Responses to applied forces and the Jarzynski equality in classical oscillator systems coupled to finite baths: An exactly solvable nondissipative nonergodic model

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Responses of small open oscillator systems to applied external forces have been studied with the use of an exactly solvable classical Caldeira-Leggett model in which a harmonic oscillator (system) is coupled to finite N-body oscillators (bath) with an identical frequency (ω_n = ω_0 for n = 1 to N). We have derived exact expressions for positions, momenta, and energy of the system in nonequilibrium states and for work performed by applied forces. A detailed study has been made on an analytical method for canonical averages of physical quantities over the initial equilibrium state, which is much superior to numerical averages commonly adopted in simulations of small systems. The calculated energy of the system which is strongly coupled to a finite bath is fluctuating but nondissipative. It has been shown that the Jarzynski equality is valid in nondissipative nonergodic open oscillator systems regardless of the rate of applied ramp force.

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I. INTRODUCTION

In the past decade, significant progress has been made in our understanding of nonequilibrium statistics. Experimental and theoretical studies have been developed on small systems such as quantum dots and biological molecular machines which generally operate away from equilibrium (for reviews, see Refs. [1–3]). The development of modern techniques of microscopic manipulation has promoted experimental studies of small systems. It has become possible to study the response of small systems to applied external forces. In parallel theorists have developed three important theorems: the Jarzynski equality (JE) [4], the steady-state and transient fluctuation theorems [5–7], and Crook’s theorem [6,7]. These fluctuation theorems may be applicable to nonequilibrium systems driven far from the equilibrium states. In this paper we direct our attention to a remarkable JE given by

\[ e^{-\beta \Delta F} = \langle e^{-\beta W} \rangle = \int dW P(W) e^{-\beta W}, \]

where \( W \) denotes work made in a system when its parameter is changed, the bracket \( \langle \cdot \rangle \) expresses the average over the work distribution function (WDF) \( P(W) \) of work performed by a prescribed protocol, \( \Delta F \) stands for the free-energy difference between the initial and final equilibrium states, and \( \beta (=1/k_B T) \) is the inverse temperature of the initial state. Equation (1) includes the second law of thermodynamics, \( \langle W \rangle \geq \Delta F \), where the equality holds only for the reversible process. The JE was originally proposed for a classical isolated system and open system weakly coupled to baths which are described by the Hamiltonian [4] and the stochastic models [8]. Jarzynski later proved that the JE is valid for strongly coupled open systems [9]. A generalization of the JE to quantum systems has been made in Refs. [10–17].

A validity of the JE has been confirmed by some experiments [18–23]. Lifshitz et al. [18] have determined the free energy required to unfold a single RNA chain from nonequilibrium work measurements. Wang et al. [19] have considered a colloidal particle pulled through liquid water by an optical trap. Douarche et al. [20,21] have verified the JE for a mechanical oscillator that is driven out of equilibrium by an external force. By using a torsion pendulum composed of a brass wire, Joubaud et al. [22,23] have experimentally studied the JE of the harmonic oscillator in contact with a thermostat and driven out of equilibrium by an external force.

Some criticisms, however, have been raised for the validity of the JE [24–35]. Cohen and Mauzerall [24] pointed out that it is difficult to define the distribution and the temperature during the irreversible process. In response to this criticism, Jarzynski [9] has claimed that the JE holds if the initial state is in the equilibrium state with a definite temperature [9]. It has been pointed out that the JE may be violated in an ideal gas model [25,31,32,34,35] and in a rigid rotator model [26,28,29]. Therefore it is currently an important issue to examine the validity condition of the JE.

Many studies have been reported for harmonic oscillator systems by both experimental [3,18,20–23] and theoretical methods [36–46]. Theoretical analyses have been made for oscillators with the use of the Markovian Langevin model [20–23,36], the non-Markovian Langevin model [37–40], the Fokker-Planck equation [41], and the Hamiltonian model [42–46]. All of these studies have shown that the JE holds in isolated and open oscillators, assuming dissipative memory kernels or overdamped models. This assumption seems reasonable in the situation under which the relevant experiments [20–23] have been performed. Recent theoretical studies, however, have demonstrated that the energy dissipation is not realized in a small system coupled to finite thermal baths [47,48]. This is quite different from the case of infinite baths in which dissipation is realized. Indeed, it is commonly believed that the dissipation is realized only when the system is coupled to an infinite bath (except for chaotic baths) [49]. Poincaré recurrence time is finite for a finite bath.

It is necessary to make detailed calculations of the responses of small systems to the applied force such as variations of position and energy of the system, which have not been reported as far as we are aware of. The purpose of the
present study is twofold: to make a detailed study of the response to an applied force and to examine the validity of the JE in open harmonic oscillator systems in a nondissipative situation. We consider the Caldeira-Leggett (CL) Hamiltonian model [50,51], adopting a single-ω bath containing uncoupled N-body oscillators with an identical frequency \( \omega_n = \omega_o \) for \( n = 1 \) to N Eq. (13). The CL model with a single-ω bath is exactly solvable. A similar optic-phonon-mode model for the bath was adopted in a different context from the present study [52]. In the conventional approach, we obtain the Langevin equation from the CL model, with which its properties are investigated. In this study, we have directly obtained the Laplace-transformed equation of motion of the system. The energy and work of the system induced by the applied force are analytically averaged over the canonical distribution of initial equilibrium states. Our nondissipative system plus bath yields nonergodic solutions, for which the JE will be shown to be valid in contrast with Refs. [39,40], which claim the importance of the ergodicity.

The paper is organized as follows. In Sec. II, we derive expressions of the response of positions, momenta, and system energy induced by an applied ramp force in open oscillator systems, by using the CL model with the single-ω bath mentioned above. We obtain the WDF and the averaged work with which the validity of the JE have been investigated. Some numerical calculations are presented. In Sec. III an application of other types of external forces to the system is studied. We compare our study with the method using the Langevin model derived from the CL model. Section IV is devoted to our conclusion.

II. THE ADOPTED MODEL

A. Equations of motion

We consider a system of a classical oscillator coupled to a bath consisting of N-body uncoupled oscillators described by the CL model [50,51],

\[
H = H_S + H_B + H_I,
\]

(2)

with

\[
H_S = \frac{p^2}{2M} + \frac{M \Omega^2 Q^2}{2} - f(t)Q, \tag{3}
\]

\[
H_B = \sum_{n=1}^{N} \left( \frac{p_n^2}{2m} + \frac{m \omega_n^2 q_n^2}{2} \right), \tag{4}
\]

\[
H_I = -\sum_{n=1}^{N} \left( c_n q_n \frac{Q}{\omega_n^2} - \frac{c_n^2 Q^2}{2} \right), \tag{5}
\]

where \( H_S, H_B, \) and \( H_I \) express one-dimensional Hamiltonians of the system, bath, and interaction, respectively, \( M \) (\( m \)), \( \Omega \) (\( \omega_n \)), \( Q \) (\( q_n \)), and \( P \) (\( p_n \)) denote mass, frequency, position, and momentum, respectively, of the system (bath), \( c_n \) is the interaction between the system and bath, and \( f(t) \) is an applied external force. Equations of motion for \( Q \) and \( q_n \) are given by

\[
M \dot{Q} = -M \Omega^2 Q + \sum_{n=1}^{N} c_n \left( q_n - \frac{c_n Q}{m \omega_n^2} \right) + f(t), \tag{6}
\]

\[
m \ddot{q}_n = -m \omega_n^2 q_n + c_n Q. \tag{7}
\]

Applying the Laplace transformation to Eqs. (6) and (7), we obtain

\[
M[s^2 \hat{Q}(s) - \dot{Q}(0) - s \dot{Q}(0)]
\]

\[
= -M \Omega^2 \hat{Q}(s) - \sum_{n=1}^{N} \left( \frac{c_n^2}{m \omega_n^2} \right) \hat{q}_n(s) + \sum_{n=1}^{N} c_n \hat{q}_n(s) + \hat{f}(s), \tag{8}
\]

\[
m[s^2 \hat{q}_n(s) - \dot{q}_n(0) - s q_n(0)] = -m \omega_n^2 \hat{q}_n(s) + c_n \hat{Q}(s), \tag{9}
\]

where

\[
\hat{Q}(s) = \int_0^\infty dt \ e^{-st} Q(t), \tag{10}
\]

and similar expressions for \( \hat{q}_n(s) \) and \( \hat{f}(s) \). Solving Eq. (9) in terms of \( \hat{q}_n(s) \) and substituting it into Eq. (8), we obtain

\[
\hat{Q}(s) = \hat{G}(s) \left[ \hat{Q}(0) + \frac{s}{M} \hat{Q}(0) \right. \right.
\]

\[
+ \sum_{n=1}^{N} \frac{c_n \hat{q}_n(0) + s q_n(0)}{M(s^2 + \omega_n^2)} + \frac{\hat{f}(s)}{M} \bigg] , \tag{11}
\]

where the Green’s function \( \hat{G}(s) \) is given by

\[
\hat{G}(s) = \left( s^2 + \Omega^2 + \sum_{n=1}^{N} \frac{c_n^2 s^2}{M m \omega_n^2 \left( s^2 + \omega_n^2 \right)} \right)^{-1}. \tag{12}
\]

In order to make an analytic calculation feasible, we consider a bath containing N-body uncoupled oscillators with an identical frequency \( \omega_n \) and a uniform coupling \( c_o \), as given by

\[
\omega_n = \omega_o, \tag{13}
\]

\[
c_n = \frac{c_o}{\sqrt{N}} \text{ for } n = 1 \text{ to } N. \tag{14}
\]

We have chosen \( c_n \) such that it yields a nondivergent result in the limit of \( N \to \infty \) in Eq. (12) (a related discussion being given in Sec. III B) [53]. With the use of Eqs. (13) and (14), \( \hat{Q}(s) \) becomes

\[
\hat{Q}(s) = \hat{G}(s) \left[ \frac{P_0}{M} + s Q_0 \right. \right.
\]

\[
+ \sum_{n=1}^{N} \frac{c_o}{M \sqrt{N} \left( s^2 + \omega_o^2 \right)} \left( \frac{p_{n0}}{m} + s q_{n0} \right) \bigg] , \tag{15}
\]

with

\[
\hat{G}(s) = \left( s^2 + \Omega^2 + \frac{c_o^2 s^2}{M m \omega_o^2 \left( s^2 + \omega_o^2 \right)} \right)^{-1} , \tag{16}
\]

where \( P_0 = M \hat{Q}(0), Q_0 = Q(0), p_{n0} = m \hat{q}_n(0), \) and \( q_{n0} = q_n(0). \) Equation (16) may be rewritten as

\[
\hat{G}(s) = \frac{s^2 + \omega_o^2}{(s^2 + \Omega^2)(s^2 + \omega_o^2) + c_o^2 s^2 / M m \omega_o^2} \tag{17}
\]

\[
= \sum_{i=1}^{2} \frac{b_i}{(s^2 + a_i^2)}. \tag{18}
\]
with
\[ a_i^2 = \frac{1}{2} \left[ \Omega^2 + \omega_o^2 + \frac{c_i^2}{M \omega_o^2} \right] + (-1)^{i-1} \sqrt{D_o} \]  
\[ (i = 1, 2), \]
\[ D_o = (\Omega^2 - \omega_o^2)^2 + \frac{2c_o^2(\Omega^2 + \omega_o^2)}{M \omega_o^2} + \frac{c_o^4}{M^2 \omega_o^4}, \quad \alpha > 0, \]
\[ b_1 = \frac{a_1^2 - \omega_o^2}{a_1^2 - a_2^2}, \quad b_2 = \frac{\omega_o^2 - a_2^2}{a_1^2 - a_2^2}. \]

Then Eq. (15) becomes
\[
\hat{Q}(s) = \frac{2}{s^2 + \omega_o^2} \left\{ \frac{P_0}{M} + s \bar{Q}_0 \right\} + \frac{c_o}{M \sqrt{N} (s^2 + \omega_o^2)} \sum_{n=1}^{N} \left( \frac{p_n \omega o}{m} + s q_n \right) + \frac{\dot{f}(t)}{M},
\]

whose inverse Laplace transformation yields
\[
\hat{Q}(t) = \Phi(t) + X_{\bar{Q}}(t) \bar{Q}_0 + X_P(t) P_0 \]
\[ + Y_q(t) \sum_{n=1}^{N} q_n + Y_p(t) \sum_{n=1}^{N} p_n, \]

with
\[
\Phi(t) = \frac{2}{\bar{M} a_i} \int_0^t \sin a_i(t - t') f(t') dt',
\]
\[
X_{\bar{Q}}(t) = \frac{2}{\bar{M} a_i} \cos a_i t,
\]
\[
X_P(t) = \frac{2}{\bar{M} a_i} \sin a_i t,
\]
\[
Y_q(t) = \frac{2}{M \sqrt{N}} \left( \frac{b_1 c_o}{M \omega_o} \right) \left( \cos \omega_o t - \cos a_i t \right) \left( \frac{a_1^2 - a_2^2}{a_1^2 - a_i^2} \right),
\]
\[
Y_p(t) = \frac{2}{M \sqrt{N}} \left( \frac{b_1 c_o}{M \omega_o} \right) \left( \frac{a_1 \sin \omega_o t - a_i \sin a_i t}{m \omega_o a_i} \right) \left( \frac{a_1^2 - a_i^2}{a_1^2 - a_2^2} \right).
\]

B. Position, momentum, and system energy

It is necessary to evaluate physical quantities averaged over the canonical distribution of the initial states \( Q_0, P_0, \{ q_n \}, \) and \( \{ p_n \} \) of the equilibrium-coupled system-and-bath \( H(t = 0) \).

In order to make such evaluations, we need the following (fluctuation-dissipation) relations for \( f(t) = 0 \) given by
\[
M \Omega^2 \langle Q_0^2 \rangle = \frac{\langle P_0^2 \rangle}{M} = k_B T = \frac{1}{\beta},
\]
\[
M \omega_o^4 \langle q_n q_0 \rangle = k_B T \delta_{n0} + \frac{c_o c_i k_B T}{m \omega_o^2 M \Omega^2},
\]
\[
\frac{\langle p_n p_0 \rangle}{m} = k_B T \delta_{n0},
\]
\[
\langle Q_0 q_0 \rangle = \frac{c_o k_B T \omega_o^2}{M \Omega^2},
\]
\[
\langle P_0 Q_0 \rangle = \frac{c_i k_B T \omega_o^2}{M \Omega^2}.
\]

Then Eq. (15) becomes
\[
\hat{O}(s) = \left( \frac{2}{s^2 + \omega_o^2} \right) \left\{ \frac{P_0}{M} + s \bar{Q}_0 \right\} + \frac{c_o}{M \sqrt{N} (s^2 + \omega_o^2)} \sum_{n=1}^{N} \left( \frac{p_n \omega o}{m} + s q_n \right) + \frac{\dot{f}(t)}{M},
\]

whose inverse Laplace transformation yields
\[
\hat{O}(t) = \Phi(t) + X_{\bar{Q}}(t) \bar{Q}_0 + X_P(t) P_0 \]
\[ + Y_q(t) \sum_{n=1}^{N} q_n + Y_p(t) \sum_{n=1}^{N} p_n, \]

with
\[
\Phi(t) = \frac{2}{\bar{M} a_i} \int_0^t \sin a_i(t - t') f(t') dt',
\]
\[
X_{\bar{Q}}(t) = \frac{2}{\bar{M} a_i} \cos a_i t,
\]
\[
X_P(t) = \frac{2}{\bar{M} a_i} \sin a_i t,
\]
\[
Y_q(t) = \frac{2}{M \sqrt{N}} \left( \frac{b_1 c_o}{M \omega_o} \right) \left( \cos \omega_o t - \cos a_i t \right) \left( \frac{a_1^2 - a_2^2}{a_1^2 - a_i^2} \right),
\]
\[
Y_p(t) = \frac{2}{M \sqrt{N}} \left( \frac{b_1 c_o}{M \omega_o} \right) \left( \frac{a_1 \sin \omega_o t - a_i \sin a_i t}{m \omega_o a_i} \right) \left( \frac{a_1^2 - a_i^2}{a_1^2 - a_2^2} \right).
\]

The system energy \( \bar{E}_S \) averaged over the initial state is given by
\[
\bar{E}_S = \langle E_S \rangle = \frac{M}{2} \langle \bar{Q}^2 \rangle + \frac{M \Omega^2}{2} \langle \bar{Q}^2 \rangle - \langle f(t) \rangle \langle Q(t) \rangle.
\]

By using Eqs. (29)–(34) and (43), we obtain \( \bar{E}_S \) given by
\[
\bar{E}_S = \bar{E}_S^{(0)} + \bar{E}_S^{(f)},
\]

with
\[
\bar{E}_S^{(0)} = \frac{k_B T}{2 M \Omega^2} \left[ M \dot{X}_P(t)^2 + M \Omega^2 \dot{X}_Q(t)^2 \right] + \frac{2 k_B T}{M \Omega^2} \left[ M \dot{X}_P(t)^2 + M \Omega^2 \dot{X}_Q(t)^2 \right] + \frac{Nm k_B T}{2} \left[ M \dot{Y}_P(t)^2 + M \Omega^2 \dot{Y}_P(t)^2 \right]}

Here $\hat{E}_S$ expresses the system energy depending on the temperature but independent of the applied force; $\hat{E}_S^{(f)}$ denotes the response to the force, $\Phi(t)$, $X_Q(t)$, $X_P(t)$, $Y_Q(t)$, and $Y_P(t)$ are given by Eqs. (24)–(28); $\dot{X}_Q(t)$, $\dot{X}_P(t)$, $\dot{Y}_Q(t)$, and $\dot{Y}_P(t)$ are their derivatives with respect to time. It is noted that $\hat{Q}(t)$ and $\hat{P}(t)$ are independent of $N$ because of the $N$-independent $\Phi(t)$ in Eq. (24). Furthermore, $\hat{E}_S$ does not depend on $N$ because the $N$ factor in the fourth term of Eq. (45) is canceled out by the $1/N$ term in $Y_Q(t)^2$ in Eq. (27) and because the $\sqrt{N}$ term of the last term of Eq. (45) is canceled out by the $1/\sqrt{N}$ of $Y_Q(t)$. These properties arise from our adopted model with $c_\alpha = c_\alpha /\sqrt{N}$ in Eq. (14) [53].

The advantage of expressions given by Eqs. (37), (38), and (44)–(46) is that canonical averages over the initial state have been analytically made and they are free from the numerical averaging, which is one of difficulties in direct simulations of small systems [47,48,58–60].

We have so far not specified the form of an external force $f(t)$. For a while we consider a ramp force given by

$$f(t) = \begin{cases} 0 & \text{for } t < 0, \\ \frac{g}{\tau} & \text{for } 0 \leq t < \tau, \\ g & \text{for } t \geq \tau. \end{cases}$$

where $\tau$ stands for a duration of the applied force and $g$ the magnitude of the force at $t \geq \tau$. For the ramp force, Eq. (24) leads to

$$\Phi(t) = \sum_{i=1}^{2} \left( \frac{g b_i}{M a_i \tau} \right) \left( a_i t - \sin a_i t \right) \text{ for } 0 \leq t < \tau,$$

$$= \sum_{i=1}^{2} \left( \frac{g b_i}{Ma_i^2} \right) \left( \frac{1}{a_i \tau} \left[ a_i \tau + \sin a_i (t - \tau) - \sin a_i \tau \right] \right) \text{ for } t \geq \tau.$$  

In the following, we examine the three cases of (1) no couplings ($c_\alpha = 0$), (2) transient force ($\tau = 0$), and (3) quasistatic force ($\tau \to \infty$).

(1) In the case of $c_\alpha = 0$ where Eqs. (19)–(21) lead to $a_1 = \Omega$, $b_1 = 1$, and $b_2 = 0$, we obtain

$$\Phi(t) = \frac{g}{M \Omega^2 \tau} \left( \Omega t - \sin \Omega t \right) \text{ for } 0 \leq t < \tau,$$

$$= \frac{g}{M \Omega^2} \left( \frac{1}{\Omega \tau} \left[ \Omega \tau + \sin \Omega (t - \tau) - \sin \Omega \tau \right] \right) \text{ for } t \geq \tau.$$  

Equations (25) and (26) lead to

$$X_Q(t) = \cos \Omega t.$$  

$\tilde{E}_S(t)$ becomes

$$\tilde{E}_S(t) = k_B T - \frac{g^2}{2M \Omega^2} \left[ \left( \frac{t}{\tau} \right)^2 - \frac{2(1 - \cos \Omega t)}{\Omega^2 \tau^2} \right]$$

for $0 \leq t < \tau,$

$$= k_B T - \frac{g^2}{2M \Omega^2} \left( 1 - \frac{2(1 - \cos \Omega t)}{\Omega^2 \tau^2} \right) \text{ for } t \geq \tau.$$  

(2) In the case of $\tau = 0$, Eq. (49) yields

$$\Phi(t) = \sum_{i=1}^{2} \left( \frac{g b_i}{Ma_i^2} \right) \left( 1 - \cos a_i t \right) \text{ for } t \geq 0,$$

which becomes for $c_\alpha = 0$,

$$\Phi(t) = \frac{g}{M \Omega^2} \left( \frac{t}{\tau} \right) \text{ for } 0 \leq t < \infty,$$

yielding

$$\tilde{E}_S(t) = k_B T \text{ for } t \geq 0.$$  

(3) In the case of $\tau \to \infty$, Eq. (48) yields

$$\Phi(t) = \sum_{i=1}^{2} \left( \frac{g b_i}{Ma_i^2} \right) \left( \frac{t}{\tau} \right) \text{ for } 0 \leq t < \infty,$$

which becomes for $c_\alpha = 0$,

$$\Phi(t) = \frac{g}{M \Omega^2} \left( \frac{t}{\tau} \right) \text{ for } 0 \leq t < \infty,$$

leading to

$$\tilde{E}_S(t) = k_B T - \frac{g^2}{2M \Omega^2} \left( \frac{t}{\tau} \right)^2 \text{ for } t \to \infty.$$  

We have performed numerical calculations for averaged position, momentum, and energy of the system with $M = m = 1.0$, $\Omega = \omega_o = 1.0$, and $g = 1.0$, which are adopted in all our calculations and are otherwise noticed. Position, momentum, and energy (work) are measured in units of $\sqrt{k_B T / M \Omega^2}$, $\sqrt{M k_B T}$, and $k_B T$, respectively. Model calculations of averaged positions and momenta are presented in Figs. 1(a)–1(h), where solid and dashed curves express $\hat{Q}(t)$ and $\hat{P}(t)$, respectively. Figures 1(a) and 1(b) show the results of $c_\alpha = 0.0$ and $c_\alpha = 1.0$, respectively, when a ramp force with $\tau = 100$ is applied. Figure 1(a) shows that $\hat{Q}(t)$ is linearly increased at $0 \leq t < 100.0$, and it becomes constant at $t \geq 100.0$ where a force $g$ is still applied. This behavior is not changed even when the system-bath coupling is introduced as shown in Fig. 1(b). Figures 1(c), 1(e), and 1(g) show $\hat{Q}(t)$ and $\hat{P}(t)$ for ramp forces with $\tau = 10.0, 5.0, 0.0$, respectively, applied to uncoupled systems ($c_\alpha = 0.0$), where regular oscillations are induced. Figures 1(d), 1(f), and
1(h), however, show that irregular oscillations are induced by external forces with \( \tau = 10.0, 5.0, \) and 0.0 in coupled systems.

Model calculations of system energy \( \bar{E}_S(t) \) are plotted in Figs. 2(a)–2(j). Figures 2(a) and 2(b) show \( \bar{E}_S(t) \) for \( c_o = 0.0 \) and \( c_o = 1.0, \) respectively, without external forces \( f(t) = g = 0.0 \) for which \( \bar{E}_S \) is constant. Figures 2(c) and 2(e) [Figs. 2(d) and 2(f)] show \( \bar{E}_S \) for \( c_o = 0.0 \) (\( c_o = 1.0, \) with applied forces of \( \tau = 100.0 \) and 10.0, respectively, where \( \bar{E}_S \) is gradually decreased by an applied force. As far as the uncoupled system is concerned, this behavior is not modified when the force with smaller \( \tau \) is applied, as shown by Figs. 2(g) and 2(i) for \( \tau = 5.0 \) and \( \tau = 0.0, \) respectively. However, when the ramp force with smaller \( \tau \) is applied to coupled systems, the behavior is changed: Irregular oscillations are induced in \( \bar{E}_S \) as shown by Figs. 2(h) and 2(j) for \( \tau = 5.0 \) and \( \tau = 0.0, \) respectively. These oscillations in coupled systems are realized for ramp forces with \( \tau \) \( \leq T_o \) where \( T_o = (2\pi/\Omega) \) denotes the period of system oscillation. We note in Figs. 2(h) and 2(j) that this irregular oscillation is not a dissipate, which has been confirmed with calculations for \( t \in [0, 10,000] \) (relevant results not shown). The averaged system energy in the coupled small systems shows irregular nondissipative oscillations, although the total energy of the system plus bath is constant [47,48].

![Figure 1](image1.png)

**FIG. 1.** (Color online) The time dependence of the averaged position \( \bar{Q} \) (solid curves) and momentum \( \bar{P} \) (dashed curves): (a) \( \tau = 100.0, c_o = 0.0, \) (b) \( \tau = 100.0, c_o = 1.0, \) (c) \( \tau = 10.0, c_o = 0.0, \) (d) \( \tau = 10.0, c_o = 1.0, \) (e) \( \tau = 5.0, c_o = 0.0, \) (f) \( \tau = 5.0, c_o = 1.0, \) (g) \( \tau = 0.0, c_o = 0.0, \) and (h) \( \tau = 0.0, c_o = 1.0. \)

![Figure 2](image2.png)

**FIG. 2.** (Color online) The time dependence of the averaged system energy \( \bar{E}_S; \) for no forces \( (f = 0) \) with (a) \( c_o = 0.0, \) (b) \( c_o = 1.0; \) for the ramp forces with (c) \( \tau = 100.0, c_o = 0.0, \) (d) \( \tau = 100.0, c_o = 1.0, \) (e) \( \tau = 10.0, c_o = 0.0, \) (f) \( \tau = 10.0, c_o = 1.0, \) (g) \( \tau = 5.0, c_o = 0.0, \) (h) \( \tau = 5.0, c_o = 1.0, \) (i) \( \tau = 0.0, c_o = 0.0, \) and (j) \( \tau = 0.0, c_o = 1.0. \)

### C. Work and work distribution function

Next we consider work performed by an applied external force. By using \( Q(t) \) given by Eq. (23), we obtain the work performed by the force \( f(t) \) applied for \( 0 \leq t < \tau \) [4].

\[
W_0 = -\int_0^\tau dt \, f(t) Q(t)
\]

\[
= \phi + C_Q Q_0 + C_P P_0 + D_q \sum_{n=1}^N q_{n0} + D_p \sum_{n=1}^N p_{n0},
\]

where

\[
\phi = -\int_0^\tau dt \, f(t) \Phi(t),
\]

\[
\Phi(t) = \frac{1}{2} \left[ f(t) \frac{d^2}{dt^2} + \Omega^2 \right] Q(t) - \frac{1}{2} \left[ f(t) \frac{d}{dt} + \Omega \right] Q(t) - f(t) Q(t).
\]
Performing the Gauss integrals, we obtain

\[
\langle \exp(-iuW_0) \rangle_0 = \exp(-iu\phi) \left( \frac{\beta \Omega}{2\pi} \right)^N \int dQ_0 \exp \left[ -\frac{\beta \Omega^2 Q_0^2}{2} - iuC_Q Q_0 \right] \int dP_0 \exp \left[ -\frac{\beta P_0^2}{2M} - iuC_P P_0 \right]
\]

\[
\times \prod_{n=1}^{N} \int dq_{n0} \exp \left[ -\frac{\beta m\omega_n^2}{2} \left( q_{n0} - \frac{c_n Q_0}{m\omega_0^2} \right)^2 - iuD_q \left( q_{n0} - \frac{c_n Q_0}{m\omega_0^2} \right) - \frac{iuD_p c_n Q_0}{m\omega_0^2} \right]
\]

\[
\times \prod_{n=1}^{N} \int dp_{n0} \exp \left[ -\frac{\beta p_{n0}^2}{2m} - iuD_p p_{n0} \right].
\]

With the use of Eqs. (64)–(67), the WDF of \( P(W) \) is given by

\[
P(W) = \langle \delta(W - W_0) \rangle_0 = \frac{1}{2\pi} \int du \exp(iuW)\exp(-iuW_0),
\]

where

\[
\phi = -\left( \frac{g^2}{M} \right) \sum_{i=1}^{2} b_i \left[ \frac{1}{2a_i} - \frac{(1 - \cos a_i\tau)}{a_i^2\tau^2} \right],
\]

\[
C_Q = -g \sum_{i=1}^{2} b_i \frac{\sin a_i\tau}{a_i\tau},
\]

\[
C_P = -\left( \frac{g}{\sqrt{N}} \right) \sum_{i=1}^{2} b_i \frac{(1 - \cos a_i\tau)}{a_i^2\tau},
\]

\[
D_q = -\left( \frac{c_0 g}{\sqrt{NM}} \right) \sum_{i=1}^{2} b_i \frac{\sin a_i\omega_0\tau - \omega_0 \sin a_i\tau}{a_i\omega_0\tau (a_i^2 - a_0^2)},
\]

\[
D_p = -\left( \frac{c_0 g}{\sqrt{NMm}} \right) \sum_{i=1}^{2} b_i \frac{\sin a_i\omega_0\tau - \omega_0 \sin a_i\tau}{a_i^2\omega_0^2 \tau (a_i^2 - a_0^2)},
\]

For a ramp force given by Eq. (47), Eqs. (65)–(67) become

\[
\phi = -\left( \frac{g^2}{M} \right) \sum_{i=1}^{2} b_i \left[ \frac{1}{2a_i} - \frac{(1 - \cos a_i\tau)}{a_i^2\tau^2} \right],
\]

\[
C_Q = -g \sum_{i=1}^{2} b_i \frac{\sin a_i\tau}{a_i\tau},
\]

\[
C_P = -\left( \frac{g}{\sqrt{N}} \right) \sum_{i=1}^{2} b_i \frac{(1 - \cos a_i\tau)}{a_i^2\tau},
\]

\[
D_q = -\left( \frac{c_0 g}{\sqrt{NM}} \right) \sum_{i=1}^{2} b_i \frac{\sin a_i\omega_0\tau - \omega_0 \sin a_i\tau}{a_i\omega_0\tau (a_i^2 - a_0^2)},
\]

\[
D_p = -\left( \frac{c_0 g}{\sqrt{NMm}} \right) \sum_{i=1}^{2} b_i \frac{\sin a_i\omega_0\tau - \omega_0 \sin a_i\tau}{a_i^2\omega_0^2 \tau (a_i^2 - a_0^2)},
\]

It is noted that \( R \) given by Eqs. (72), (77), and (79)–(83) is independent of \( N \) because the \( \sqrt{N} \) factor in the first term of Eq. (72) is canceled out by \( 1/\sqrt{N} \) of \( D_q \) in Eq. (82), and because \( N \) factors in the third and fourth terms in Eq. (72) are canceled out by \( 1/N \) factors of \( D_q \) in Eqs. (82) and (83). This is the consequence of our choice of \( c_0 \) in Eq. (14): A different choice of the \( N \) dependence of \( c_0 \) leads to \( N \)-dependent \( R \). Furthermore, \( R \) is independent of \( \beta \) because the \( \beta \) factor in the second term of Eq. (77) is canceled out by \( 1/\beta \) in Eq. (72).

Figure 3(a) shows the \( \tau \) dependence of \( \mu \) (=\langle W \rangle) for \( c_0 = 0.0 \) (solid curves), 0.5 (dashed curves), and 1.0 (chain curves). For \( \tau \lessapprox T_o \) (\( \simeq 6 \)), we obtain \( \langle W \rangle > \Delta F \) (=\( -0.5 \)), signaling the occurrence of the irreversibility. At the same time, \( \sigma \) (=\( \sqrt{(\langle W \rangle - \langle W \rangle)^2} \)) is rapidly increased for \( \tau \lessapprox T_o \), where fluctuation in \( W \) grows significantly, as shown in Fig. 3(b). For \( \tau = 2m\pi/\Omega \) (\( m = 1, 2, \ldots \)) with \( c_0 = 0.0 \), \( \sigma \) vanishes [Eq. (93)]. Figure 3(c) will be explained shortly.
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FIG. 3. (Color online) The \( \tau \) dependence of (a) \( \mu = \langle W \rangle \), (b) \( \sigma = \sqrt{\langle (W - \langle W \rangle)^2 \rangle} \), and (c) \( R = -\beta^{-1} \ln \langle e^{-\beta W} \rangle \) for \( c_o = 0 \) (solid curves), 0.5 (dashed curves), and 1.0 (chain curves); arrows along the right-hand side ordinates in (a) and (c) express \( \Delta F = -0.5 \). In (c) \( R = \Delta F \) for \( c_o = 0, 0.5, \) and 1.0.

Figure 4 shows three-dimensional plots of WDF of \( P(W) \) as functions of \( W \) and \( \tau \) for \( c_o = 0 \). The result for \( c_o = 1 \) is not very different from that of \( c_o = 0 \) at first glance. With decreasing \( \tau \), the center of \( P(W) \) moves to zero and its width is considerably increased as Figs. 3(a) and 3(b) show.

D. Jarzynski equality

In this section, we consider the JE given by Eq. (1). From Eqs. (1) and (75)–(77), the JE is satisfied if the relation given by

\[
R = \phi - \frac{\beta \sigma^2}{2} = \Delta F, \tag{84}
\]

holds. Here \( \Delta F \) denotes the free-energy difference between the two equilibrium systems with and without a force \( g \) defined by [9]

\[
\Delta F = F(g) - F(0) = -\frac{1}{\beta} \ln \frac{Z_S(g)}{Z_S(0)}, \tag{85}
\]

with

\[
Z_S(g) = \frac{\text{Tr}[e^{-\beta(H_S(g)+H_B+H_I)}]}{\text{Tr}[e^{-\beta H_B}]}, \tag{86}
\]

where

\[
H_S(g) = \frac{P^2}{2M} + \frac{M\Omega^2}{2} \left( Q - \frac{g}{M\Omega} \right)^2 - \frac{g^2}{2M\Omega^2}, \tag{87}
\]

yielding

\[
\Delta F = -\frac{g^2}{2M\Omega^2}, \tag{91}
\]

which is independent of the coupling \( c_o \).

In what follows, we examine \( \mu, \sigma^2, \) and \( R \) in the three limits of (1) no couplings \( (c_o = 0) \), (2) transient force \( (\tau \to 0) \), and (3) quasistatic force \( (\tau \to \infty) \).
(1) In the limit of $c_o = 0$, we obtain from Eqs. (72) and (79)–(83)

$$
\mu = -\frac{g^2}{2M \Omega^2} + \frac{g^2(1 - \cos \Omega \tau)}{M^2 \Omega^2 \tau^2},
$$

$$
\sigma^2 = \frac{2g^2(1 - \cos \Omega \tau)}{\beta M \Omega^2 \tau^2},
$$

leading to

$$
R = -\frac{g^2}{2M \Omega^2} = \Delta F, \quad (94)
$$

where $\Delta F$ is given by Eq. (91).

(2) In the limit of $\tau \to 0$, Eqs. (72) and (79)–(83) lead to

$$
\mu = 0, \quad (95)
$$

$$
\sigma^2 = \frac{g^2}{\beta M \Omega^2}, \quad (96)
$$

where we employ the relations $C_G = -g$ and $C_P = D_G = D_P = 0$. A substitution of Eqs. (95) and (96) into Eq. (77) leads to

$$
R = -\frac{g^2}{2M \Omega^2} = \Delta F. \quad (97)
$$

(3) In limit of $\tau \to \infty$, we obtain

$$
\mu = -\frac{g^2}{2} \sum_{i=1}^{N} \frac{b_i}{2Ma_i^2} = -\frac{g^2}{2M \Omega^2}, \quad (98)
$$

$$
\sigma^2 = 0, \quad (99)
$$

employing the relations $\sum_{i=1}^{N} (b_i/a_i^2) = 1/\Omega^2$ and $C_G = C_P = D_G = D_P = 0$. Equations (77) and (99) lead to

$$
R = -\frac{g^2}{2M \Omega^2} = \Delta F. \quad (100)
$$

Equations (94), (97), and (100) imply that the JE holds in the three limits of (1) $c_o = 0$, (2) $\tau \to 0$, and (3) $\tau \to \infty$.

Figure 3(c) shows that the JE is numerically verified for $10^{1} \leq \tau \leq 10^{2}$ with $c_o = 0.0, 0.5, \text{ and } 1.0$. The JE is valid even when we adopt other sets of model parameters. It is surprising that complicated expressions of $\mu (=\phi)$ and $\sigma^2$ given by Eqs. (79) and (72), respectively, satisfy the JE given by Eq. (84). Although the validity of the JE is confirmed by numerical calculations, we have not succeeded in its analytical proof except for the three cases of $c_o = 0, \tau \to 0$, and $\tau \to \infty$.

III. DISCUSSION

A. Canonical average over initial equilibrium state

It should be noted that the canonical average in Eq. (35) must be performed over the total Hamiltonian $H = H_S + H_B + H_I$ in the initial equilibrium state [61]. If the average in Eq. (35) is performed over the Hamiltonian of the uncoupled state $(H_S + H_B)$ in place of $H$, we obtain a wrong result. Figures 5(a) and 5(b) show $\bar{E}_t(t) = \langle E_t(t) \rangle_{00}$ with no forces ($f = 0$) and a ramp force of $\tau = 100$, respectively, with $c_o = 1$ when the average is performed over the initial uncoupled state of $(H_S + H_B)$,

$$
\langle O \rangle_{00} = \frac{\text{Tr}[e^{-\beta[H_S(0)+H_B(0)]}O]}{\text{Tr}[e^{-\beta[H_S(0)+H_B(0)]}]}, \quad (101)
$$

with $\langle O \rangle_{00}$ being the average over the initial uncoupled state of $(H_S + H_B)$.

![Figure 5](image-url)

**FIG. 5.** (Color online) The time dependence of $\bar{E}_t(t)$ with (a) no forces ($f = 0$) and (b) a ramp force of $\tau = 100.0$ with $c_o = 1.0$ when the average is performed over initial uncoupled state of $H_S + H_B$: (a) and (b) should be compared to Figs. 2(b) and 2(d), respectively, which are averaged over the initial coupled state of $H_S + H_B + H_I$ (see text).

where $O$ stands for an operator. Results in Figs. 5(a) and 5(b) are quite different from the corresponding ones averaged over $H$ which have been shown in Figs. 2(b) and 2(d). In particular, the irregular energy exchange between the system and bath occurs even when $f(t) = 0.0$ in Fig. 5(a), while the initial serene state persists in Figs. 2(b). Figure 5(a) denotes the result of the case where the system-bath coupling is suddenly added at $t = 0.0$ to the uncoupled system in an equilibrium state at $t < 0.0$. The perturbation of the added coupling induces an irregular energy exchange between the system and bath which does not dissipate for $\tau \geq 0.0$.

If the canonical average in Eq. (78) is performed over $H_S + H_B$, we obtain

$$
\langle e^{-\beta Q(t)} \rangle_{00} = e^{-\beta(\phi - \sigma^2/2)}, \quad (102)
$$

with

$$
\sigma^2 = \frac{1}{\beta} \left[ \frac{C_G^2}{M \Omega^2} + MC_P^2 + \frac{ND_P^2}{m\sigma_o^2} + mN \sigma_f^2 \right], \quad (103)
$$

where $\phi$ is given by Eq. (65). Because $\sigma^2$ is different from $\sigma^2$ in Eq. (72), it wrongly leads to a violation of the JE: $R = \phi - \beta \sigma^2/2 \neq \phi - \beta \sigma^2/2 = \Delta F$. A related discussion will be given also in Sec. III D.

B. A two-step ramp force

Besides the ramp force given by Eq. (47), we have employed a two-step ramp force given by

$$
f(t) = \begin{cases} 
0, & \text{for } t < 0, \\
g \left(\frac{b}{\kappa}\right), & \text{for } 0 \leq t < \tau_m, \\
g \left[1 - \kappa(\tau - \tau_m)/\kappa(\tau_m - \tau)\right], & \text{for } \tau_m \leq t < \tau, \\
g, & \text{for } t \geq \tau,
\end{cases}
$$

(104)

where $h$ stands for a magnitude at a middle time of $\tau_m$ ($< \tau$). Figures 6(a) and 6(b) show $\mu$ and $\sigma$, respectively, as a function of $\tau$ when a two-step ramp input $f(t)$ given by Eq. (104) with $g = 1.0, h = 1.5$, and $\tau_m = \tau/2$ is applied $f(t)$ is shown in the inset of Fig. 6(b). The input force $f(t)$ first linearly increases to $1.5g$ at $t = \tau_m$ and then it linearly decreases to the final value of $g$ at $t \geq \tau$. The $\tau$ dependences of $\mu$ and $\sigma$ shown in Fig. 6 are rather different from those for a single-step ramp input shown in Fig. 3. In particular, magnitudes of $\mu$ and $\sigma$ have resonancelike peaks at $\tau \sim \tau_m$. Nevertheless the JE holds also for the two-step ramp force.
by integral over a continuous spectrum and it may be expressed performed in the same way as was made in Sec. II. Then the expression for the corresponding eigenfunction \[62\].

FIG. 6. (Color online) The \(\tau\) dependence of (a) \(\mu (W)\) and (b) \(\sigma (\sqrt{\langle W - W \rangle^2})\) for a two-step ramp force \(f(t)\) given by Eq. (104) with \(g = 1.0, h = 1.5,\) and \(\tau_n = \tau/2\) [see the inset of (b)] with \(c_o = 0.0\) (solid curves), 0.5 (dashed curves), and 1.0 (chain curves); an arrow along the right-hand side ordinate in (a) expresses \(\Delta F = \langle\rangle\).

Our study in the preceding section has been made for the bath. The Green’s function given by Eq. (12) may be generally expressed by

\[
\hat{G}(s) = \sum_{i=1}^{N+1} \frac{b_i}{s^2 + \omega_i^2},
\]

where \(\omega_i\) denotes the normal-mode frequency of the coupled system plus bath and \(b_i\) is expressed in terms of the corresponding eigenfunction \[62\].

The Green’s function given by Eqs. (105) or (106) has the same structure as that for the single-\(\omega\) bath given by Eq. (18). Calculations of \(Q(t), W_0,\) and \(P(W)\) may be formally performed in the same way as was made in Sec. II. Then the properties of the CL model with a finite-\(N\) multiple-\(\omega\) bath are essentially the same as those with a single-\(\omega\) bath.

On the other hand, in the limit of \(N \to \infty\), the summation over \(n\) in the Green’s function of Eq. (12) is converted to an integral over a continuous spectrum and it may be expressed by

\[
\hat{G}(s) = \left[s^2 + \Omega^2 + \frac{s^2 c_o^2}{M m} \int \frac{D(\omega)}{w^2(s^2 + \omega^2)} d\omega\right]^{-1},
\]

where \(D(\omega)\) denotes the density of state

\[
D(\omega) = \frac{1}{N} \sum_{n=1}^{N} \delta(\omega - \omega_n).
\]

When we assume the Debye-type density of states \(D(\omega) = a\omega^2\) \((a\) is a constant), \(\hat{G}(s)\) is given by

\[
\hat{G}(s) = \frac{1}{(s + c_1)(s + c_2)},
\]

with

\[
c_{1,2} = \pm i \sqrt{\frac{\Omega^2 - \pi a c_o^2}{4Mm}} + \left(\frac{\pi a c_o^2}{4Mm}\right).
\]

Because of the real parts in \(c_1\) and \(c_2\), the inverse Laplace transformation of \(\hat{G}(s)\) in Eq. (109) yields dissipative \(G(t)\), which vanishes at \(t \to \infty\). For dissipation it is necessary that the frequencies \(\{\omega_n\}\) have a continuous spectrum in the limit of \(N \to \infty\) \[62\]. With a discrete spectrum for finite \(N\), however, the Green’s function \(G(t)\) in Eq. (12) is nondissipative and not vanishing in the limit of \(t \to \infty\).

**D. The Generalized Langevin Approach**

In the conventional approach to the CL model, we derive the Langevin equation given by

\[
M \ddot{\hat{Q}} = -M\Omega^2 \hat{Q} - \int_0^t \gamma(t' - t) \hat{\dot{Q}}(t') dt' + \xi(t) + f(t),
\]

with \(\xi(t) = \xi(t) - \gamma(t) Q(0),\)

\[
\gamma(t) = \sum_{n=1}^{N} \left(\frac{c_n^2}{mo_n^2}\right) \cos \omega_n t,
\]

\[
\xi(t) = \sum_{n=1}^{N} c_n \left[q_n(0) \cos \omega_n t + \left(\frac{p_n(0)}{m\omega_n}\right) \sin \omega_n t\right].
\]

After obtaining a formal solution of \(q_n(0)\) from Eq. (7) and substituting it into Eq. (6) \[50,51\]. Equations (111)–(114) express the non-Markovian Langevin equation with colored noise.

When we adopt the single-\(\omega\) bath given by Eq. (13), \(\gamma(t)\) and \(\xi(t)\) are given by

\[
\gamma(t) = \left(\frac{c_o^2}{m\omega_o^2}\right) \cos \omega_o t,
\]

\[
\xi(t) = \frac{c_o}{\sqrt{N}} \left[\cos \omega_o t \sum_{n=1}^{N} q_n + \sin \omega_o t \sum_{n=1}^{N} p_n\right].
\]

By using the Laplace transformation yielding

\[
\hat{\gamma}(s) = \frac{c_o^2 s}{m\omega_o^2(s^2 + \omega_o^2)},
\]

\[
\hat{\xi}(s) = \frac{c_o}{\sqrt{N}} \left[\frac{s}{s^2 + \omega_o^2} \sum_{n=1}^{N} q_n + \frac{1}{m(s^2 + \omega_o^2)} \sum_{n=1}^{N} p_n\right].
\]
we obtain an equation for $\dot{Q}(t)$ which is exactly the same as Eqs. (15) and (16).

It has been shown that the JE is satisfied in the non-Markovian Langevin model with colored noise (generalized Langevin model) [37–40], which is different from our Langevin equation given by Eqs. (111), (115), and (116) in two ways: (a) The second term of Eq. (112) includes an additional term of $-\gamma(t)Q(0)$ which is missing in the conventional generalized Langevin model, and (b) the memory kernel given by Eq. (115) is oscillating and nondissipative while that in the generalized Langevin model is dissipative. In the literature (e.g., Ref. [63]), the additional term of the generalized Langevin model is dissipative. In the literature (e.g., Ref. [63]), the additional term of

$$f = f_1.$$  

It is noted that the general validity condition reported in Ref. [29] is satisfied for our system even though it is a nondissipative one.

**IV. CONCLUSION**

We have studied the response to an applied force of a small open oscillator system described by the exactly solvable CL model with a nondissipative single-$\omega$ bath. Although the model adopted in our study seems to be a pedagogical toy model, it is expected not to be unrealistic because nondissipative properties are realized in small systems coupled to finite baths [47,48]. We have obtained exact expressions for position, momentum, and energy of the system whose canonical averages have been analytically performed over initial equilibrium states. Our calculations of system energy and work have shown the following: (i) The energy of the system strongly coupled to a finite bath is fluctuating but nondissipative in general, and (ii) the JE is valid in nondissipative nonergodic systems.

Item (i) supports direct simulations for open systems coupled to finite baths [47,48], although it is contrast to the result showing the dissipation for $N \gtrsim 10–20$ [58]. Item (ii) is consistent with Jarzynski’s proof for arbitrary classical open systems [9]. Our study is complementary to previous studies for dissipative oscillator systems with the use of the Markovian [20–23] and non-Markovian Langevin models [37–40], the Fokker-Planck equation [41], and Hamiltonian models [42–46].

Although items (i) and (ii) hold for open systems described by the CL [50,51] and Ford-Kac models [63], it is not certain whether they are valid for any nondissipative nonergodic open system. In this respect, it would be interesting to examine work in the $(N_S + N_B)$ model for a classical $N_S$-body system coupled to an $N_B$-body bath [48]. The $(N_S + N_B)$ model clarifies some interesting issues, such as the $N_S$-dependent non-Gaussian energy distribution of the system [48], which, to the best of our knowledge, has been not realized in previous studies for CL-type models with $N_S = 1$ [50,51,63]. Such a calculation is in progress and will be reported in a separate paper.

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Two methods have been proposed for calculating the system energy in the system plus bath [55]:

\[ E_S^{(2)}(t) = \text{Tr} \left( e^{-\beta H} \omega \right) \text{Tr} e^{-\beta H} \]

and

\[ E_S^{(3)} = \beta H \text{Tr} e^{-\beta H} \]

with the reduced partition function

\[ Z_S = \text{Tr} e^{-\beta H} \]

and where the kernel \( \gamma(t) \) includes the \( c_n^2 \) term, \( \gamma(t) = \sum_n c_n^2 \text{Tr} \left( e^{-\beta H} \cos \omega_{n} t / m \omega_n \right) \). 

In the limit of \( N \to \infty \), \( D(\omega) \) standing for the density of states.

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where \( \text{Tr} \omega \) stands for the partial trace over the bath. We obtain \( E_S^{(2)} = E_S^{(3)} \) for the classical CL model [55–57].

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