Classical double-well systems coupled to finite baths

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Abstract

We have studied properties of a classical $N_S$-body double-well system coupled to an $N_B$-body bath, performing simulations of $2(N_S + N_B)$ first-order differential equations with $N_S \simeq 1 - 10$ and $N_B \simeq 1 - 1000$. A motion of Brownian particles in the absence of external forces becomes chaotic for appropriate model parameters such as $N_B$, $c_o$ (coupling strength), and $\{\omega_n\}$ (oscillator frequency of bath): For example, it is chaotic for a small $N_B$ ($\lesssim 100$) but regular for a large $N_B$ ($\gtrsim 500$). Detailed calculations of the stationary energy distribution of the system $f_S(u)$ ($u$: an energy per particle in the system) have shown that its properties are mainly determined by $N_S$, $c_o$ and $T$ (temperature) but weakly depend on $N_B$ and $\{\omega_n\}$. The calculated $f_S(u)$ is analyzed with the use of the $\Gamma$ distribution. Difference and similarity between properties of double-well and harmonic-oscillator systems coupled to finite bath are discussed.

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I. INTRODUCTION

Many studies have been made with the use of a model describing a classical or quantum open system which is coupled to baths consisting of a collection of harmonic oscillators. Such a model is conventionally referred to as the Caldeira-Leggett (CL) model \[1, 2\], although equivalent models had been proposed earlier by Magalinskii \[3\] and Ullersma \[4\]. From the CL model, we may derive the Langevin model with dissipation and diffusion (noise) terms. Originally the CL model was introduced for \(N_B\)-body bath with \(N_B \to \infty\), for which the Ohmic and Drude-type spectral densities with continuous distributions are adopted. Furthermore in the original CL model, the number of particles in a systems, \(N_S\), is taken to be unity (\(N_S = 1\)). We expect that a generic open system may contain any number of particles and that a system may be coupled to a bath consisting of finite harmonic oscillators in general. In recent years, the CL model has been employed for a study of properties of open systems with finite \(N_S\) and/or \(N_B\) \[5–13\]. Specific heat anomalies of quantum oscillator (system) coupled to finite bath have been studied \[5, 6, 12\]. A thermalization \[7, 8\], energy exchange \[9\], dissipation \[11\] and the Jarzynski equality \[13, 14\] in classical systems coupled to finite bath have been investigated.

In a previous paper \[10\], we have studied the \((N_S + N_B)\) model for finite \(N_S\)-body systems coupled to baths consisting of \(N_B\) harmonic oscillators. Our study for open harmonic oscillator systems with \(N_S \simeq 1 – 10\) and \(N_B \simeq 10 – 1000\) has shown that stationary energy distribution of the system has a significant and peculiar dependence on \(N_S\), but it weakly depends on \(N_B\) \[10\]. These studies mentioned above \[5–13\] have been made for harmonic-oscillator systems with finite \(N_S\) and/or \(N_B\).

Double-well potential models have been employed in a wide range of fields including physics, chemistry and biology (for a recent review on double-well system, see Ref. \[15\]). Various phenomena such as the stochastic resonance (SR), tunneling through potential barrier and thermodynamical properties \[16\] have been studied. The CL model for the double-well systems with \(N_S = 1\) and \(N_B = \infty\) has been extensively employed for a study on the SR \[17\]. Properties of SR for variations of magnitude of white noise \[17, 20\] and relaxation time of colored noise \[21, 22\] have been studied. However, studies for open double-well systems with finite \(N_S\) and/or \(N_B\) have not been reported as far as we are aware of. It would be interesting and worthwhile to study open classical double-well systems described by the
(\(N_S + N_B\)) model with finite \(N_S\) and \(N_B\), which is the purpose of the present paper.

The paper is organized as follows. In Sec. II, we briefly explain the \((N_S + N_B)\) model proposed in our previous study \[10\]. In Sec. III, direct simulations (DSs) of \(2(N_S + N_B)\) first-order differential equations for the adopted model have been performed. Dynamics of a single double-well system \((N_S = 1)\) coupled to a finite bath \((2 \leq N_B \leq 1000)\) in the phase space is investigated (Sec. III B). We study stationary energy distributions in the system and bath, performing detailed DS calculations, changing \(N_S, N_B\), the coupling strength and the distribution of bath oscillators (Sec. III C). Stationary energy and position distributions obtained by DSs are analyzed in Sec. IV. The final Sec. V is devoted to our conclusion.

II. ADOPTED \((N_S + N_B)\) MODEL

We consider a system including \(N_S\) Brownian particles coupled to a bath consisting of independent \(N_B\) harmonic oscillators. We assume that the total Hamiltonian is given by \[10\]

\[
H = H_S + H_B + H_I, \tag{1}
\]

with

\[
H_S = \sum_{k=1}^{N_S} \left[ \frac{P_k^2}{2M} + V(Q_k) \right], \tag{2}
\]

\[
H_B = \sum_{n=1}^{N_B} \left[ \frac{p_n^2}{2m} + \frac{m\omega_n^2}{2}q_n^2 \right], \tag{3}
\]

\[
H_I = \frac{1}{2} \sum_{k=1}^{N_S} \sum_{n=1}^{N_B} c_{kn} (Q_k - q_n)^2, \tag{4}
\]

where \(H_S\), \(H_B\) and \(H_I\) express Hamiltonians for the system, bath and interaction, respectively. Here \(M\) (\(m\)) denotes the mass, \(P_k\) (\(p_n\)) the momentum, \(Q_k\) (\(q_n\)) position of the oscillator in the system (bath), \(V(Q_k)\) signifies the potential in the system, \(\omega_n\) stands for oscillator frequency in the bath, and \(c_{nk}\) is coupling constant. The model is symmetric with respect to an exchange of system ↔ bath if \(V(Q)\) is the harmonic potential. From Eqs.
we obtain \( 2(N_S + N_B) \) first-order differential equations,

\[
\dot{Q}_k = \frac{P_k}{M},
\]

(5)

\[
\dot{P}_k = -V'(Q_k) - \sum_{n=1}^{N_B} c_{kn}(Q_k - q_n),
\]

(6)

\[
\dot{q}_n = \frac{p_n}{m},
\]

(7)

\[
\dot{p}_n = -m\omega_n^2 q_n - \sum_{k=1}^{N_S} c_{kn}(q_n - Q_k),
\]

(8)

which yield

\[
M\ddot{Q}_k = -V'(Q_k) - \sum_{n=1}^{N_B} c_{kn}(Q_k - q_n),
\]

(9)

\[
m\ddot{q}_n = -m\omega_n^2 q_n - \sum_{k=1}^{N_S} c_{kn}(q_n - Q_k),
\]

(10)

with prime (\('\)) and dot (\(\cdot\)) denoting derivatives with respect to the argument and time, respectively. It is noted that the second term of Eq. (6) or (9) given by

\[
F_k^{(e f f)} = -\sum_{n=1}^{N_B} c_{kn}(Q_k - q_n),
\]

(11)

plays a role of the effective force to the \( k \)th system.

A formal solution of Eq. (10) for \( q_n(t) \) is given by

\[
q_n(t) = q_n(0) \cos \tilde{\omega}_n t + \frac{\dot{q}_n(0)}{\tilde{\omega}_n} \sin \tilde{\omega}_n t + \sum_{\ell=1}^{N_S} \frac{c_{\ell n}}{m\tilde{\omega}_n} \int_0^t \sin \tilde{\omega}_n (t - t') Q_\ell(t') dt',
\]

(12)

with

\[
\tilde{\omega}_n^2 = \frac{b_n}{m} + \sum_{k=1}^{N_S} \frac{c_{kn}}{m} = \omega_n^2 + \sum_{k=1}^{N_S} \frac{c_{kn}}{m}.
\]

(13)

Substituting Eq. (12) to Eq. (9), we obtain the non-Markovian Langevin equation given by

\[
M\ddot{Q}_k(t) = -V'(Q_k) - M\sum_{\ell=1}^{N_S} \xi_{k\ell} Q_\ell(t) - \sum_{\ell=1}^{N_S} \int_0^t \gamma_{k\ell}(t - t') \dot{Q}_\ell(t') dt' - \sum_{\ell=1}^{N_S} \gamma_{k\ell}(t) Q_\ell(0) + \zeta_k(t) \quad (k = 1 \text{ to } N_S),
\]

(14)
with

\[ M \xi_{k\ell} = \sum_{n=1}^{N_B} \left[ c_{kn} \delta_{k\ell} - \frac{c_{kn} c_{\ell n}}{m \tilde{\omega}_n^2} \right], \quad (15) \]

\[ \gamma_{k\ell}(t) = \sum_{n=1}^{N_B} \left( \frac{c_{kn} c_{\ell n}}{m \tilde{\omega}_n^2} \right) \cos \tilde{\omega}_n t, \quad (16) \]

\[ \zeta_k(t) = \sum_{n=1}^{N_B} c_{kn} \left[ q_n(0) \cos \tilde{\omega}_n t + \frac{\dot{q}_n(0)}{\omega_n} \sin \tilde{\omega}_n t \right], \quad (17) \]

where \( \xi_{k\ell} \) denotes the additional interaction between \( k \) and \( \ell \)th particles in the system induced by couplings \( \{ c_{kn} \} \), \( \gamma_{k\ell}(t) \) the memory kernel and \( \zeta_k \) the stochastic force.

If the equipartition relation is realized in initial values of \( q_n(0) \) and \( \dot{q}(0) \),

\[ \langle m \tilde{\omega}_n^2 q_n(0)^2 \rangle_B = \langle m \dot{q}_n(0)^2 \rangle_B = k_B T, \quad (18) \]

we obtain the fluctuation-dissipation relation:

\[ \langle \zeta_k(t) \zeta_k(t') \rangle_B = k_B T \gamma_{kk}(t - t'), \quad (19) \]

where \( \langle \cdot \rangle_B \) stands for the average over variables in the bath.

In the case of \( N_B \to \infty \), summations in Eqs. (15)-(17) are replaced by integrals. When the spectral density defined by

\[ J(\omega) = \frac{\pi}{2} \sum_n \frac{c_n^2}{m_n \omega_n^2} \delta(\omega - \omega_n), \quad (20) \]

is given by the Ohmic form: \( J(\omega) \propto \omega \) for \( 0 \leq \omega < w_D \), the kernel becomes

\[ \gamma(t) \propto \frac{\sin \omega_D t}{\pi t} \propto \delta(t), \quad (21) \]

which leads to the Markovian Langevin equation.

In the case of \( N_S = 1 \), we obtain \( \xi \) and \( \gamma \) in Eqs. (15) and (16) where the subscripts \( k \) and \( \ell \) are dropped (e.g., \( c_{kn} = c_n \)),

\[ M \xi(t) = \sum_{n=1}^{N_B} c_n \left( 1 - \frac{c_n}{m \tilde{\omega}_n^2} \right), \quad (22) \]

\[ \gamma(t) = \sum_{n=1}^{N_B} \left( \frac{c_n^2}{m \tilde{\omega}_n^2} \right) \cos \tilde{\omega}_n t. \quad (23) \]

The additional interaction vanishes (\( \xi = 0 \)) if we choose \( c_n = m \tilde{\omega}_n^2 \) in Eq. (22).

In the case of \( N_S \neq 1 \), however, it is impossible to choose \( \{ c_{kn} \} \) such that \( \xi_{k\ell} = 0 \) is realized for all pairs of \( (k, \ell) \) in Eq. (15). Then \( Q_k \) is inevitably coupled to \( Q_\ell \) for \( \ell \neq k \) with the superexchange-type interaction of antiferromagnets: \( -\sum_n c_{kn} c_{\ell n} / m \tilde{\omega}_n^2 \) in Eq. (15).
III. MODEL CALCULATIONS FOR DOUBLE-WELL SYSTEMS

A. Calculation methods

We consider a system with the double-well potential

$$V(Q) = \left( \frac{\Delta}{Q_0^4} \right) (Q^2 - Q_0^2)^2, \quad (24)$$

which has the stable minima of $V(\pm Q_0) = 0$ at $Q = \pm Q_0$ and locally unstable maximum of $V(0) = \Delta$ at $Q = 0$ with the barrier height $\Delta$. We have adopted $Q_0 = 1.0$ and $\Delta = 1.0$ in our DSs.

It is easier to solve $2(N_S + N_B)$ first-order differential equations given by Eqs. (5)-(8) than to solve the $N_S$ Langevin equations given by Eqs. (14)-(17) although the latter provides us with clearer physical insight than the former. In order to study the $N_S$ and $N_B$ dependences of various physical quantities, we have assumed that the coupling $c_{kn}$ is given by

$$c_{kn} = \frac{c_o N_S N_B}{N_S N_B}, \quad (25)$$

because the interaction term includes summations of $\sum_{k=1}^{N_S}$ and $\sum_{n=1}^{N_B}$ in Eq. (4). It is noted that with our choice of $c_{kn}$, the interaction contribution is finite even in the thermodynamical limit of $N_B \to \infty$ because the summation over $n$ runs from 1 to $N_B$ in Eq. (4). DSs of Eqs. (5)-(8) have been performed with the use of the fourth-order Runge-Kutta method with the time step of 0.01. We have adopted $k_B = 1.0$, $M = m = 1.0$, $c_o = 1.0$, and $\omega_n = 1.0$ otherwise noticed.

We consider energies per particle $u_{\eta}(t)$ in the system ($\eta$=S) and the bath ($\eta$=B) which are assume to be given by

$$u_S = \frac{1}{N_S} \sum_{k=1}^{N_S} \left[ \frac{P_k^2}{2M} + V(Q_k) \right], \quad (26)$$

$$u_B = \frac{1}{N_B} \sum_{n=1}^{N_B} \left[ \frac{p_n^2}{2m} + \frac{m \omega_n^2 q_n^2}{2} \right], \quad (27)$$

which is valid for the weak interaction, although a treatment of the finite interaction is ambiguous and controversial \cite{5, 6}.
B. Dynamics of a particle in the \((Q, P)\) phase space

1. Effect of \(c_o\)

First we consider an isolated double-well system \((N_S = 1\) and \(c_o = 0.0\)). Figure 1 shows the phase-space trajectories in the \((Q, P)\) phase space for this system with six different initial system energies \(E_{S_0}\). For \(E_{S_0} = 0.0\), the system has two stable fixed points at \((Q, P) = (\pm1.0, 0.0)\), and for \(E_{S_0} = \Delta = 1.0\) it has one unstable fixed point at \((Q, P) = (0.0, 0.0)\). In the case of \(0.0 < E_{S_0} < 1.0\), the trajectory is restricted in the region of \(Q > 0.0\) (or \(Q < 0.0\)). In contrast in the case of \(E_{S_0} > 1.0\), trajectory may visit both regions of \(Q > 0.0\) and \(Q < 0.0\). The case of \(E_{S_0} = 1.0\) is critical between the two cases.

Next the double-well system is coupled to a bath. In our DSs, we have assumed that system and bath are decoupled at \(t < 0\) where they are in equilibrium states with \(E_{S_0} = T\), the temperature \(T\) being defined by \(T = u_B\). We have chosen initial values of \(Q(0) = 1.0\) and \(P(0) = \sqrt{2M[E_{S_0} - V(Q(0))]\)} for a given initial system energy \(E_{S_0}\). Initial conditions for \(q_n(0)\) and \(p_n(0)\) are given by random Gaussian variables with zero means and variance proportional to \(T\) [Eq. (18)] [10]. Results to be reported in this subsection have been obtained by single runs for \(t = 0\) to 1000.

Figures 2(a) and 2(b) show a strobe plot in the \((Q, P)\) phase space (with a time interval of 1.0) and the time-dependence of \(Q(t)\), respectively, for \(E_{S_0} = 1.0\), \(N_S = 1\), \(N_B = 100\) and \(c_o = 0.2\). The trajectory starting from \(Q(0) = 1.0\) goes to the negative-\(Q\) region because a particle may go over the potential barrier with a help of a force (noise) originating from bath given by Eq. (11). The system energy fluctuates as shown in Fig. 2(c), whose distribution is plotted in Fig. 2(d).

Results in Fig. 2 are regular. In contrast, when a coupling strength is increased to \(c_o = 1.0\), the system becomes chaotic as shown in Figs. 3(a) and 3(b) where a strobe plot in the \((Q, P)\) phase space and the time-dependence of \(Q(t)\) are plotted, respectively. This is essentially the force-induced chaos in classical double-well system [23]: although an external force is not applied to our system, a force arising from a coupling with bath given by Eq. (11) plays a role of an effective external force for the system. Figures 3(c) and 3(d) show that in the case of \(c_o = 1.0\), \(u_S\) has more appreciable temporal fluctuations with a wider energy distribution in \(f_S(u)\) than in the case of \(c_o = 0.2\). Although system energies fluctuate, they
FIG. 1: Plot of phase-space trajectories for a particle in an isolated double-well system ($c_o = 0.0$). Trajectories are plotted for energies of $E_{So}/\Delta = 0.0, 0.5, 0.8, 1.0, 1.2$ and 1.5. are not dissipative at $0.0 \leq t < 1000.0$ in DSs both for $c_o = 0.2$ and $c_o = 1.0$ with $N_B = 100$.

2. Effect of $\omega_n$ distributions

We have so far assumed $\omega_n = 1.0$ in the bath, which is now changed. Figures 4(a) and 4(c) show strobe plots for $\omega_n = 0.5$ and 2.0, respectively, which are regular and which are different from a chaotic result for $\omega_n = 1.0$ shown in Fig. 4(b). When we adopt \{\omega_n\} which is randomly distributed in $[0.5, 2.0]$, a motion of a system particle becomes chaotic as shown
FIG. 2: (Color online) (a) Strobe plot in the \((Q, P)\) phase space (with a time interval of 1.0), (b) \(Q(t)\), (c) \(u_S(t)\), and (d) the system energy distribution \(f_S(u)\) obtained by a single run for \(E_{So} = 1.0, N_S = 1, N_B = 100, T = 1.0\) and \(c_o = 0.2\).

in Fig. 3(d). This is because contributions from \(\omega_n \sim 1.0\) among \([0.5, 2.0]\) induce chaotic behavior.
FIG. 3: (Color online) (a) Strobe plot in the \((Q, P)\) phase space, (b) \(Q(t)\), (c) \(u_S(t)\), and (d) the system energy distribution \(f_S(u)\) obtained by a single run for \(E_{So} = 1.0\), \(N_S = 1\), \(N_B = 100\), \(T = 1.0\) and \(c_o = 1.0\).

3. Effect of \(N_B\)

We have repeated calculations by changing \(N_B\), whose results are plotted in Figs. 5(a)-5(d). Figures 5(a), 5(b) and 5(c) show that chaotic behaviors for \(N_B = 2\) and \(N_B = 10\) are
more significant than that for $N_B = 100$. On the contrary, chaotic behavior is not realized for $N_B = 1000$ in Fig. 5(d), which is consistent with the fact that chaos has not been reported for the double-well system subjected to infinite bath.
FIG. 5: Strobe plots in the \((Q,P)\) phase space for various \(N_B\): (a) \(N_B = 2\), (b) \(N_B = 10\), (c) \(N_B = 100\) and (d) \(N_B = 1000\) with \(E_{So} = 1.0\), \(N_S = 1\), \(T = 1.0\) and \(c_o = 1.0\).

4. **Effect of initial system energy \(E_{So}\)**

Next we change the initial system energy of \(E_{So}\). Figures 6(a)-(d) show strobe plots in the \((Q,P)\) phase space for various \(E_{So}\) with \(N_S = 1\), \(N_B = 100\), \(T = 1.0\) and \(c_o = 1.0\). Figure 6(a) shows that for \(E_{So} = 0.5\), the regular trajectory starting from \(Q = 1.0\) remains
in the positive-$Q$ region because a particle cannot go over the potential barrier of $\Delta = 1.0$. For $E_{So} = 0.8$, chaotic trajectories may go to the negative-$Q$ region with a help of force from bath [Eq. [11]]. Figure [6(d)] shows that when $E_{So}$ is too large compared to $\Delta$ ($E_{So}/\Delta = 1.2$), the trajectory again becomes regular, going between positive- and negative-$Q$ regions.

Figure [7] shows the system energy distribution $f_S(u)$ for various $E_{So}$. $f_S(u)$ moves upward as $E_{So}$ is increased. It is noted that peak positions of $f_S(u)$ for $E_{So} = 0.5 - 1.0$ locate at $u \simeq 1.0$ while that for $E_{So} = 1.2$ locates at $u \simeq 1.35$.

C. Stationary energy probability distributions

In this subsection, we will study stationary energy probability distributions of system and bath which are averaged over $N_r (\approx 10,000)$ runs stating from different initial conditions. Assuming that the system and bath are in the equilibrium states with $T = u_B = u_S$ at $t < 0.0$, we first generate exponential derivatives of initial system energies $\{E_j\}$: $p(E_j) \propto \exp(-\beta E_j) \ (j = 1 \text{ to } N_SN_r)$ for our DSs where $\beta = 1/k_B T$. A pair of initial values of $Q_j(0)$ and $P_j(0)$ for a given $E_j$ is randomly chosen such that they meet the condition given by $E_j = P_j(0)^2/2M + V(Q_j(0))$. The procedure for choosing initial values of $q_n(0)$ and $p_n(0)$ is the same as that adopted in the preceding subsection [10]. We have discarded results for $t < 200$ in our DSs performed for $t = 0$ to 1000.

Before discussing cases where $N_S$ and $N_B$ may be greater than unity, we first study a pedagogical simple case of $N_S = N_B = 1$: a particle with double-well potential is subjected to a single harmonic oscillator. Double-chain curves in Fig. [8(a)] and [8(b)] show energy distributions of the system [$f_S(u)$] and bath [$f_B(u)$], respectively, with $c_o = 0.0$, where $u = u_S \ (u = u_B)$ for the system (bath). Both $f_S(u_S)$ and $f_B(u_B)$ follow the exponential distribution because the assumed initial equilibrium states of decoupled system and bath persist at $t \geq 0.0$. When they are coupled by a weak coupling of $c_o = 0.1$ at $t \geq 0.0$, $f_S(u)$ and $f_B(u)$ almost remain exponential distributions except for that $f_S(u)$ has a small peak at $u = 1.0$, as shown by dashed curve in Fig. [8(a)]. This peak has been realized in Figs. [2(d)] and [3(d)]. It is due to the presence of a potential barrier with $\Delta = 1.0$ in double-well potential because the peak at $u = 1.0$ in $f_S(u)$ is realized even when $T \neq 1.0$, as will be discussed later in 4. Effect of $T$ (Fig. [12]). This peak is developed for stronger couplings of $c_o = 1.0$ and 2.0, for which magnitudes of $f_S(u)$ at small $u$ are decreased, as shown by solid
FIG. 6: Strobe plots in the $(Q,P)$ phase space for various $E_{So}$: (a) $E_{So} = 0.5$, (b) $E_{So} = 0.8$ (c) $E_{So} = 1.0$ and $E_{So} = 1.2$ with $N_{S} = 1$, $N_{B} = 100$, $T = 1.0$ and $c_o = 1.0$.

and chain curves in Figs. 8(a) and 8(b).
FIG. 7: (Color online) System energy distributions $f_S(u)$ for $E_{S_0} = 0.5, 0.8, 1.0$ and $1.2$ with $N_S = 1, N_B = 100, T = 1.0$ and $c_0 = 1.0$, curves being successively shifted upward by two for clarity of figures.

1. Effect of $c_0$

We change the coupling strength of $c_0$. Figures 9(a) and 9(b) show $f_S(u)$ and $f_B(u)$, respectively, for $c_0 = 0.2, 1.0, 5.0$ and $10.0$ with $N_S = 1, N_B = 100$ and $T = 1.0$. $f_S(u)$ for $c_0 = 0.2$ nearly follows the exponential distribution. When $c_0$ becomes larger, magnitudes of $f_S(u)$ at $u < 1.0$ are decreased while that at $u > 1.0$ is increased. In particular, the magnitude of $f_S(0)$ is more decreased for larger $c_0$. 

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FIG. 8: (Color online) Stationary distributions of (a) $f_S(u)$ and (b) $f_B(u)$ for various $c_o$: $c_o = 0.0$ (double-chain curves), 0.1 (dashed curves), 1.0 (solid curves) and 2.0 (chain curves) obtained by 10 000 runs with $N_S = N_B = 1$ and $T = 1.0$.

2. Effect of $\omega_n$ distributions

Although we have assumed $\omega_n = 1.0$ in bath oscillators, we will examine the effect of their distribution, taking into account two kinds of random distributions given by $\omega_n \in [0.5, 2.0]$
FIG. 9: (Color online) Stationary distributions of (a) $f_S(u)$ and (b) $f_B(u)$ for various $c_o$: $c_o = 0.2$ (dashed curves), 1.0 (chain curves), 5.0 (double-chain curves) and 10.0 (solid curves) with $N_S = 1$, $N_B = 100$ and $T = 1.0$.

and $\omega_n \in [2.0, 3.0]$. From calculated results shown in Figs. [10(a) and 10(b)], we note that $f_S(u)$ and $f_B(u)$ are not much sensitive to the distribution of $\{\omega_n\}$ in accordance with our previous calculation for harmonic oscillator system [10, 25]. This conclusion, however, might
not be applied to the case of infinite bath where distribution of \( \{ \omega_n \} \) becomes continuous distribution. Ref. [8] reported that the relative position between oscillating frequency ranges of system and bath is very important for a thermalization of the harmonic oscillator system subjected to finite bath.

3. Effect of \( N_B \)

We have calculated \( f_S(u) \) and \( f_B(u) \), changing \( N_B \) but with fixed \( N_S = 1 \), whose results are shown in Figs. 11(a) and 11(b). For larger \( N_B \), the width of \( f_B(u) \) becomes narrower as expected. However, shapes of \( f_S(u) \) are nearly unchanged for all cases of \( N_B = 1, 10, 100 \) and 1000.

4. Effect of \( T \)

We change the temperature of the bath. Figures 12(a) and 12(b) show \( f_S(u) \) and \( f_B(u) \), respectively, for \( T = 0.5, 1.0 \) and 1.5 with \( N_S = 1, N_B = 100 \) and \( c_o = 1.0 \). When \( T \) is decreased (increased), positions of \( f_B(u) \) move to lower (higher) energy such that mean values of \( u_B \) correspond to \( T \). For a lower temperature of \( T = 0.5 \), magnitude of \( f_S(u) \) at \( u < 1.0 \) is increased while that at \( u > 1.0 \) is decreased. The reverse is realized for higher temperature of \( T = 1.5 \). We should note that the peak position in \( f_S(u) \) at \( u = 1.0 \) is not changed even if \( T \) is changed because this peak is related to the barrier with \( \Delta = 1.0 \) of the double-well potential.

5. Effect of \( N_S \)

Although \( N_S = 1 \) has been adopted so far, we will change \( N_s \) to investigate its effects on stationary energy distributions. Figure 13(a) shows \( f_S(u) \) for \( N_S = 1, 2, 5 \) and 10. \( f_S(u) \) for \( N_S = 1 \) shows an exponential-like distribution with \( f_S(0) \neq 0 \) at \( u = 0.0 \). In contrast, \( f_S(u) \) vanishes at \( u = 0.0 \) for \( N_S = 2, 5 \) and 10. Figure 13(a) shows that shapes of \( f_S(u) \) much depend on \( N_S \) while those of \( f_B(u) \) are almost unchanged in Fig. 13(b).
FIG. 10: (Color online) Stationary distributions of (a) $f_S(u)$ and (b) $f_B(u)$ for various distributions of $\{\omega_n\}$: $\omega = 1.0$ (dashed curves), $\omega_n \in [0.5, 2.0]$ (solid curves) and $\omega_n \in [2.0, 3.0]$ (chain curves) with $N_S = 1$, $N_B = 100$, $T = 1.0$ and $c_o = 1.0$. 
FIG. 11: (Color online) Stationary distributions of (a) $f_S(u)$ and (b) $f_B(u)$ for various $N_B$: $N_B = 1$ (solid curves), 10 (dashed curves), 100 (chain curves) and 1000 (bold solid curves) with $N_S = 1$, $T = 1.0$ and $c_0 = 1.0$. $f_B(u)$ for $N_B = 1000$ is multiplied by a factor of $1/3$. 
FIG. 12: (Color online) Stationary distributions of (a) $f_S(u)$ and (b) $f_B(u)$ for various $T$: $T = 0.5$ (chain curves), 1.0 (solid curves) and 1.5 (dashed curves) with $N_S = 1$, $N_B = 100$ and $c_0 = 1.0$. 
FIG. 13: (Color online) Stationary distributions of (a) $f_S(u)$ and (b) $f_B(u)$ for various $N_S$: $N_S = 1$ (dashed curves), 2 (dotted curves), 5 (chain curves) and 10 (solid curves) with $N_B = 100$, $T = 1.0$ and $c_o = 1.0$. 
IV. DISCUSSION

A. Analysis of stationary energy distributions

Our DSs in the preceding section have shown that \( f_S(u) \) depends mainly on \( N_S, c_o \) and \( T \) while \( f_B(u) \) depends mostly on \( N_B \) and \( T \) for \( N_S \ll N_B \). We will try to analyze \( f_S(u) \) and \( f_B(u) \) in this subsection. It is well known that when variables of \( x_i (i = 1 - N) \) are independent and follow the exponential distributions with the same mean, the distribution of its sum: \( X = \sum_i x_i \) is given by the \( \Gamma \) distribution. Then for an uncoupled system \( (c_o = 0.0) \), \( f_S(u) \) and \( f_B(u) \) are expressed by the \( \Gamma \) distribution given by \[ f_\eta(u) = \frac{1}{Z_{\eta}} u^{a_\eta - 1} e^{-b_\eta u} \equiv g(u; a_\eta, b_\eta), \] (28)

with

\[
\begin{align*}
    a_\eta &= N_\eta, \\
    b_\eta &= N_\eta \beta, \\
    Z_\eta &= \frac{\Gamma(a_\eta)}{b_\eta^{a_\eta}},
\end{align*}
\] (30)

where \( \eta \) = S and B for a system and bath, respectively, and \( \Gamma(x) \) is the gamma function. In the limit of \( N_S = 1 \), the \( \Gamma \) distribution reduces to the exponential distribution. Mean \( (\mu_\eta) \) and variance \( (\sigma^2_\eta) \) of the \( \Gamma \) distribution are given by

\[
\mu_\eta = \frac{a_\eta}{b_\eta}, \quad \sigma^2_\eta = \frac{a_\eta}{b_\eta^2},
\] (31)

from which \( a_\eta \) and \( b_\eta \) are expressed in terms of \( \mu_\eta \) and \( \sigma_\eta \)

\[
\begin{align*}
    a_\eta &= \frac{\mu_\eta^2}{\sigma^2_\eta}, \\
    b_\eta &= \frac{\mu_\eta}{\sigma_\eta^2}.
\end{align*}
\] (32)

We have tried to evaluate \( f_S(u) \) and \( f_B(u) \) for the coupled system \( (c_o \neq 0.0) \) as follows: From mean \( (\mu_\eta) \) and root-mean-square (RMS) \( (\sigma_\eta) \) calculated by DSs, \( a_\eta \) and \( b_\eta \) are determined by Eq. (32), with which we obtain the \( \Gamma \) distributions for \( f_S(u) \) and \( f_B(u) \). Filled and open squares in Fig. 14 show \( \mu_B \) and \( \sigma_B \), respectively, as a function of \( N_S \). We obtain \( \mu_B = 1.0 \) and \( \sigma_B = 0.1 \) nearly independently of \( N_S \), which yield \( a_B = b_B = 100.0 \) in agreement with Eq. (29). Filled and open triangles in Fig. 14 express the \( N_S \) dependence of \( \mu_S \) and \( \sigma_S \) obtained by DSs with \( c_o = 1.0, N_B = 100 \) and \( T = 1.0 \). Calculated mean and RMS values of \( (\mu_S, \sigma_S) \) are \((1.07, 0.98), (0.99, 0.70), (0.99, 0.44) \) and \((0.99, 0.319) \) for \( N_S = 1, 2, 5 \).
FIG. 14: (Color online) $N_S$ dependences of $\mu_\eta$ and $\sigma_\eta$ of system ($\eta = S$) and bath ($\eta = B$) with $N_B = 100$ and $T = 1.0$: filled (open) triangles denote $\mu_S$ ($\sigma_S$) with $c_o = 1.0$: filled (open) circles express $\mu_S$ ($\sigma_S$) with $c_o = 10.0$: filled (open) squares show $\mu_B$ ($\sigma_B$) with $c_o = 1.0$.

and 10, respectively, for which Eq. (32) yields $(a_S, b_S) = (1.18, 1.11), (2.04, 2.05), (4.50, 5.06)$ and $(9.82, 9.97)$. These values of $a_S$ and $b_S$ are not so different from $N_S$ and $N_S \beta$ given by Eq. (29). We have employed the $\Gamma$ distribution with these parameters $a_S$ and $b_S$ for our analysis of $f_S(u)$ having been shown in Fig. 13(a). Dashed curves in Figs. 15(a)-(d) express calculated $\Gamma$ distributions, which are in fairly good agreement with $f_S(u)$ plotted by solid curves, except for $N_S = 1$ for which $g(0) = 0.0$ because $a_S = 1.18 > 1.0$ while $f_S(0) \neq 0.0$.

Similar analysis has been made for another result obtained with a larger $c_o = 10.0$ for
FIG. 15: (Color online) u dependences of $f_S(u)$ for (a) $N_S = 1$, (b) $N_S = 2$, (c) $N_S = 5$ and (d) $N_S = 10$ with $T = 1.0$, $c_o = 1.0$ and $N_B = 100$ obtained by DSs (solid curves): dashed and chain curves express $\Gamma$ and exponential distributions, respectively (see text).

$N_B = 100$ and $T = 1.0$. $N_S$-dependences of calculated $\mu_S$ and $\sigma_S$ are plotted by filled and open circles, respectively, in Fig. 14. Calculated ($\mu_S, \sigma_S$) are $(2.88, 2.61)$, $(1.81, 1.12)$, $(1.21, 0.47)$ and $(1.07, 0.31)$ for $N_S = 1$, 2, 5 and 10, respectively, which lead to $(a_S, b_S) =$
FIG. 16: (Color online) $u$ dependences of $f_S(u)$ for (a) $N_S = 1$, (b) $N_S = 2$, (c) $N_S = 5$ and (d) $N_S = 10$ with $T = 1.0$, $c_0 = 10.0$ and $N_B = 100$ obtained by DSs (solid curves): dashed and chain curves express $\Gamma$ and exponential distributions, respectively (see text).

$(1.22, 0.42), (2.62, 1.45), (6.57, 5.44)$ and $(11.54, 10.81)$ by Eq. (32). Obtained $a_S$ and $b_S$ are rather different from $N_S$ and $N_S\beta$ given by Eq. (29). Dashed curves in Figs. 16(a)-(d) show $\Gamma$ distributions with these parameters, which may approximately explain $f_S(u)$ obtained by
DSs in the *phenomenologically* sense, except for \( N_S = 1 \) for which \( g(0) = 0.0 \) but \( f_S(0) \neq 0.0 \).

We note in Fig. 15(a) or 16(a) that an agreement between \( g(u) \) and \( f_S(u) \) with \( N_S = 1 \) is not satisfactory. We have tried to obtain a better fit between them, by using the \( q \)-\( \Gamma \) distribution \( g_q(u) \) given by [10]

\[
g_q(u) = \frac{1}{Z_q} u^{a-1} e^{-bu^q}, \tag{33}
\]

with

\[
e_q^x = [1 + (1 - q)x]_{+}^{1/(1-q)}, \tag{34}
\]

where \([y]_+ = \max(y, 0)\) and \( Z_q \) is the normalization factor. Note that \( g_q(u) \) reduces to the \( \Gamma \) distribution in the limit of \( q \to 1.0 \). Although the \( q \)-\( \Gamma \) distribution was useful for \( f_S(u) \) of harmonic-oscillator systems subjected to finite bath [10], it does not work for \( f_S(u) \) of double-well systems. This difference may be understood from a comparison between \( f_S(u) \) for \( N_S = 1 \) of a double-well system shown in Fig. 15(a) [or 16(a)] and its counterpart of a harmonic oscillator system shown in Fig. 9(a) of Ref. [10]. Although the latter shows an exponential-like behavior with a monotonous decrease with increasing \( u \), the former with a characteristic peak at \( u = 1.0 \) cannot be expressed by either the exponential, \( \Gamma \), or \( q \)-\( \Gamma \) distribution.

**B. Analysis of stationary position distributions**

We have studied also the \( N_S \) dependence of stationary position distributions of \( p(Q) \) and \( P(\bar{Q}) \), where \( Q \) denotes the position of a particle in the system and \( \bar{Q} \) expresses the averaged position given by

\[
\bar{Q} = \frac{1}{N_S} \sum_{k=1}^{N_S} Q_k. \tag{35}
\]

Figures 17(a) and 17(b) show \( p(Q) \) and \( P(\bar{Q}) \), respectively, obtained by DSs for various \( N_S \) with \( N_B = 100, T = 1.0 \) and \( c_o = 1.0 \). For \( N_S = 1 \), we obtain \( p(Q) = P(\bar{Q}) \) with the characteristic double-peaked structure. We note, however, that \( P(\bar{Q}) \) is different from \( p(Q) \) for \( N_S > 1 \) for which \( P(\bar{Q}) \) has a single-peaked structure despite the double-peaked \( p(Q) \). This is easily understood as follows: For example, in the case of \( N_S = 2 \), two particles in
FIG. 17: (Color online) Stationary distributions of (a) \( p(Q) \) as a function of particle position \( Q \) and (b) \( P(\bar{Q}) \) as a function of the averaged position \( \bar{Q} \) for various \( N_S \): \( N_S = 1 \) (dashed curve), 2 (solid curve), 5 (dotted curve) and 10 (chain curve) with \( N_B = 100, T = 1.0 \) and \( c_0 = 1.0 \). Open circles in (b) express an analytical result obtained by Eq. (36) with \( N_S = 2 \).

the system mainly locate at \( Q_k = 1.0 \) or \( Q_k = -1.0 \) \( (k = 1, 2) \) which yields the double-peaked distribution of \( f_S(Q) \). However, the averaged position of \( \bar{Q} = (Q_1 + Q_2)/2 \) will be dominantly \( \bar{Q} = 0.0 \), which leads to a single-peaked \( P(\bar{Q}) \). The situation is the same also for \( N_S > 2 \).
Theoretically $P(\bar{Q})$ may be expressed by

$$P(\bar{Q}) = \int \cdots \int \prod_{k=1}^{N_S} dQ_k \exp \left[ -\beta V(Q_k) \right] \delta \left( \bar{Q} - N_S^{-1} \sum_{k=1}^{N_S} Q_k \right).$$

(36)

$P(\bar{Q})$ numerically evaluated for $N_S = 2$ is plotted by open circles in Fig. 17 which are in good agreement with the solid curve expressing $P(\bar{Q})$ obtained by DS. It is impossibly difficult to numerically evaluate Eq. (36) for $N_S \geq 3$. In the limit of $N_S \to \infty$, $P(\bar{Q})$ reduces to the Gaussian distribution according to the central-limit theorem. This trend is realized already in the case of $N_S = 10$ in Fig. 17(b).

V. CONCLUDING REMARKS

We have studied the properties of classical double-well systems coupled to finite bath, employing the $(N_S + N_B)$ model [10] in which $N_S$-body system is coupled to $N_B$-body bath. Results obtained by DSs have shown the following:

(i) Chaotic oscillations are induced in the double-well system coupled to finite bath in the absence of external forces for appropriate model parameters of $c_o$, $N_B$, $T$, $\{\omega_n\}$ and $E_{So}$.

(ii) Among model parameters, $f_S(u)$ depends mainly on $N_S$, $c_o$ and $T$ while $f_B(u)$ depends on $N_B$ and $T$ for $N_S \ll N_B$.

(iii) $f_S(u)$ for $N_S > 1$ obtained by DSs may be phenomenological expressed by the $\Gamma$ distribution,

(iv) $f_S(u)$ for $N_S = 1$ with $c_o \neq 0.0$ cannot be described by either the exponential, $\Gamma$, or $q$-$\Gamma$ distribution, although that with $c_o = 0.0$ follows the exponential distribution, and

(v) The dissipation is not realized in the system energy for DSs at $t = 0 - 1000$ with $N_S = 1 - 100$ and $N_B = 10 - 1000$.

The item (i) is in consistent with chaos in a closed classical double-well system driven by external forces [23], although chaos is induced without external forces in our open classical double-well system. This is somewhat reminiscent of chaos induced by quantum noise in the absence of external force in closed quantum double-well systems [27]. Effects of induced chaos in the item (i) are not apparent in $f_S(u)$ because $u (= u_S)$ is ensemble averaged over 10 000 runs (realizations) with exponentially distributed initial system energies. Items (ii) and (v) are the same as in the harmonic-oscillator system coupled to finite bath [10]. The item (v) suggests that for the energy dissipation of system, we might need to adopt a much larger
$N_B \gg 1000$ \cite{26}. The item (iv) is in contrast to $f_\Sigma(u)$ for $N_\Sigma = 1$ in the open harmonic-oscillator system which may be approximately accounted for by the $q$-Γ distribution \cite{10}. It would be necessary and interesting to make a quantum extension of our study which is left as our future subject.

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