^\star=\langle\hat{p}^2\rangle_\beta/\langle\hat{q}^2\rangle_\beta$. We will use the effective oscillator with $(M_{\text{eff}}^\star,k_{\text{eff}}^\star,T_{\text{eff}}^\star)$ in Sec. IV for a generalization of the Clausius inequality.

Let us consider the thermal entropy of the effective uncoupled oscillator $\hat{H}_{\text{eff}}$ (of course, $\hat{H}_{\text{eff}}^\star$, too, as its special case), which is

$$S_{\text{eff}}(=S_{\text{eff}}^\star) = k_B \ln Z_{\text{eff}} + k_B\beta_{\text{eff}}U_{\text{eff}} = -k_B\left\{\ln(1-\xi_\beta) + \frac{\xi_\beta}{1-\xi_\beta}\ln \xi_\beta\right\}. \tag{40}$$

We can immediately verify that this is identical to the von-Neumann entropy of the coupled oscillator,

$$S_N = k_B\left(\upsilon+\frac{1}{2}\right)\ln\left(\upsilon+\frac{1}{2}\right) - k_B\left(\upsilon-\frac{1}{2}\right)\ln\left(\upsilon-\frac{1}{2}\right) \tag{41}$$

(note again that $\hat{\rho}_s=\hat{\rho}_{\text{eff}}=\hat{\rho}_{\text{eff}}^\star$). From Fig. 2, it is shown that S_N increases with the magnitude of the damping parameter and also with the temperature of the total system.

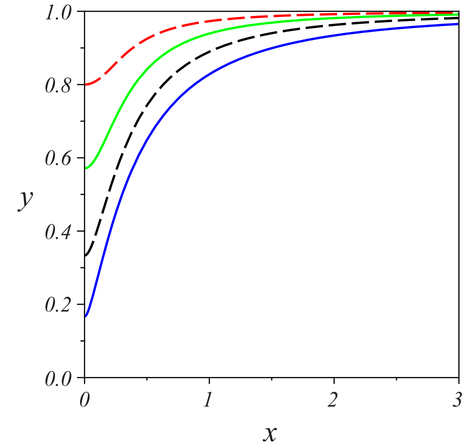

FIG. 1. (Color online) $y=k_0/k_{\text{eff}}^\star=2/(1+(\Omega+\gamma)\langle\hat{p}^2\rangle_\beta/\{\Omega(M\mathbf{w}_0)^2\langle\hat{q}^2\rangle_\beta\})$ versus $x=k_BT/\hbar\mathbf{w}_0$ (dimensionless temperature), where $\mathbf{w}_0$ is the renormalized eigen frequency of the oscillator $\hat{H}_s$ [cf. Eq. (9)]; for $k_{\text{eff}}^\star$ refer to Eq. (39). From bottom to top, (blue solid: damping parameter $\gamma=10$, overdamped), (black dash: $\gamma=4$, overdamped), (green solid: $\gamma=3/2$, underdamped) and (red dash: $\gamma=1/2$, underdamped). We have $y\leq 1$ so that $M/M_{\text{eff}}^\star=1/(2-y)\leq 1$. Here $\hbar=k_B=\mathbf{w}_0=\Omega=M=1$.

Now we briefly comment on the introduction of effective parameters: First, it has been shown in [22] that the coupled oscillator with (M,ω_0) at zero temperature of the total system $(T=0)$ can be interpreted as an uncoupled one with $(M,\bar{\omega}_{\text{eff}})$ in a thermal state with a finite effective temperature $\bar{T}_{\text{eff}}$ (with $\beta=\infty$), where $\bar{\omega}_{\text{eff}}=\sqrt{\langle\hat{p}^2\rangle_\infty/\langle\hat{q}^2\rangle_\infty}/M$. Using the very same technique, we have generalized this result into $(M_{\text{eff}},\omega_{\text{eff}},T_{\text{eff}})$ in Eqs. (32) and (33) for an arbitrary temperature of the total system. It is interesting to note here that $\bar{U}_{\text{eff}}\neq U_s(\beta=\infty)$ though, where $\bar{U}_{\text{eff}}=\langle\hat{p}^2\rangle_\infty/(2M)+\{M(\bar{\omega}_{\text{eff}})^2/2\}\langle\hat{q}^2\rangle_\infty$. Second, it is also known [16,24] that the coupled oscillator can exactly be seen as an uncoupled oscillator with an effective frequency

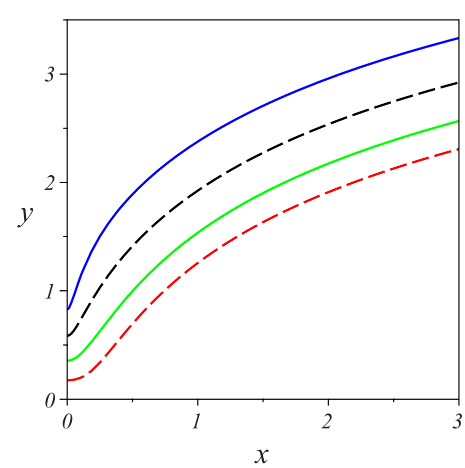

FIG. 2. (Color online) $y=S_N$ (von-Neumann entropy) versus $x=k_BT/\hbar\mathbf{w}_0$ (dimensionless temperature); for S_N refer to Eq. (41). From top to bottom, (blue solid: $\gamma=10$), (black dash: $\gamma=4$), (green solid: $\gamma=3/2$) and (red dash: $\gamma=1/2$). As γ decreases, then S_N decreases. Here $\hbar=k_B=\mathbf{w}_0=\Omega=1$.

$$\tilde{\omega}_{\rm eff} = \frac{2}{\hbar\beta}\,\text{arccoth}\left(\frac{2}{\hbar}\sqrt{\langle\hat{q}^2\rangle_\beta\langle\hat{p}^2\rangle_\beta}\right) \tag{42}$$

and an effective mass $\tilde{M}_{\rm eff}=\sqrt{\langle\hat{p}^2\rangle_\beta/\langle\hat{q}^2\rangle_\beta}/\tilde{\omega}_{\rm eff}$ in the canonical thermal state $\hat{\rho}_s=e^{-\beta\hat{H}_s}/Z_\beta$ (i.e., $\tilde{T}_{\rm eff}=T$), which can be well understood simply as a special case of $(M_{\rm eff},\omega_{\rm eff},T_{\rm eff})$ in Eqs. (32) and (33) (note again that these are not the starred quantities). However, $\tilde{U}_{\rm eff}\neq U_s$, either, whereas $U_s=U^\star_{\rm eff}$ introduced below Eq. (38).

It is also interesting to compare the internal energy $U^\star_{\rm eff}$ of the coupled oscillator with an alternative definition [7–9,25–27]

$$\mathcal{U} = -\frac{\partial}{\partial\beta}\ln\mathcal{Z}_\beta, \tag{43}$$

where the partition function $\mathcal{Z}_\beta=\text{Tr}\,e^{-\beta\hat{H}}/\text{Tr}_b\,e^{-\beta\hat{H}_b}$. Here, Tr_b denotes the partial trace for the bath alone (in the absence of a coupling between system and bath, the function $\mathcal{Z}_\beta$ would exactly correspond to the partition function of the system only). Then it immediately follows that $\mathcal{U}=U_s+\langle\hat{H}_b\rangle_\beta+\langle\hat{H}_{sb}\rangle_\beta-\langle\hat{H}_b\rangle_{\beta'}\neq U_s$ where $\langle\hat{H}_b\rangle_{\beta'}=\text{Tr}_b(\hat{H}_b e^{-\beta\hat{H}_b}/\text{Tr}_b\,e^{-\beta\hat{H}_b})$. Therefore the energy $\mathcal{U}$ is not valid for the reduced system alone. The entropy $\mathcal{S}=k_B(\ln\mathcal{Z}_\beta-\beta\frac{\partial}{\partial\beta}\ln\mathcal{Z}_\beta)$ can also be introduced here [26,27], which is, however, different from the von-Neumann entropy S_N ($=S^\star_{\rm eff}$) for the reduced density matrix $\hat{\rho}_s$ of the coupled oscillator. Actually, the entropy $\mathcal{S}$ cannot be derived from the Jaynes maximum entropy principle [28,29] applied for the reduced system whereas the entropy $S^\star_{\rm eff}$ can be so with the effective temperature $T^\star_{\rm eff}$. As a result, all thermodynamic quantities resulting from the partition function $\mathcal{Z}_\beta$ are not appropriate for the well-defined *local* thermodynamics of the reduced system.

IV. CLAUSIUS INEQUALITIES

We will discuss the second law of thermodynamics in terms of the Clausius inequality. To do so, we need the relationship obtained from Eq. (23),

$$dU_s = \sum_n (E_n dp_n + p_n dE_n) \tag{44}$$

where $\Sigma E_n dp_n=\text{Tr}_s(\hat{H}_s d\hat{\rho}_s)=\delta\mathcal{Q}_s$ corresponds to an amount of heat added to the coupled oscillator, and $\Sigma p_n dE_n=\text{Tr}_s(\hat{\rho}_s d\hat{H}_s)=\delta\mathcal{W}_s$ an amount of work on the oscillator [4]. For a later purpose, we first consider the well-defined Clausius inequality for a weakly coupled oscillator

$$\delta\mathcal{Q}_s \le T dS. \tag{45}$$

For a typical reversible process we have either a variation of the mass of the oscillator or a variation of its spring constant in such a way that

$$\frac{\partial}{\partial M}\mathcal{Q}_s = \frac{1}{2M}\frac{\partial}{\partial M}\langle\hat{p}^2\rangle_\beta + \frac{k_0}{2}\frac{\partial}{\partial M}\langle\hat{q}^2\rangle_\beta, \tag{46}$$

$$= \frac{\beta(\hbar\omega_0)^2}{8M}\left(\text{csch}\frac{\beta\hbar\omega_0}{2}\right)^2 = T\frac{\partial}{\partial M}S, \tag{47}$$

$$\frac{\partial}{\partial k_0}\mathcal{Q}_s = \frac{1}{2M}\frac{\partial}{\partial k_0}\langle\hat{p}^2\rangle_\beta + \frac{k_0}{2}\frac{\partial}{\partial k_0}\langle\hat{q}^2\rangle_\beta, \tag{48}$$

$$= -\frac{\beta\hbar^2}{8M}\left(\text{csch}\frac{\beta\hbar\omega_0}{2}\right)^2 = T\frac{\partial}{\partial k_0}S, \tag{49}$$

respectively (cf. it is also noted that $\partial\mathcal{W}_s/\partial M=-\langle\hat{p}^2\rangle_\beta/(2M^2)$ and $\partial\mathcal{W}_s/\partial k_0=\langle\hat{q}^2\rangle_\beta/2$). We thus confirm the equality sign in Eq. (45).

Next we consider the Clausius inequality in the process of coupling between oscillator and bath. The coupling process can be represented in terms of a variation of the damping parameter such that for a reversible process,

$$\frac{\partial}{\partial\gamma}\mathcal{Q}_s = \frac{\partial}{\partial\gamma}U_s = \frac{1}{2M}\frac{\partial}{\partial\gamma}\langle\hat{p}^2\rangle_\beta + \frac{k_0}{2}\frac{\partial}{\partial\gamma}\langle\hat{q}^2\rangle_\beta \tag{50}$$

$$\frac{\partial}{\partial\gamma}S = k_B\left(\frac{\partial v}{\partial\gamma}\right)\ln\frac{v+\frac{1}{2}}{v-\frac{1}{2}} \tag{51}$$

where $S=S_N$ and

$$\frac{\partial v}{\partial\gamma} = \frac{1}{2\hbar}\frac{\langle\hat{q}^2\rangle_\beta\frac{\partial}{\partial\gamma}\langle\hat{p}^2\rangle_\beta + \langle\hat{p}^2\rangle_\beta\frac{\partial}{\partial\gamma}\langle\hat{q}^2\rangle_\beta}{\sqrt{\langle\hat{q}^2\rangle_\beta\langle\hat{p}^2\rangle_\beta}}. \tag{52}$$

Equation (50) can be evaluated in closed form with the aid of Eqs. (6)–(9) such that

$$\frac{\partial}{\partial\gamma}\langle\hat{q}^2\rangle^{(d)}_\beta = \frac{1}{M}\sum_{l=1}^{3}\,{}_\gamma K^{(d)}_l \tag{53}$$

$$\frac{\partial}{\partial\gamma}\langle\hat{p}^2\rangle^{(d)}_\beta = -M\sum_{l=1}^{3}\left({}_\gamma K^{(d)}_l\underline{\omega_l}^2 + 2\underline{\omega_l}\lambda^{(l)}_d\left\{\frac{1}{\beta\underline{\omega_l}} + \frac{\hbar}{\pi}\psi\left(\frac{\beta\hbar\underline{\omega_l}}{2\pi}\right)\right\}\frac{\partial\underline{\omega_l}}{\partial\gamma}\right), \tag{54}$$

where $\partial\underline{\omega_1}/\partial\gamma=0$ and

$$\frac{\partial\underline{\omega_2}}{\partial\gamma} = \frac{1}{2}\left(1-\frac{1}{\sqrt{1-\left(\frac{2\mathbf{w}_0}{\gamma}\right)^2}}\right);$$

$$\frac{\partial\underline{\omega_3}}{\partial\gamma} = \frac{1}{2}\left(1+\frac{1}{\sqrt{1-\left(\frac{2\mathbf{w}_0}{\gamma}\right)^2}}\right), \tag{55}$$

and

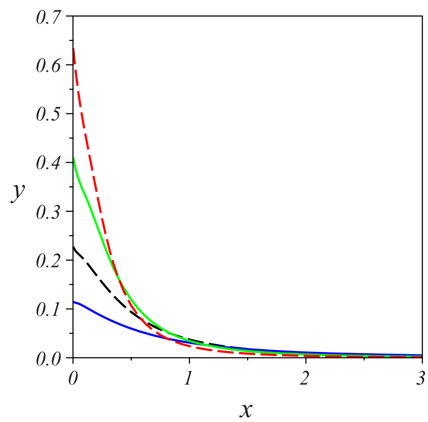

FIG. 3. (Color online) $y=10\cdot(\partial\mathcal{Q}_s/\partial\gamma - T\partial S_N/\partial\gamma)/\hbar$ (dimensionless) versus $x=k_BT/\hbar\mathbf{w}_0$ (dimensionless temperature); for y refer to Eqs. (50) and (51). From bottom to top (at $T=0$), (blue solid: $\gamma=10$), (black dash: $\gamma=4$), (green solid: $\gamma=3/2$) and (red dash: $\gamma=1/2$). Here $\hbar=k_B=\mathbf{w}_0=\Omega=M=1$.

$$
{}_\gamma K_l^{(d)} = \left\{\frac{1}{\beta\underline{\omega_l}} + \frac{\hbar}{\pi}\psi\left(\frac{\beta\hbar\underline{\underline{\omega_l}}}{2\pi}\right)\right\}\frac{\partial\lambda_d^{(l)}}{\partial\gamma} + \lambda_d^{(l)}\left\{-\frac{1}{\beta\underline{\omega_l}^2} + \frac{\hbar^2\beta}{2\pi^2}\psi^{(1)}\left(\frac{\beta\hbar\underline{\underline{\omega_l}}}{2\pi}\right)\right\}\frac{\partial\underline{\underline{\omega_l}}}{\partial\gamma} \quad (56)
$$

in terms of the digamma function $\psi(y)$ and the trigamma function $\psi^{(1)}(y)=d^2\ln\Gamma(y)/dy^2$ [18]. Here we obtained Eqs. (53) and (54) for the overdamped case ($\gamma/2>\mathbf{w}_0$), which is, still, found to hold for the underdamped case ($\gamma/2\le\mathbf{w}_0$) as well, being expressed in terms of the functions with complex-valued arguments. Then we get a violation of the Clausius inequality, $\partial\mathcal{Q}_s/\partial\gamma > T\partial S_N/\partial\gamma$ as seen from Fig. 3.

We, however, argue that this violation results from an inappropriate choice of temperature T being defined for the *total* system. We now propose a well-defined form of the Clausius inequality pertaining to the coupling process in such a way that

$$
\delta\mathcal{Q}_{\text{eff}}^\star \le T_{\text{eff}}^\star dS_N \quad (57)
$$

where $\delta\mathcal{Q}_{\text{eff}}^\star$ is the heat exchanged between the effective (weakly coupled) oscillator with $(M_{\text{eff}}^\star, k_{\text{eff}}^\star)$ in Eq. (39) and a bath at the equilibrium temperature $T_{\text{eff}}^\star=-\hbar\omega_{\text{eff}}^\star/(k_B\ln\xi_\beta)$ with Eq. (38). For an reversible process we then have

$$
\frac{\partial}{\partial\gamma}\mathcal{Q}_{\text{eff}}^\star = \frac{1}{2M_{\text{eff}}^\star}\frac{\partial}{\partial\gamma}\langle\hat{p}^2\rangle_\beta + \frac{k_{\text{eff}}^\star}{2}\frac{\partial}{\partial\gamma}\langle\hat{q}^2\rangle_\beta, \quad (58)
$$

which can be shown to be identical to $T_{\text{eff}}^\star\partial S_N/\partial\gamma$ with the aid of Eqs. (51) and (52). Therefore, there is no violation of the Clausius inequality! From $U_{\text{eff}}^\star=U_s$, we note that $\int_0^\gamma dU_{\text{eff}}^\star=\int_0^\gamma dU_s=U_s(\gamma)-U_0=\Delta U_s$ in which $U_0=(\hbar\omega_0/2)\coth(\beta\hbar\omega_0/2)$ for an uncoupled oscillator, and $\oint dU_s=\oint dU_{\text{eff}}^\star=0$, where $\oint=\int_0^\gamma+\int_\gamma^0$ represents a cyclic process of the coupling and decoupling. From the first law $dU_s=\delta\mathcal{Q}_s+\delta\mathcal{W}_s=\delta\mathcal{Q}_{\text{eff}}^\star+\delta\mathcal{W}_{\text{eff}}^\star$ with $\partial\mathcal{W}_s/\partial\gamma=0$ and thus $\partial(\mathcal{Q}_{\text{eff}}^\star-\mathcal{Q}_s)/\partial\gamma=-\partial\mathcal{W}_{\text{eff}}^\star/\partial\gamma$, it also follows that

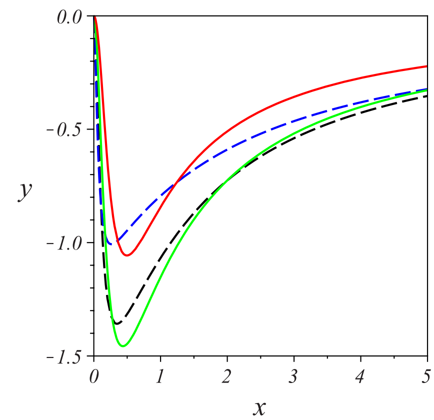

FIG. 4. (Color online) $y=100\cdot(\partial\mathcal{W}_{\text{eff}}^\star/\partial\gamma)/\hbar$ (dimensionless) versus $x=k_BT/\hbar\mathbf{w}_0$ (dimensionless temperature); for y refer to Eq. (59). From top to bottom (at $T=0.5$), (blue dash: $\gamma=10$), (red solid: $\gamma=1/2$), (black dash: $\gamma=4$) and (green solid: $\gamma=3/2$). Here $\hbar=k_B=\mathbf{w}_0=\Omega=M=1$.

$$
\frac{\partial}{\partial\gamma}\mathcal{Q}_s - \frac{\partial}{\partial\gamma}\mathcal{W}_{\text{eff}}^\star = T_{\text{eff}}^\star\frac{\partial}{\partial\gamma}S_N \quad (59)
$$

where, with the aid of (39),

$$
\begin{aligned}
\frac{\partial}{\partial\gamma}\mathcal{W}_{\text{eff}}^\star &= -\frac{1}{2M_{\text{eff}}^\star}\left(\frac{\partial M_{\text{eff}}^\star}{\partial\gamma}\right)\langle\hat{p}^2\rangle_\beta + \frac{1}{2}\left(\frac{\partial k_{\text{eff}}^\star}{\partial\gamma}\right)\langle\hat{q}^2\rangle_\beta \\
&= \frac{1}{4M}\left(1-\frac{Mk_0\langle\hat{q}^2\rangle_\beta}{\langle\hat{p}^2\rangle_\beta}\right)\frac{\partial}{\partial\gamma}\langle\hat{p}^2\rangle_\beta \\
&\quad + \frac{k_0}{4}\left(1-\frac{\langle\hat{p}^2\rangle_\beta}{Mk_0\langle\hat{q}^2\rangle_\beta}\right)\frac{\partial}{\partial\gamma}\langle\hat{q}^2\rangle_\beta. \quad (60)
\end{aligned}
$$

Figure 4 shows that $\partial\mathcal{W}_{\text{eff}}^\star/\partial\gamma\le 0$, which immediately leads to no violation of the inequality $\partial\mathcal{Q}_s/\partial\gamma\le T_{\text{eff}}^\star\partial S_N/\partial\gamma$. Here it should be noted that we have appropriately selected the effective oscillator $\hat{H}_{\text{eff}}^\star$ with $(M_{\text{eff}}^\star, \omega_{\text{eff}}^\star)$ from Eq. (32) to introduce an effective temperature $T_{\text{eff}}^\star$ without any ambiguity, which is now a critical element for the well-defined Clausius inequality in Eq. (57).

Therefore, we are now in a position to understand, by means of Clausius inequality (57), the validity of the second law in a cyclic process of the coupling and decoupling between oscillator and bath at an equilibrium temperature T. The validity has actually been shown for zero temperature ($T=0$) in [7,8] and later for an arbitrary temperature in [9] by verifying the second law in its Kelvin-Planck form [6]; it states that the minimum work $\Delta\mathcal{F}$ needed to couple the oscillator to a bath (in a reversible process), being equivalent to the Helmholtz free energy of the *coupled* total system minus the free energy of the *uncoupled* total system, cannot be less than the maximum useful work obtainable from the oscillator when it decouples from the bath such that

$$
\Delta U_s \lneq \Delta\mathcal{F} \quad (61)
$$

(note the strict inequality and see below). Here we have on the left-hand side the internal energy ΔU_s as the maximum useful work obtainable from the oscillator on completion of the decoupling process.

For the coupling-decoupling process (with a varying damping parameter $\gamma':0\to\gamma\to 0$), inequality (57) can be transformed to $\oint\delta\mathcal{Q}^\star_{\text{eff}}/T^\star_{\text{eff}}\le 0$, which means, according to the Kelvin-Planck form, that the net work obtainable from the effective uncoupled oscillator (with an accordingly varying parameter γ') on completion of this cyclic process cannot be greater than zero. For a reversible process, this inequality then reduces to

$$\int_0^\gamma \frac{d\gamma'}{T^\star_{\text{eff}}}\frac{\partial}{\partial\gamma'}\mathcal{Q}^\star_{\text{eff}}+\int_\gamma^0 \frac{d\gamma'}{T^\star_{\text{eff}}}\frac{\partial}{\partial\gamma'}\mathcal{Q}^\star_{\text{eff}}=0, \tag{62}$$

which means that the minimum work (ΔU_s) done onto the oscillator for $U_0\to U^\star_{\text{eff}}$ on completion of the coupling exactly equals the maximum useful work releasable from the oscillator on completion of the decoupling. For comparison, on the other hand, the free energy $\Delta\mathcal{F}$ is, by definition, the minimum work done on *both* oscillator and bath so that we get the inequality in Eq. (61). Anyhow, the second law holds in the coupling-decoupling process.

Now we consider the Clausius inequality (with a fixed coupling strength) after completion of the coupling, which has been discussed so far, e.g., in [4,5,12]. Note that we are now with the effective oscillator with $(M^\star_{\text{eff}},k^\star_{\text{eff}})$ at temperature $T^\star_{\text{eff}}$. We can then show that for a reversible process,

$$\begin{aligned}\frac{\partial}{\partial M}\mathcal{Q}^\star_{\text{eff}}&=\frac{1}{2M^\star_{\text{eff}}}\frac{\partial}{\partial M}\langle\hat{p}^2\rangle_\beta+\frac{k^\star_{\text{eff}}}{2}\frac{\partial}{\partial M}\langle\hat{q}^2\rangle_\beta\\&=\frac{\hbar\omega^\star_{\text{eff}}}{4}\left(\frac{\partial}{\partial M}\ln\xi_\beta\right)\left(\operatorname{csch}\frac{\ln\xi_\beta}{2}\right)^2\\&=T^\star_{\text{eff}}\frac{\partial}{\partial M}S_N,\end{aligned} \tag{63}$$

$$\begin{aligned}\frac{\partial}{\partial k_0}\mathcal{Q}^\star_{\text{eff}}&=\frac{1}{2M^\star_{\text{eff}}}\frac{\partial}{\partial k_0}\langle\hat{p}^2\rangle_\beta+\frac{k^\star_{\text{eff}}}{2}\frac{\partial}{\partial k_0}\langle\hat{q}^2\rangle_\beta\\&=\frac{\hbar\omega^\star_{\text{eff}}}{4}\left(\frac{\partial}{\partial k_0}\ln\xi_\beta\right)\left(\operatorname{csch}\frac{\ln\xi_\beta}{2}\right)^2\\&=T^\star_{\text{eff}}\frac{\partial}{\partial k_0}S_N,\end{aligned} \tag{64}$$

which follow from Eqs. (33), (36), (38), and (39), respectively. Therefore, there is no violation of the Clausius inequality at all! Note here as well that from the first law $dU_s=\delta\mathcal{Q}_s+\delta\mathcal{W}_s=\delta\mathcal{Q}^\star_{\text{eff}}+\delta\mathcal{W}^\star_{\text{eff}}$, the effective work is also well defined such as

$$\partial_{M,k_0}\mathcal{W}^\star_{\text{eff}}=-\frac{1}{2M^\star_{\text{eff}}}(\partial_{M,k_0}M^\star_{\text{eff}})\langle\hat{p}^2\rangle_\beta+\frac{1}{2}(\partial_{M,k_0}k^\star_{\text{eff}})\langle\hat{q}^2\rangle_\beta, \tag{65}$$

the closed form of which can immediately be obtained with the aid of $M^\star_{\text{eff}}=\langle\hat{p}^2\rangle_\beta/U_s$ and Eq. (39).

For comparison, we next seek to have Eqs. (46) and (48) in closed form in the Drude damping model. After making some lengthy calculations (cf. Appendix B), we then obtain the expressions

$$\frac{\partial}{\partial M}\langle\hat{q}^2\rangle^{(d)}_\beta=-\frac{1}{M}\langle\hat{q}^2\rangle^{(d)}_\beta+\frac{1}{M}\sum_{l=1}^{3}{}_MK^{(d)}_l \tag{66}$$

$$\begin{aligned}\frac{\partial}{\partial M}\langle\hat{p}^2\rangle^{(d)}_\beta=\frac{1}{M}\langle\hat{p}^2\rangle^{(d)}_\beta-M\sum_{l=1}^{3}\Bigg({}_MK^{(d)}_l\underline{\omega_l}^2\\+2\underline{\omega_l}\lambda^{(l)}_d\left\{\frac{1}{\beta\underline{\omega_l}}+\frac{\hbar}{\pi}\psi\left(\frac{\beta\hbar\underline{\omega_l}}{2\pi}\right)\right\}\frac{\partial\underline{\omega_l}}{\partial M}\Bigg)\end{aligned} \tag{67}$$

where

$$\begin{aligned}{}_MK^{(d)}_l:=\left\{\frac{1}{\beta\underline{\omega_l}}+\frac{\hbar}{\pi}\psi\left(\frac{\beta\hbar\underline{\omega_l}}{2\pi}\right)\right\}\frac{\partial\lambda^{(l)}_d}{\partial M}\\+\lambda^{(l)}_d\left\{-\frac{1}{\beta\underline{\omega_l}^2}+\frac{\hbar^2\beta}{2\pi^2}\psi^{(1)}\left(\frac{\beta\hbar\underline{\omega_l}}{2\pi}\right)\right\}\frac{\partial\underline{\omega_l}}{\partial M},\end{aligned} \tag{68}$$

and

$$\frac{\partial}{\partial k_0}\langle\hat{q}^2\rangle^{(d)}_\beta=\frac{1}{M}\sum_{l=1}^{3}{}_{k_0}K^{(d)}_l, \tag{69}$$

$$\begin{aligned}\frac{\partial}{\partial k_0}\langle\hat{p}^2\rangle^{(d)}_\beta=-M\sum_{l=1}^{3}\Bigg({}_{k_0}K^{(d)}_l\underline{\omega_l}^2+2\underline{\omega_l}\lambda^{(l)}_d\Bigg\{\frac{1}{\beta\underline{\omega_l}}\\+\frac{\hbar}{\pi}\psi\left(\frac{\beta\hbar\underline{\omega_l}}{2\pi}\right)\Bigg\}\frac{\partial\underline{\omega_l}}{\partial k_0}\Bigg),\end{aligned} \tag{70}$$

where ${}_{k_0}K^{(d)}_l$ is defined as Eq. (68) but with the replacement of $\partial/\partial M$ by $\partial/\partial k_0$. Equations (66) and (67) [as well as Eqs. (69) and (70)] hold for both overdamped and underdamped cases. To discuss the second law, we now consider an equality similar to Eq. (59) in form of

$$\frac{\partial}{\partial M}\mathcal{Q}_s-\frac{\partial}{\partial M}(\mathcal{W}^\star_{\text{eff}}-\mathcal{W}_s)=T^\star_{\text{eff}}\frac{\partial}{\partial M}S_N, \tag{71}$$

$$\frac{\partial}{\partial k_0}\mathcal{Q}_s-\frac{\partial}{\partial k_0}(\mathcal{W}^\star_{\text{eff}}-\mathcal{W}_s)=T^\star_{\text{eff}}\frac{\partial}{\partial k_0}S_N, \tag{72}$$

obtained with the aid of the first law. Here $\partial\mathcal{W}_s/\partial M=-\langle\hat{p}^2\rangle_\beta/(2M^2)$ and $\partial\mathcal{W}_s/\partial k_0=\langle\hat{q}^2\rangle_\beta/2$, whereas $\partial\mathcal{W}_s/\partial\gamma$ for Eq. (59) vanishes. Actually we have here $\partial_{M,k_0}(\mathcal{W}^\star_{\text{eff}}-\mathcal{W}_s)\ge 0$, which follows from $\partial\mathcal{Q}_s/\partial M\ge T^\star_{\text{eff}}\partial S_N/\partial M$ and $\partial\mathcal{Q}_s/\partial k_0\ge T^\star_{\text{eff}}\partial S_N/\partial k_0$, demonstrated in Figs. 5 and 6, respectively [where Eqs. (66)–(70) were used]. This can be interpreted as follows. To define a well-defined (effective) local temperature of the oscillator, we need to "project" the coupled oscillator onto the effective oscillator. In doing so, it is required here to do additional work $(\mathcal{W}^\star_{\text{eff}}-\mathcal{W}_s)$ onto the oscillator, whereas in the coupling process we need to release the work $\mathcal{W}^\star_{\text{eff}}$ from the oscillator. Without considering this work compensation we would consequently get a violation

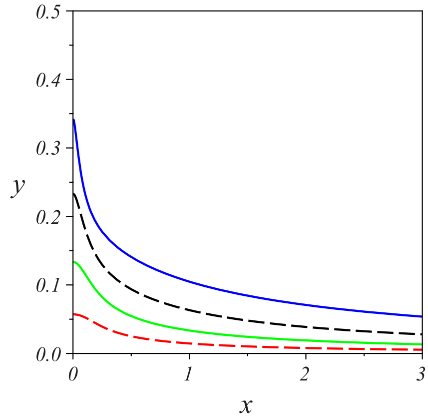

FIG. 5. (Color online) $y=(\partial \mathcal{Q}_s/\partial M - T^\star_{\mathrm{eff}} \partial S_N/\partial M)/(\hbar \mathbf{w}_0/M)$ (dimensionless) versus $x=k_B T/\hbar \mathbf{w}_0$ (dimensionless temperature); for y refer to Eq. (71). From top to bottom, (blue solid: $\gamma=10$), (black dash: $\gamma=4$), (green solid: $\gamma=3/2$) and (red dash: $\gamma=1/2$). As γ decreases, then y decreases. Here $\hbar=k_B=\mathbf{w}_0=\Omega=M=1$.

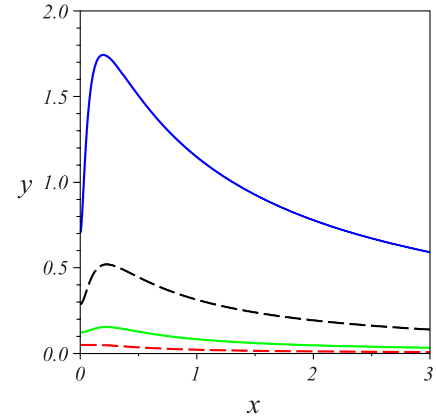

FIG. 6. (Color online) $y=(\partial \mathcal{Q}_s/\partial k_0 - T^\star_{\mathrm{eff}} \partial S_N/\partial k_0)/(\hbar/(M \mathbf{w}_0))$ (dimensionless) versus $x=k_B T/\hbar \mathbf{w}_0$ (dimensionless temperature); for y refer to Eq. (72). From top to bottom, (blue solid: $\gamma=10$), (black dash: $\gamma=4$), (green solid: $\gamma=3/2$) and (red dash: $\gamma=1/2$). As γ decreases, then y decreases. Here $\hbar=k_B=\mathbf{w}_0=\Omega=M=1$.

of the Clausius inequality. It is also interesting to rewrite Eq. (71) as

$$\frac{\partial}{\partial M}\mathcal{Q}_s = T\frac{\partial}{\partial M}S_N + Y \tag{73}$$

in terms of the temperature T of the *total* system, where $Y = (T^\star_{\mathrm{eff}} - T)\,\partial S_N/\partial M + \partial(\mathcal{W}^\star_{\mathrm{eff}} - \mathcal{W}_s)/\partial M$. Figure 7 shows that $\partial \mathcal{Q}_s/\partial M > T\partial S_N/\partial M$, which has been used in [12] for the justification of a violation of the Clausius inequality (note also the strict inequality even for a reversible process). However, we understand now that this simply represents the neglect of the additional term $Y>0$ rather than a violation proper. As a result, we have a generalized form of the Clausius inequality, $\oint \delta \mathcal{Q}^\star_{\mathrm{eff}}/T^\star_{\mathrm{eff}} \le 0$ where $\oint$ represents a cyclic process with respect to *any* variation of (M, k_0, γ). For the relevant comment on effective thermodynamic relations, see Appendix C.

V. CONCLUSION

In conclusion, we have found a well defined effective Clausius inequality appropriate for the quantum Brownian oscillator with *any* coupling strength. It satisfies the equality condition for a reversible process. We have clearly shown that there is no violation of the inequality so that the second law of thermodynamics is robust even beyond the weak-coupling limit. In doing so, we have used the effective internal energy $U^\star_{\mathrm{eff}} = \langle \hat{H}^\star_{\mathrm{eff}}\rangle_\beta$, being identical to the internal energy $U_s = \langle \hat{H}_s\rangle_\beta$, whereas the approach of apparently many other works has been based on a different energy $\mathcal{U}$ defined in Eq. (43) and discussed thereafter.

We believe that this inequality will provide a useful starting point for a consistent generalization of thermodynamics and information theory into the quantum and nanosystem regime, respectively. As an example, a generalization of the Landauer principle [30,31] is in consideration, which can be understood as a simple logical consequence of the Clausius inequality; our findings then suggest an existence of an effective Landauer principle yet to be introduced rigorously [32] which is correct even in the strong-coupling limit, whereas based on the violation of the Clausius inequality considered in [4,5] as stated in Sec. I, it was concluded in [21] that the original form of Landauer principle may not be applicable in the strong-coupling limit.

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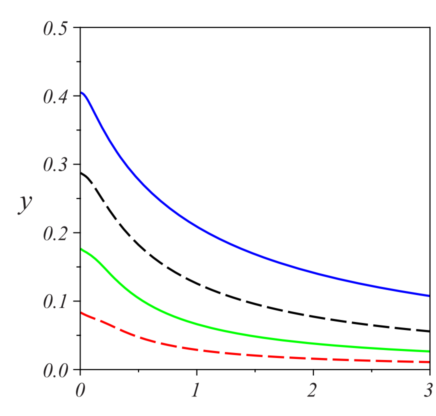

FIG. 7. (Color online) $y=(\partial \mathcal{Q}_s/\partial M - T\partial S_N/\partial M)/(\hbar \mathbf{w}_0/M)$ (dimensionless) versus $x=k_B T/\hbar \mathbf{w}_0$ (dimensionless temperature); for y refer to Eq. (73). From top to bottom, (blue solid: $\gamma=10$), (black dash: $\gamma=4$), (green solid: $\gamma=3/2$) and (red dash: $\gamma=1/2$). As γ decreases, then y decreases. Here $\hbar=k_B=\mathbf{w}_0=\Omega=M=1$.

APPENDIX A: DERIVATION OF Eqs. (14a)–(14c), (16a), and (16b)

Substituting into Eq. (13) the eigenfunction

$$\psi_\nu(q) = \sqrt{\frac{c}{2^\nu \nu!\sqrt{\pi}}}e^{-(c^2/2)q^2}H_\nu(cq) \tag{A1}$$

in terms of the Hermite polynomial H_ν where $\nu=n,m$, then we immediately obtain

$$\rho_{nm} = \frac{1}{\sqrt{2^{n+m}n!\,m!}}\frac{1}{\pi c}\frac{1}{\sqrt{2\langle\hat{q}^2\rangle_\beta}} \times \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dy dy' H_n(y)H_m(y') \times \exp\left\{-a_\beta(y^2+y'^2)+\frac{1}{c^2}\left(\frac{\langle\hat{p}^2\rangle_\beta}{\hbar^2}-\frac{1}{4\langle\hat{q}^2\rangle_\beta}\right)yy'\right\} \tag{A2}$$

where $y=cq$ and $y'=cq'$, and $a_\beta=\frac{1}{2}+\frac{1}{8c^2\langle\hat{q}^2\rangle_\beta}+\frac{\langle\hat{p}^2\rangle_\beta}{2\hbar^2c^2}$. The substitution of the relations [18]

$$H_n(y) = \left(\frac{\partial}{\partial t}\right)^n e^{2yt-t^2}|_{t=0} \tag{A3a}$$

$$H_m(y') = \left(\frac{\partial}{\partial s}\right)^m e^{2y's-s^2}|_{s=0} \tag{A3b}$$

into Eq. (A2) subsequently allows us to have

$$\rho_{nm} = \frac{1}{\sqrt{2^{n+m}n!\,m!}}\frac{1}{\pi c}\frac{1}{\sqrt{2\langle\hat{q}^2\rangle_\beta}}\left(\frac{\partial}{\partial t}\right)^n\left(\frac{\partial}{\partial s}\right)^m \times e^{-(t^2+s^2)}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dy dy' e^{-(a_\beta y^2-2ty)}e^{-\{a_\beta y'^2+2b_\beta(y)\cdot y'\}}|_{t,s=0} \tag{A4}$$

where $b_\beta(y)=\frac{y}{2c^2}\left(\frac{1}{4\langle\hat{q}^2\rangle_\beta}-\frac{\langle\hat{p}^2\rangle_\beta}{\hbar^2}\right)-s$. By using the identity [18]

$$\int_{-\infty}^{\infty} dz e^{-(az^2+2bz)} = \sqrt{\frac{\pi}{a}}e^{b^2/a} \tag{A5}$$

we can first carry out the integration over y' in (A4) and then over y, which will give rise to

$$\rho_{nm} = \frac{1}{\sqrt{2^{n+m}n!\,m!}}\frac{1}{c}\frac{1}{\sqrt{2\langle\hat{q}^2\rangle_\beta A_\beta}}\left(\frac{\partial}{\partial t}\right)^n\left(\frac{\partial}{\partial s}\right)^m \times e^{-\Upsilon_\beta(t^2+s^2)+2\Lambda_\beta ts}|_{t,s=0} = \sqrt{\frac{(\Upsilon_\beta)^{m-n}}{2^{n+m}n!\,m!}}\frac{(\Lambda_\beta)^n}{c}\frac{1}{\sqrt{2\langle\hat{q}^2\rangle_\beta A_\beta}}\left(\frac{\partial}{\partial u}\right)^n \times e^{-\Delta_\beta u^2}H_m(u)|_{u=0} \tag{A6}$$

in terms of A_β, Υ_β, Λ_β, and Δ_β in Eq. (15). Here we used Eq. (A3b), and $u=\frac{\Lambda_\beta t}{\sqrt{\Upsilon_\beta}}$. From the Heisenberg uncertainty relation with $\langle\hat{q}\rangle_\beta=\langle\hat{p}\rangle_\beta=0$ [cf. Eq. (19)], it follows that $1>\Lambda_\beta\geq 0$. For a later purpose it is useful to confirm that for an uncoupled oscillator, $\Upsilon_\beta=\Delta_\beta=0$ and $\Lambda_\beta=e^{-\beta\hbar\omega_0}$.

To arrive at a closed form for ρ_{nm}, we consider the expression in Eq. (A6),

$$_{nm}\Xi_\beta := \left(\frac{\partial}{\partial u}\right)^n e^{-\Delta_\beta u^2}H_m(u)|_{u=0} = \sum_{r=0}^{n}\binom{n}{r}(e^{-\Delta_\beta u^2})^{(n-r)}\{H_m(u)\}^{(r)}\Big|_{u=0} \tag{A7}$$

where $\binom{n}{r}=\frac{n!}{(n-r)!r!}$, and $(\cdots)^{(r)}=(\frac{\partial}{\partial u})^r(\cdots)$. The Hermite polynomial $H_m(u)={}_mh_m u^m+{}_mh_{m-2}u^{m-2}+\cdots$ can be expressed as [18]

$$H_{2l}(u) = (-1)^l\frac{(2l)!}{l!}{}_1F_1\left(-l;\frac{1}{2};u^2\right) \tag{A8a}$$

$$H_{2l+1}(u) = (-1)^l\frac{2\cdot(2l+1)!}{l!}u\,{}_1F_1\left(-l;\frac{3}{2};u^2\right) \tag{A8b}$$

in terms of the confluent hypergeometric function ${}_1F_1(a;b;z)=\frac{\Gamma(b)}{\Gamma(a)}\sum_{k=0}^{\infty}\frac{\Gamma(a+k)}{\Gamma(b+k)}\frac{z^k}{k!}$ with $\frac{1}{\Gamma(-k)}=0$, $k=0,1,2,\cdots$. Then it immediately follows that

$$\{H_{2l}(u)\}^{(r)}|_{u=0} = \begin{cases}(2p)!\,{}_{2l}h_{2p} & \text{for } r=2p \text{ even, where } p\leq l\\ 0 & \text{otherwise}\end{cases} \tag{A9}$$

and from Eq. (A8a),

$$\{H_{2l}(u)\}^{(2p)}|_{u=0} = \sqrt{\pi}(-1)^l\frac{(2l)!}{l!}\frac{(2p)!}{p!}\frac{(-l)_p}{\Gamma\left(p+\frac{1}{2}\right)} \tag{A10}$$

where the Pochhammer symbol $(z)_k=\frac{\Gamma(z+k)}{\Gamma(z)}$. Similarly, we can also find that

$$\{H_{2l+1}(u)\}^{(r)}|_{u=0} = \begin{cases}(2p+1)!\,{}_{2l+1}h_{2p+1} & \text{for } r=2p+1 \text{ odd, where } p\leq l\\ 0 & \text{otherwise}\end{cases} \tag{A11}$$

and from Eq. (A8b),

$$\{H_{2l+1}(u)\}^{(2p+1)}|_{u=0} = \sqrt{\pi}(-1)^l \frac{(2l+1)!}{l!}\frac{(2p+1)!}{p!}\frac{(-l)_p}{\Gamma\left(p+\frac{3}{2}\right)}. \tag{A12}$$

Also, in Eq. (A7) we have

$$(e^{-\Delta_\beta u^2})^{(n-r)}|_{u=0} = \begin{cases} \dfrac{(-\Delta_\beta)^q(2q)!}{q!} & \text{for } n-r=2q \text{ even} \\ 0 & \text{otherwise.} \end{cases} \tag{A13}$$

With the aid of Eqs. (A9)–(A13), Eq. (A7) reduces to

$${}_{n,2l+1}\Xi_\beta = 0, \tag{A14}$$

$${}_{n,2l}\Xi_\beta = \frac{\sqrt{\pi}(-1)^{k+l}(2k)!\,(2l)!\,(\Delta_\beta)^k}{l!\,\Gamma(-l)} \times \sum_{p=0}^{k} \frac{\Gamma(-l+p)}{\Gamma\left(\frac{1}{2}+p\right)\Gamma(k-p+1)} \frac{\left(\frac{-1}{\Delta_\beta}\right)^p}{p!}, \tag{A15}$$

$$= (-1)^{k+l}\frac{(2k)!}{k!}\frac{(2l)!}{l!}(\Delta_\beta)^k {}_2F_1\left(-k,-l;\frac{1}{2};\frac{1}{\Delta_\beta}\right) \tag{A16}$$

for $n=2k$ even, and similarly

$${}_{n,2l}\Xi_\beta = 0, \tag{A17}$$

$${}_{n,2l+1}\Xi_\beta = 2(-1)^{k+l}\frac{(2k+1)!}{k!}\frac{(2l+1)!}{l!} \times (\Delta_\beta)^k {}_2F_1\left(-k,-l;\frac{3}{2};\frac{1}{\Delta_\beta}\right), \tag{A18}$$

for $n=2k+1$ odd. In Eq. (A15) we used the identity

$$\frac{1}{\Gamma(k-p+1)} = \frac{(-1)^p\Gamma(-k+p)}{\Gamma(k+1)\Gamma(-k)} \tag{A19}$$

to get the hypergeometric function ${}_2F_1(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)}\sum_{k=0}^{\infty}\frac{\Gamma(a+k)\Gamma(b+k)}{\Gamma(c+k)}\frac{z^k}{k!}$ in Eq. (A16). From Eqs. (A6), (A7), and (A14)–(A18) with the relation [18]

$$\Gamma(2\nu) = \frac{1}{\sqrt{\pi}}2^{2\nu-1}\Gamma(\nu)\Gamma\left(\nu+\frac{1}{2}\right) \tag{A20}$$

where $\nu=k,l$, we finally get Eqs. (14a)–(14c). We will below simplify the closed forms in Eqs. (14b) and (14c), respectively,

Now we use the relation [18]

$$P_n^{(\mu,\nu)}(z) = \binom{n+\mu}{n}\left(\frac{1+z}{2}\right)^n {}_2F_1\left(-n,-n-\nu;\mu+1;\frac{z-1}{z+1}\right) \tag{A21}$$

to express the matrix elements $(\hat{\rho}_s)_{nm}$ in terms of the Jacobi polynomial [18]

$$P_n^{(\mu,\nu)}(z) = \frac{1}{2^n}\sum_{k=0}^{n}\binom{n+\mu}{k}\binom{n+\nu}{n-k}(z-1)^{n-k}(z+1)^k, \tag{A22}$$

where $\mu,\nu > -1$. Equation (A21) allows us to have

$${}_2F_1\left(-k,-l;\frac{1}{2};\frac{1}{\Delta_\beta}\right) = \frac{\Gamma\left(\frac{1}{2}\right)\Gamma(l+1)}{\Gamma\left(l+\frac{1}{2}\right)}\left(\frac{2}{1+v}\right)^l P_l^{(-1/2,k-l)}(v) \tag{A23a}$$

$${}_2F_1\left(-k,-l;\frac{3}{2};\frac{1}{\Delta_\beta}\right) = \frac{\Gamma\left(\frac{3}{2}\right)\Gamma(l+1)}{\Gamma\left(l+\frac{3}{2}\right)}\left(\frac{2}{1+v}\right)^l P_l^{(1/2,k-l)}(v) \tag{A23b}$$

for $k \geq l$ where $v=1-\frac{2}{1-\Delta_\beta}$. Further, we find that [33]

$$P_{2n}^{(\nu,\nu)}(z) = (-1)^n\frac{\Gamma(2n+\nu+1)\Gamma(n+1)}{\Gamma(n+\nu+1)\Gamma(2n+1)}P_n^{(-1/2,\nu)}(1-2z^2) \tag{A24a}$$

$$P_{2n+1}^{(\nu,\nu)}(z) = (-1)^n\frac{\Gamma(2n+\nu+2)\Gamma(n+1)}{\Gamma(n+\nu+1)\Gamma(2n+2)}zP_n^{(1/2,\nu)}(1-2z^2), \tag{A24b}$$

which can be verified, respectively, by using Eq. (A22) and then comparing each coefficient of z^k on both sides. Note here that $P_{2n}^{(\nu,\nu)}(z)=P_{2n}^{(\nu,\nu)}(-z)$ and $P_{2n+1}^{(\nu,\nu)}(z)=-P_{2n+1}^{(\nu,\nu)}(-z)$. With the aid of Eqs. (A23a), (A23b), (A24a), and (A24b), Eqs. (14b) and (14c) can then be transformed into Eqs. (16a) and (16b), respectively.

APPENDIX B: DERIVATION OF EQS. (66)–(70)

Using the relations in Eq. (9) with $\partial\omega_0/\partial M = -\omega_0/(2M)$ we can easily obtain

$$\frac{\partial\Omega}{\partial M} = \frac{\Omega}{\Omega+\gamma}\frac{\mathbf{w}_0^2\gamma}{M\{\Omega(\gamma-\Omega)-\mathbf{w}_0^2\}};\quad \frac{\partial\gamma}{\partial M} = -\frac{\partial\Omega}{\partial M};$$

$$\frac{\partial\mathbf{w}_0}{\partial M} = \frac{\mathbf{w}_0\Omega(\mathbf{w}_0^2+\Omega^2-\gamma^2)}{2M(\Omega+\gamma)\{\Omega(\gamma-\Omega)-\mathbf{w}_0^2\}}. \tag{B1}$$

From $\partial\omega_0/\partial k_0 = -(\partial\omega_0/\partial M)/\omega_0^2$, it immediately follows as well that

$$\frac{\partial\Omega}{\partial k_0} = -\frac{1}{(\mathbf{w}_0)^2}\frac{\Omega+\gamma}{\Omega}\frac{\partial\Omega}{\partial M};\quad \frac{\partial\gamma}{\partial k_0} = -\frac{\partial\Omega}{\partial k_0};$$

$$\frac{\partial\mathbf{w}_0}{\partial k_0} = -\frac{1}{(\mathbf{w}_0)^2}\frac{\Omega+\gamma}{\Omega}\frac{\partial\mathbf{w}_0}{\partial M}. \tag{B2}$$

We also have $\partial\underline{\omega_1}/\partial M = \partial\Omega/\partial M$ and

$$\frac{\partial \underline{\underline{\omega_2}}}{\partial M} = \frac{1}{\sqrt{\left(\frac{\gamma}{2\mathbf{w}_0}\right)^2 - 1}} \frac{\partial \mathbf{w}_0}{\partial M} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{1 - \left(\frac{2\mathbf{w}_0}{\gamma}\right)^2}}\right)\frac{\partial \Omega}{\partial M} \tag{B3}$$

$$\frac{\partial \underline{\underline{\omega_3}}}{\partial M} = - \frac{1}{\sqrt{\left(\frac{\gamma}{2\mathbf{w}_0}\right)^2 - 1}} \frac{\partial \mathbf{w}_0}{\partial M} - \frac{1}{2}\left(1 + \frac{1}{\sqrt{1 - \left(\frac{2\mathbf{w}_0}{\gamma}\right)^2}}\right)\frac{\partial \Omega}{\partial M}, \tag{B4}$$

and from Eq. (8),

$$\frac{\partial \lambda_d^{(1)}}{\partial M} = \frac{(2\Omega\gamma - \gamma^2 + \Omega^2 + \mathbf{w}_0^2)\frac{\partial \Omega}{\partial M} + 2\gamma \mathbf{w}_0 \frac{\partial \mathbf{w}_0}{\partial M}}{(\Omega - z_1)^2(\Omega - z_2)^2};$$

$$\frac{\partial \lambda_d^{(2)}}{\partial M} = \frac{(z_2^2 - z_1^2)\frac{\partial \Omega}{\partial M} + (\Omega + z_2)(2z_1 - z_2 - \Omega)\frac{\partial z_1}{\partial M} + (\Omega^2 - z_1^2)\frac{\partial z_2}{\partial M}}{(z_1 - \Omega)^2(z_1 - z_2)^2} \tag{B5}$$

and $\partial\lambda_d^{(3)}/\partial M \rightarrow \partial\lambda_d^{(2)}/\partial M$ with $(z_1 \leftrightarrow z_2)$. Then we finally arrive at the expressions in Eqs. (66) and (67), respectively. With the replacement of $\partial/\partial M$ in Eqs. (B3)–(B5) by $\partial/\partial k_0$, we can also have Eqs. (69) and (70).

APPENDIX C: COMMENT ON EFFECTIVE THERMODYNAMIC RELATIONS

In ordinary thermodynamics, the notion of temperature T appears conceptually as a partial derivative of internal energy U with respect to entropy S such that $T=\partial U/\partial S$. This also holds for the effective temperature $T^\star_{\text{eff}}$: Combining the first law $dU_s=\delta\mathcal{Q}^\star_{\text{eff}}+\delta\mathcal{W}^\star_{\text{eff}}$ with the second law $\delta\mathcal{Q}^\star_{\text{eff}}=T^\star_{\text{eff}} dS_N$ for a reversible process, we have

$$T^\star_{\text{eff}} = \left(\frac{\partial U_s}{\partial S_N}\right)_{\partial\mathcal{W}^\star_{\text{eff}}=0}. \tag{C1}$$

It is also interesting to note that Eq. (37) can be recovered by the relation

$$U_s = U^\star_{\text{eff}} = -\frac{\partial}{\beta^\star_{\text{eff}}} \ln Z^\star_{\text{eff}}, \tag{C2}$$

which is well defined in terms of a generating function

$$\frac{\partial}{\partial \beta^\star_{\text{eff}}} \ln Z^\star_{\text{eff}} = \frac{\partial}{\partial A} \ln \sum_n e^{A\hbar\omega^\star_{\text{eff}}(n+1/2)}\Big|_{A=\beta^\star_{\text{eff}}}. \tag{C3}$$

From Eq. (40) it then follows as well that the effective free energy $F^\star_{\text{eff}}=U_s-T^\star_{\text{eff}} S_N$, where $F^\star_{\text{eff}}=-k_B T^\star_{\text{eff}} \ln Z^\star_{\text{eff}}$.

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