Responses of small quantum systems subjected to finite baths

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Abstract

We have studied responses to applied external forces of the quantum \((N_S + N_B)\) model for \(N_S\)-body interacting harmonic oscillator (HO) system subjected to \(N_B\)-body HO bath, by using canonical transformations combined with Husimi’s method for a driven quantum HO [K. Husimi, Prog. Theor. Phys. 9, 381 (1953)]. It has been shown that the response to a uniform force expressed by the Hamiltonian: \(H_f = -f(t) \sum_{k=1}^{N_S} Q_k\) is generally not proportional to \(N_S\) except for no system-bath couplings, where \(f(t)\) expresses its time dependence and \(Q_k\) denotes a position operator of \(k\)th particle of the system. We have calculated also the response to a space- and time-dependent force expressed by \(H_f = -f(t) \sum_{k=1}^{N_S} Q_k e^{i 2\pi ku/N_S}\), where the wavevector \(u\) is \(u = 0\) and \(u = -N_S/2\) for uniform and staggered forces, respectively. The spatial correlation \(\Gamma_m\) for a pair of positions of \(Q_k\) and \(Q_{k+m}\) has been studied as functions of \(N_S\) and the temperature. Our calculations have indicated an importance of taking account of finite \(N_S\) in studying quantum open systems which generally include arbitrary numbers of particles.

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I. INTRODUCTION

In recent years, there has been considerable interest in open small systems, whose physical properties have been studied both by experimental and theoretical methods [1]. We may prepare desired small systems by advanced new techniques. Theoretical studies of open systems have been made with the use of the Caldeira-Leggett (CL) type models [2–6]. CL-type models have been extensively studied by using various methods such as quantum Langevin equation and master equation [6]. The original CL model considers a system of a single particle ($N_S = 1$) which is subjected to a bath consisting of infinite numbers of uncoupled harmonic oscillators (HOs) ($N_B = \infty$). Recent studies with the CL model have tried to go beyond this restriction on $N_S$ and $N_B$. References [7–9] have employed the CL model with $N_S = 1$ and $N_B \approx 1 - 800$ for studies of properties of small system coupled to finite bath. CL-type models with $N_S = 2$ and $N_B = \infty$ have been investigated [10, 11]. Reference [12] discusses the master equation of arbitrary $N_S$ system coupled to an arbitrary $N_B$ bath. In our previous study [13], we have adopted the $(N_S + N_B)$ model for $N_S$-body system subjected to $N_B$-body bath in order to calculate energy distributions of a system, which show intrigue properties as functions of $N_S$, $N_B$ and a system-bath coupling.

In adopting the CL-type model, we have implicitly assumed that physical quantities such as the energy and specific heat of a system with finite $N_S$ ($> 1$) are given as $N_S$ times of results of a system with $N_S = 1$. Our recent calculation [14], however, has pointed out that it is generally not the case because the system specific heat, $C_S(T; N_S, N_B)$, of the $(N_S + N_B)$ model at temperature $T$ is given by

$$C_S(T; N_S, N_B) \neq N_S C_S(T; 1, N_B),$$

except for no system-bath couplings and/or in the high-temperature limit. Furthermore it has been shown that the low-temperature specific heat may be negative for finite $N_S$ with a strong system-bath coupling [14]. This is in contrast with Refs. [15, 16, 18] showing a non-negative system specific heat for HO system in CL-type models with $(N_S, N_B) = (1, 1)$ and $(1, \infty)$. These results imply that we should explicitly take into account finite $N_S$ in studying open systems which may generally include arbitrary numbers of particles. It is interesting and necessary to study responses to applied external forces of the $(N_S + N_B)$ model, which is the purpose of the present paper. Responses of the CL models have been
mostly made for infinite baths for which Ohmic and Drude models are adopted (e.g., Ref. [19]) [6]. In this study, we employ the identical-frequency model for finite baths [14].

The paper is organized as follows. In Sec. II, we briefly explain the \((N_S + N_B)\) model [13, 14], to which we apply the canonical transformations in order to obtain the diagonalized Hamiltonian including external forces. By using Husimi’s method for a driven quantum HO [21], we calculate the response of the open HO system to sinusoidal and step forces. In Sec. III, we calculate also the response to space- and time-dependent forces. The spatial correlation \(\Gamma_m\) between positions of two particles separated by a distance \(m\) is evaluated. The final Sec. IV is devoted to our conclusion.

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

A. Quantum Langevin equation

We consider the \((N_S + N_B)\) model in which a one-dimensional \(N_S\)-body system \((H_S)\) is subjected to an \(N_B\)-body bath \((H_B)\) by the interaction \((H_I)\) [13, 14]. The total Hamiltonian is assumed to be given by

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

with

\[
H_S = \sum_{k=1}^{N_S} \left[ \frac{P_k^2}{2M} + \frac{DQ_k^2}{2} + \frac{K}{2}(Q_k - Q_{k+1})^2 \right] + H_f,
\]

\[
H_f = -f(t) \sum_{k=1}^{N_S} Q_k,
\]

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

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

Here \(P_k (p_n)\) and \(Q_k (q_n)\) express the momentum and position operators, respectively, of a HO with a mass of \(M (m)\) in the system (bath), \(D\) and \(K\) denote force constants in the system, \(\omega_n\) is the oscillator frequency of the bath, \(c_{kn}\) is a system-bath coupling and \(f(t)\) stands for an applied force. Operators satisfy commutation relations,

\[
[Q_k, P_\ell] = i\hbar \delta_{k\ell}, \quad [q_n, p_m] = i\hbar \delta_{nm}, \quad [Q_k, Q_\ell] = [P_k, P_\ell] = [q_n, q_m] = [p_n, p_m] = 0.
\]
Equation (3) expresses the interacting HO system for $D \neq 0$ and $K \neq 0$. In the limiting case of $K = 0$, the system consists of a collection of uncoupled (independent) HOs. The system is subjected to a bath consisting of a collection of uncoupled HOs with oscillator frequencies of $\{\omega_n\}$.

In conventional approaches to the quantum system-plus-bath model, we obtain equations of motion for $Q_k$ and $q_n$, employing the Heisenberg equation,

$$i\hbar \dot{O} = [O, H],$$

where $O$ expresses an arbitrary operator and a dot stands for a derivative with respect of time. We obtain the quantum Langevin equations given by [14]

$$M \ddot{Q}_k(t) = -DQ_k(t) - K [2Q_k(t) - Q_{k-1}(t) - Q_{k+1}(t)] - M \sum_{\ell=1}^{N_S} \xi_{k\ell} Q_\ell(t)$$

$$- \sum_{\ell=1}^{N_S} \int_0^t \gamma_{k\ell}(t-t') \dot{Q}_\ell(t') \, dt' - \sum_{\ell=1}^{N_S} \gamma_{k\ell}(t) Q_\ell(0) + \zeta_k(t) + f(t),$$

with

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

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

$$\zeta_k(t) = \sum_{n=1}^{N_B} c_{kn} \left( q_n(0) \cos \tilde{\omega}_n t + \frac{\dot{q}_n(0)}{\tilde{\omega}_n} \sin \tilde{\omega}_n t \right).$$

Here $\xi_{k\ell}$ denotes the additional interaction between $k$ and $\ell$th particles in the system induced by couplings $\{c_{kn}\}$, $\gamma_{k\ell}(t)$ stands for the memory kernel and $\zeta_k$ is the stochastic force. By using averages over initial values of $q_n(0)$ and $\dot{q}_n(0)$,

$$\langle m \tilde{\omega}_n^2 q_n(0)^2 \rangle_B = m \langle \dot{q}_n(0)^2 \rangle_B = \left( \frac{\hbar \tilde{\omega}_n}{2} \right) \coth \left( \frac{\beta \hbar \tilde{\omega}_n}{2} \right),$$

we obtain the fluctuation-dissipation relation,

$$\frac{1}{2} \langle \zeta_k(t) \zeta_\ell(t') + \zeta_\ell(t') \zeta_k(t) \rangle_B = \sum_{n=1}^{N_B} \left( \frac{c_{kn} c_{\ell n}}{m \tilde{\omega}_n^2} \right) \left( \frac{\hbar \tilde{\omega}_n}{2} \right) \coth \left( \frac{\beta \hbar \tilde{\omega}_n}{2} \right) \cos \tilde{\omega}_n (t - t'),$$

$$\rightarrow k_B T \gamma_{k\ell}(t-t') \quad \text{for} \quad \beta \rightarrow 0,$$

where $\langle \cdot \rangle_B$ expresses the average over initial states of the bath. $\xi_{k\ell}$ in Eq. (10) denotes a shift of oscillator frequency due to an introduced coupling, and it vanishes if we adopt...
\( c_n = m \tilde{\omega}_n^2 \) for \( N_S = 1 \). In the case of \( N_S \neq 1 \), however, it is impossible to choose \( \{c_{kn}\} \) such as \( \xi_{k\ell} = 0 \) for all pairs of \((k, \ell)\), then \( Q_k \) is inevitably coupled with \( Q_\ell \) \((\ell \neq k)\). Because of these couplings between HOs, the \( N_S \)-body system cannot be simply regarded as a sum of systems with \( N_S = 1 \). Although Eqs. (9)-(12) are formally exact, it is difficult to solve \( N_S \)-coupled integrodifferential equations.

### B. The canonical transformation

In order to obtain a tractable Langevin equation, we apply the canonical transformation to the model Hamiltonian. We assume that \( N_S \) is even without a loss of generality. Imposing a periodic boundary condition,

\[
Q_{N_S+k} = Q_k, \quad P_{N_S+k} = P_k, \tag{16}
\]

we employ the canonical transformation \[20\],

\[
Q_k = \frac{1}{\sqrt{N_S}} \sum_{s=-N_S/2}^{N_S/2-1} e^{i(2\pi ks/N_S)} \tilde{Q}_s, \tag{17}
\]

\[
P_k = \frac{1}{\sqrt{N_S}} \sum_{s=-N_S/2}^{N_S/2-1} e^{i(2\pi ks/N_S)} \tilde{P}_s. \tag{18}
\]

Note that the boundary condition is satisfied in Eqs. (17) and (18) and that the set \( \{(1/\sqrt{N_S})e^{i(2\pi ks/N_S)}\} \) is orthogonal and complete in a periodic domain of the oscillator label \( k \). By the canonical transformation, \( H_S \) in Eq. (3) becomes

\[
H_S = \sum_{s=-N_S/2}^{N_S/2-1} \left[ \frac{\tilde{P}_s^* \tilde{P}_s}{2M} + \frac{(D + M\Omega_s^2)\tilde{Q}_s^* \tilde{Q}_s}{2} \right] - \sqrt{N_S} \tilde{Q}_0 f(t), \tag{19}
\]

with

\[
M\Omega_s^2 = 4K \sin^2 \left( \frac{\pi s}{N_S} \right), \quad \text{for } s = -\frac{N_S}{2}, -\frac{N_S}{2} + 1, \ldots, \frac{N_S}{2} - 1, \tag{20}
\]

where the commutation relations:

\[
[\tilde{Q}_s, \tilde{P}_{s'}^*] = i\hbar \delta_{ss'}, \quad [\tilde{Q}_s, \tilde{Q}_{s'}] = [\tilde{P}_s, \tilde{P}_{s'}] = 0, \tag{21}
\]

hold with \( \tilde{Q}_s^* = \tilde{Q}_{-s} \) and \( \tilde{P}_s^* = \tilde{P}_{-s} \).
For a simplicity of our calculation, we assume an identical frequency bath \[14\],

\[
\omega_n = \omega_0, \quad c_{kn} = c.
\]  

(22)

We furthermore assume that \(N_B\) is even, imposing the periodic boundary condition given by

\[
q_{N_B+n} = q_n, \quad p_{N_B+n} = p_n.
\]  

(23)

We apply the canonical transformation \[14, 20\],

\[
q_n = \frac{1}{\sqrt{N_B}} \sum_{r=-N_B/2}^{N_B/2-1} e^{i(2\pi nr/N_B)} \tilde{q}_r, \\
p_n = \frac{1}{\sqrt{N_B}} \sum_{r=-N_B/2}^{N_B/2-1} e^{i(2\pi nr/N_B)} \tilde{p}_r,
\]  

(24)

(25)

to the bath with the periodic condition given by Eq. (23). The bath Hamiltonian \(H_B\) in Eqs. (5) becomes \[25\]

\[
H_B = \frac{N_B}{2} \sum_{r=-N_B/2}^{N_B/2-1} \left( \frac{\tilde{p}_r^* \tilde{p}_r}{2m} + \frac{m \omega_r^2 \tilde{q}_r^* \tilde{q}_r}{2} \right)
\]  

(26)

where the commutation relations:

\[
[q_r, \tilde{p}_{r'}^*] = i\hbar \delta_{rr'}, \quad [\tilde{q}_r, \tilde{q}_{r'}] = [\tilde{p}_r, \tilde{p}_{r'}] = 0,
\]  

(27)

hold with \(\tilde{q}_r^* = \tilde{q}_{-r}\) and \(\tilde{p}_r^* = \tilde{p}_{-r}\). By canonical transformations given by Eqs. \[17\], \[18\], \[24\] and \[25\], \(H_I\) in Eq. \[6\] becomes \[25\]

\[
H_I = \frac{c N_B}{2} \sum_{s=-N_S/2}^{N_S/2-1} \tilde{Q}_s^* \tilde{Q}_s + \frac{c N_S}{2} \sum_{r=-N_B/2}^{N_B/2-1} \tilde{q}_r^* \tilde{q}_r - c \sqrt{N_S N_B} \tilde{Q}_0 \tilde{q}_0.
\]  

(28)

Summing up Eqs. (19), (26) and (28), we obtain the total Hamiltonian expressed by

\[
H = H_0 + H'_S + H'_B,
\]  

(29)

where

\[
H_0 = \frac{\tilde{P}_0^2}{2M} + \frac{M \tilde{Q}_0^2}{2} + \frac{m \tilde{P}_0^2}{2} + \frac{m \omega_0^2}{2} - c \sqrt{N_S N_B} \tilde{Q}_0 \tilde{q}_0 - \sqrt{N_S} \tilde{Q}_0 f(t),
\]  

(30)

\[
H'_S = \sum_{s(\neq 0)} \left[ \frac{\tilde{P}_s^* \tilde{P}_s}{2M} + \frac{M \tilde{Q}_s^2 \tilde{Q}_s}{2} \right],
\]  

(31)

\[
H'_B = \sum_{r(\neq 0)} \left[ \frac{\tilde{p}_r^* \tilde{p}_r}{2m} + \frac{m \omega_r^2 \tilde{q}_r^* \tilde{q}_r}{2} \right],
\]  

(32)
\[ M\tilde{\Omega}^2_s = D + 4K\sin^2\left(\frac{\pi s}{N_S}\right) + cN_B \quad \text{for } s = -\frac{N_S}{2}, \ldots, \frac{N_S}{2} - 1, \quad (33) \]

\[ m\tilde{\omega}^2_r = m\omega_0^2 + cN_S \quad \text{for } r = -\frac{N_B}{2}, \ldots, \frac{N_B}{2} - 1. \quad (34) \]

It is noted that \( H_0 \) expresses the Hamiltonian for a uniform mode with \( s = u = 0 \) and that a summation over \( s \) (\( r \)) in the \( H'_S \) \( (H'_B) \) is excluded for \( s = 0 \) \( (r = 0) \).

C. Eigenfrequencies with \( f(t) = 0 \)

Eigenfrequencies of the system-plus-bath with \( f(t) = 0 \) may be obtained when we diagonalize \( H_0 \) given by Eq. (30). We employ the canonical transformation given by

\[ \tilde{Q}_0 = M^{-1/2}(X_1\cos \theta + X_2\sin \theta), \quad \tilde{P}_0 = M^{1/2}(Y_1\cos \theta + Y_2\sin \theta), \quad (35) \]

\[ \tilde{q}_0 = m^{-1/2}(-X_1\sin \theta + X_2\cos \theta), \quad \tilde{p}_0 = m^{1/2}(-Y_1\sin \theta + Y_2\cos \theta), \quad (36) \]

where \( Y_i = \dot{X}_i \) and their commutation relations are given by

\[ [X_i, Y_j] = i\hbar \delta_{ij}, \quad [X_i, X_j] = [Y_i, Y_j] = 0 \quad \text{for } i, j = 1, 2. \quad (37) \]

The canonical transformation yields the diagonalized Hamiltonian given by

\[ H = H_0 + H'_S + H'_B, \quad (38) \]

with

\[ H_0 = \frac{Y_1^2}{2} + \frac{\phi_1^2X_1^2}{2} + \frac{Y_2^2}{2} + \frac{\phi_2^2X_2^2}{2}, \quad (39) \]

\[ \tan 2\theta = \frac{2c\sqrt{N_SN_B}}{\sqrt{Mm} (\tilde{\Omega}_0^2 - \tilde{\omega}_0^2)}, \quad (40) \]

\[ \phi_1^2 = \tilde{\Omega}_0^2\cos^2 \theta + \tilde{\omega}_0^2\sin^2 \theta + \left(\frac{2c\sqrt{N_SN_B}}{\sqrt{Mm}}\right)\cos \theta \sin \theta, \quad (41) \]

\[ \phi_2^2 = \tilde{\Omega}_0^2\sin^2 \theta + \tilde{\omega}_0^2\cos^2 \theta - \left(\frac{2c\sqrt{N_SN_B}}{\sqrt{Mm}}\right)\cos \theta \sin \theta, \quad (42) \]

where \( H'_S \) and \( H'_B \) are given by Eqs. (31) and (32), respectively. With the use of Eq. (40), \( \phi_1^2 \) and \( \phi_2^2 \) are alternatively expressed by

\[ \phi_{1,2}^2 = \frac{1}{2} \left[ \tilde{\Omega}_0^2 + \tilde{\omega}_0^2 \pm \sqrt{(\tilde{\Omega}_0^2 - \tilde{\omega}_0^2)^2 + \frac{4N_SN_Bc^2}{Mm}} \right], \quad (43) \]
where $+ (-)$ of a double sign is applied to $\phi_1^2$ ($\phi_2^2$).

In the equilibrium state with $f(t) = 0$, Eqs. (31), (32) and (43) yield eigenfrequencies of \{\nu_i\} ($i = 1$ to $N_S + N_B$) for $H$ given by

$$
\begin{array}{cccccccc}
  i & 1 & \cdots & N_S/2 + 1 & \cdots & N_S & N_S + 1 & \cdots & N_S + N_B/2 + 1 & \cdots & N_S + N_B \\
\nu_i^2 & \tilde{\Omega}_{-N_S/2}^2 & \cdots & \phi_1^2 & \cdots & \tilde{\Omega}_{N_S/2-1}^2 & \tilde{\omega}_0^2 & \cdots & \phi_2^2 & \cdots & \tilde{\omega}_0^2 \\
\end{array}
$$

In the limit of $c = 0$, eigenfrequencies become

$$
\begin{array}{cccccccc}
  i & 1 & \cdots & N_S/2 + 1 & \cdots & N_S & N_S + 1 & \cdots & N_S + N_B/2 + 1 & \cdots & N_S + N_B \\
\nu_i^2 & \Omega_{-N_S/2}^2 & \cdots & \Omega_0^2 & \cdots & \Omega_{N_S/2-1}^2 & \omega_0^2 & \cdots & \omega_0^2 & \cdots & \omega_0^2 \\
\end{array}
$$

Reference [14] obtained the same eigenfrequencies by an alternative method: $\phi_1$ and $\phi_2$ given by Eq. (43) correspond to $\nu_+$ and $\nu_-$, respectively, in Ref. [14]. With the use of these eigenfrequencies, the system energy $E_S$ is given by [14]

$$
E_S = -\frac{\partial \ln Z_S}{\partial \beta},
$$

(44)

$$
= \sum_{i=1}^{N_S+N_B} \left( \frac{\hbar \nu_i}{2} \right) \coth \left( \frac{\beta \hbar \nu_i}{2} \right) - \left( \frac{N_B \hbar \omega_0}{2} \right) \coth \left( \frac{\beta \hbar \omega_0}{2} \right),
$$

(45)

where

$$
Z_S = \frac{Z}{Z_B},
$$

(46)

with

$$
Z = \text{Tr} \ e^{-\beta H} = \prod_{i=1}^{N_S+N_B} \left[ \frac{1}{2 \sinh(\beta \hbar \nu_i/2)} \right],
$$

(47)

$$
Z_B = \text{Tr}_B \ e^{-\beta H_B} = \left[ \frac{1}{2 \sinh(\beta \hbar \omega_0/2)} \right]^{N_B}.
$$

(48)

$\text{Tr}$ and $\text{Tr}_B$ denoting a full trace over all variables and a partial trace over bath variables, respectively.

**D. Responses to external forces**

1. *Driven quantum harmonic oscillators*

Quantum HOs driven by an external force have been discussed in Refs. [21–23]. It has been shown that the average position of a quantum HO is expressed by an equation of
motion of relevant classical HO [21–23] as follows. The Hamiltonian of a single HO with mass \( m \) and oscillating frequency \( \omega_0 \) driven by a force \( F(t) \) is given by [21–23]

\[
H = \frac{p^2}{2m} + \frac{m\omega_0^2 x^2}{2} - xF(t),
\]

(49)

for which the Schrödinger equation is expressed by

\[
\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega_0^2 x^2}{2} - xF(t)\right] \Phi(x, t) = i\hbar \frac{\partial \Phi(x, t)}{\partial t}.
\]

(50)

By using a unitary transformation, we may obtain a solution of \( \Phi(x, t) \) expressed by [24]

\[
\Phi_n(x, t) = \phi_n(x - w(t)) \exp\left\{i\hbar \left[ m\dot{w}(x - w(t)) - E_n t + \int_0^t L(t') \, dt' \right] \right\},
\]

(51)

with

\[
L(t) = \frac{1}{2} mw^2 - \frac{1}{2} m\omega_0^2 w^2 + wF(t),
\]

(52)

\[
E_n = \hbar \omega_0 \left(n + \frac{1}{2}\right) \quad \text{for } n = 0, 1, 2, \ldots
\]

(53)

Here \( \phi_n(x) \) and \( E_n \) are wavefunction and eigenvalue, respectively, of the Schrödinger equation with \( F(t) = 0 \) in Eq. (49), and \( w(t) \) obeys an equation of motion for a classical driven HO,

\[
m\ddot{w}(t) + m\omega_0^2 w(t) = F(t).
\]

(54)

Equation (51) shows that the center of a wave packet moves with \( w(t) \). It implies that an average of time-dependent position is given by [21–23]

\[
\bar{x}(t) = w(t),
\]

(55)

where an overline denotes the quantum average and \( w(t) \) is a solution of Eq. (54). This is consistent with Ehrenfest’s theorem.

2. Open quantum system of harmonic oscillators

In order to study the response of the open quantum HO under consideration, it is necessary to pursue equations of classical motions after Husimi’s method [21–23]. From Eqs. (30) and (35), the total Hamiltonian with \( f(t) \neq 0 \) becomes

\[
H = H_0 + H'_S + H'_B,
\]

(56)
with

\[ H_0 = H_{01} + H_{02}, \]  
\[ H_{01} = \frac{Y_1^2}{2} + \frac{\phi_1^2 X_1^2}{2} - \sqrt{\frac{N_S}{M}} X_1 f(t) \cos \theta, \]  
\[ H_{02} = \frac{Y_2^2}{2} + \frac{\phi_2^2 X_2^2}{2} - \sqrt{\frac{N_S}{M}} X_2 f(t) \sin \theta, \]

where \( H'_S \) and \( H'_B \) are given by Eqs. (31) and (32), respectively, and \( \phi_1 \) and \( \phi_2 \) are given by Eqs. (41) and (42). Hamiltonians \( H_{01} \) and \( H_{02} \) in Eqs. (58) and (59) express HOs driven by forces of \( \sqrt{N_S/M} f(t) \cos \theta \) and \( \sqrt{N_S/M} f(t) \sin \theta \), respectively. From \( H'_S \) in Eq. (31), equations of motion for \( \tilde{Q}_s \) with \( s \neq 0 \) are given by

\[ M \ddot{\tilde{Q}}_s = -M \Omega_s^2 \tilde{Q}_s \quad \text{for} \ s \neq 0, \]  
while Eqs. (57) and (58) lead to those for \( s = 0 \), \( X_1 \) and \( X_2 \), given by

\[ \ddot{X}_1 = -\phi_1^2 X_1 + \sqrt{\frac{N_S}{M}} f(t) \cos \theta, \]  
\[ \ddot{X}_2 = -\phi_2^2 X_2 + \sqrt{\frac{N_S}{M}} f(t) \sin \theta. \]

A solution for \( \tilde{Q}_0(t) \) may be evaluated from solutions of \( X_1(t) \) and \( X_2(t) \) with the canonical transformation given by Eq. (35).

After some manipulations, quantum-averaged solutions of \( \tilde{Q}_s \) are given by

\[ \overline{\tilde{Q}_s(t)} = \tilde{Q}_s(0) \cos \Omega_s t + \frac{\tilde{P}_s(0)}{M \Omega_s} \sin \Omega_s t \quad \text{for} \ s \neq 0, \]  
\[ \overline{\tilde{Q}_0(t)} = \tilde{Q}_0(0) A_Q(t) + \tilde{P}_0(0) A_P(t) + \tilde{q}_0(0) B_q(t) + \tilde{p}_0(0) B_p(t) + \Phi(t) \quad \text{for} \ s = 0, \]

with

\[ A_Q(t) = \sum_{i=1}^{2} a_i \cos \phi_i t, \]  
\[ A_P(t) = \frac{1}{M} \sum_{i=1}^{2} \frac{a_i \sin \phi_i t}{\phi_i}, \]  
\[ B_q(t) = -\sqrt{\frac{m}{M}} \cos \theta \sin \theta \left( \cos \phi_1 t - \cos \phi_2 t \right), \]  
\[ B_p(t) = -\frac{1}{\sqrt{Mm}} \cos \theta \sin \theta \left( \frac{\sin \phi_1 t}{\phi_1} - \frac{\sin \phi_2 t}{\phi_2} \right), \]  
\[ \Phi(t) = \frac{\sqrt{N_S}}{M} \sum_{i=1}^{2} \left( \frac{a_i}{\phi_i} \right) \int_{0}^{t} \sin \phi_i (t - t') f(t') \, dt', \]  
\[ a_1 = 1 - a_2 = \cos^2 \theta, \]
where $\tilde{Q}_s(0)$, $\tilde{P}_s(0)$, $\tilde{q}_s(0)$ and $\tilde{p}_s(0)$ denote initial states. The response of the total output averaged over initial states is given by

$$ R(t) \equiv \left\langle \sum_k \tilde{Q}_k(t) \right\rangle_0 = \sqrt{N_S} \left\langle \tilde{Q}_0(t) \right\rangle_0, \quad (71) $$

$$ = \frac{N_S}{M} \sum_{i=1}^{2} \left( \frac{a_i}{\phi_i} \right) \int_0^t \sin \phi_i(t - t') f(t') \, dt', \quad (72) $$

where we employ the relations given by

$$ \left\langle \tilde{Q}_s(0) \right\rangle_0 = \left\langle \tilde{P}_s(0) \right\rangle_0 = \langle \tilde{q}_s(0) \rangle_0 = \langle \tilde{p}_s(0) \rangle_0 = 0, \quad (73) $$

the bracket $\langle \cdot \rangle_0$ expressing an average over initial states. Equation (72) leads to the susceptibility,

$$ \chi(t) = \frac{N_S}{M} \sum_{i=1}^{2} a_i \sin \phi_i t \frac{\phi_i}{\phi_i^2 - \omega^2}, \quad (74) $$

whose Fourier transformation is given by

$$ \hat{\chi}(\omega) = \frac{N_S}{M} \sum_{i=1}^{2} a_i \left( \phi_i^2 - \omega^2 \right), \quad (75) $$

with poles at $\omega = \pm \phi_i$.

It should be noted that $R(t)$ in Eq. (72) is generally not proportional to $N_S$ except for the $c = 0$ case because $\phi_i$ and $a_i$ depend on $N_S$ as shown in Eqs. (41), (42) and (70). This point will be shortly demonstrated in numerical model calculations for sinusoidal and step forces in the following.

A. Sinusoidal forces

We apply a periodic monochromatic force,

$$ f(t) = g \sin \omega t, \quad (76) $$

where $\omega$ and $g$ stand for the frequency and magnitude, respectively, of the force. Equations (72) and (70) yield

$$ R(t) = \left( \frac{N_S g}{M} \right) \sum_{i=1}^{2} \frac{a_i \left( \phi_i \sin \omega t - \omega \sin \phi_i t \right)}{\phi_i \left( \phi_i^2 - \omega^2 \right)} \quad \text{for } \omega \neq \phi_i. \quad (77) $$

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FIG. 1: (Color online) Eigenfrequencies $\nu_i$ of HO systems with $N_S = 10$ subjected to a bath with $N_B = 100$ for $c_0 = 0.0$ (open circles) and $c_0 = 10.0$ (filled circles) ($D = K = M = m = 1.0$ and $\omega_0 = 1.0$), solid and dashed curves being plotted only for a guide of the eye.

In the resonant case of $\omega = \phi_1$, $R(t)$ is given by

$$R(t) = \left(\frac{N_S g}{M}\right) \left[ \frac{a_1 (\sin \omega t - \omega t \cos \omega t)}{2\omega^2} + \frac{a_2 (\phi_2 \sin \omega t - \omega \sin \phi_2 t)}{\phi_2 (\phi_2^2 - \omega^2)} \right].$$  \hspace{1cm} (78)

Expressions of $R(t)$ in the resonance cases of $\omega = \phi_2$ and $\omega = \phi_1 = \phi_2$ are similarly given.

In the limit of $c = 0$ where $\phi_1 = \Omega_0$, $\phi_2 = \omega_0$, $\theta = 0.0$, $a_1 = 1.0$ and $a_2 = 0.0$, Eq. (77) reduces to

$$R(t) = \left(\frac{N_S g}{M}\right) \left[ \frac{\Omega_0 \sin \omega t - \omega \sin \Omega_0 t}{\Omega_s (\Omega_0^2 - \omega^2)} \right] \quad \text{for} \quad c = 0 \quad \text{and} \quad \omega \neq \Omega_0,$$

which expresses the response of a HO isolated from a bath.

We have performed numerical model calculations, choosing a coupling $[14]$, $c = \frac{c_0}{N_S N_B}$, \hspace{1cm} (80)

such that the interaction term in Eq. (6) including summations over $\sum_{k=1}^{N_S}$ and $\sum_{n=1}^{N_B}$ yield finite contributions even in the limits of $N_S \to \infty$ and/or $N_B \to \infty$. We have adopted parameters of $D = K = M = m = \omega_0 = 1.0$ for a given system-plus-bath.

Figure 1 shows eigenfrequencies $\nu_i$ for $c_0 = 0.0$ (open circles) and $c_0 = 10.0$ (filled circles) of a HO system ($N_S = 10$) subjected to a bath ($N_B = 100$). Eigenfrequencies $\nu_i$ for...
FIG. 2: (Color online) Responses of $R(t)/N_S$ of HO systems with $N_S = 1$ (chain curves), 2 (dashed curves), 10 (dotted curves) and 20 (solid curves) for (a) $c_0 = 1.0$ and (b) $c_0 = 10.0$ to an applied sinusoidal force with $\omega = 0.5$ and $g = 1.0$ ($D = K = M = m = 1.0$, $\omega_0 = 1.0$ and $N_B = 100$).

$1 \leq i \leq 10$ show a dispersion relation of the HO system while those for $11 \leq \nu_i \leq 110$ of the bath are almost constant. For $c_0 = 0.0$, we obtain $\tilde{\Omega}_0 = 1.0$ and $\tilde{\omega}_0 = 1.0$. When the system-bath coupling of $c_0 = 10.0$ is introduced, they become 1.414 and 1.048, respectively, which lead to $\phi_1 = 1.449$ and $\phi_2 = 1.0$.

Figure 2(a) shows responses of $R(t)/N_S$ to a sinusoidal force with $\omega = 0.5$ and $g = 1.0$ of HO systems with $N_S = 1$, 2, 10 and 20 coupled to $N_B = 100$ baths with a coupling
FIG. 3: (Color online) $N_S$ dependences of (a) $\phi_i$, and (b) $\theta$ and $a_i$ ($i = 1, 2$) for $c_0 = 1.0$ (dashed curves) and 10.0 (solid curves) ($D = K = M = m = \omega_0 = 1.0$ and $N_B = 100$). $\theta$ and $a_i$ in (b) are independent of $c_0$ for the adopted parameters (see the text).

of $c_0 = 1.0$. Results of $R(t)/N_S$ are almost the same independently of $N_S$, although some discrepancies among the four results are realized at $t \gtrsim 50$. These discrepancies become more evident for a larger coupling of $c_0 = 10.0$, whose results are shown in Fig. 2(b). These results clearly suggest

$$R(t; N_S) = N_S R(t; 1) \quad \text{for } c = 0,$$

$$\neq N_S R(t; 1) \quad \text{for } c \neq 0.$$
In order to elucidate $N_S$ and $c_0$ dependences of $R(t)/N_S$, we show in Figs. 3, $\phi_i$, $\theta$ and $a_i$ ($i = 1, 2$) as a function of $N_S$ for $c_0 = 1.0$ (dashed curves) and 10.0 (solid curves). Figure 3(a) shows that with increasing $N_S$, $\phi_1$ is slightly increased while $\phi_2$ is constant. We note in Fig. 3(b) that an increase of $N_S$ yields an increase in $\theta$, by which $a_2$ is increased but $a_1$ is decreased. For adopted parameters, $\theta$, $a_1$ and $a_2$ are independent of $c$ because the denominator of Eq. (40) becomes $\tilde{\Omega}_0^2 - \tilde{\omega}_0^2 = (N_B - N_S)c$ whose $c$ is cancelled out by that in its numerator. With increasing $N_S$, a contribution from a lower eigenfrequency of $\phi_2$ is increased. The effect of the system-bath coupling for $c_0 = 10.0$ is more significant than that for $c_0 = 1.0$ because the difference of $\phi_1 - \phi_2$ in the former is larger than that in the latter: if $\phi_1 = \phi_2$ results are independent of $a_i$ (and then $N_S$).

B. Step forces

Next we apply a step force given by

$$f(t) = g \Theta(t_s - t),$$

(83)

where $\Theta(x)$ stands for the Heaviside function and $t_s$ is the starting time of a force with a magnitude of $g$. The averaged output is given by

$$R(t) = \left( \frac{N_S g}{M} \right) \sum_{i=1}^{2} a_i \frac{1 - \cos \phi_i(t - t_s)}{\phi_i^2}.$$  \hspace{1cm} (84)

Figure 4(a) shows $R(t)/N_S$ for a step force with $t_s = 10.0$ and $g = 1.0$ of HO systems with $N_S = 1, 2, 10$ and 20 coupled to $N_B = 100$ baths with a coupling of $c_0 = 1.0$ ($D = 1.0$ and $\omega_0 = 1.0$). Result of $R(t)/N_S$ for $N_S \geq 2$ are almost the same as that for $N_S = 1$. However, when the interaction is increased to $c_0 = 10.0$, the discrepancy between results of $N_S = 1$ and $N_S \geq 2$ become evident. Fig. 4(b) shows similar plots but with stronger coupling of $c_0 = 10.0$, for which shape and magnitude of $R(t)/N_S$ are significantly modified for $N_S \geq 2$.

III. DISCUSSION

A. Responses to space- and time-dependent forces

It is interesting to calculate responses to a space- and time-dependent force which yields $H_f$ in Eq. (3),

$$H_f = -f(t)S(u),$$

(85)
FIG. 4: (Color online) Responses of $R(t)/N_S$ of HO systems with $N_S = 1$ (chain curves), 2 (dashed curves), 10 (dotted curves) and 20 (solid curves) for (a) $c_0 = 1.0$ and (b) $c_0 = 10.0$ to an applied step force with $t_s = 10.0$ and $g = 1.0$ ($B = K = M = m = 1.0$, $\omega_0 = 1.0$ and $N_B = 100$). Results for all $N_S$ in (a) are indistinguishable.

with

$$S(u) = \sum_{k=1}^{N_B} Q_k e^{i2\pi ku/N_S} \quad \text{for } u \in \{-N_S/2, -N_S/2 + 1, \cdots, N_S/2 - 1\}. \quad (86)$$
FIG. 5: (Color online) Responses of $R(t)/N_S$ of an isolated HO system ($c_0 = 0.0$) to an applied sinusoidal force with $\omega = 0.5$ and $g = 1.0$ for various $u$ ($N_S = 12$, $N_B = 100$ and $K = D = M = m = \omega_0 = 1.0$). Results for $u = -6.0$, $-4.0$ and $-2.0$ are shifted by 6.0, 4.0 and 2.0, respectively, for clarity of the figures. Here the wavevector $u$ is, for example, $u = 0$ and $u = -N_S/2$ for uniform and staggered forces, respectively, for which $S(u)$ is represented by

$$S(u) = \sum_{k=1}^{N_S} Q_k, \quad \text{for } u = 0,$$

$$= \sum_{k=1}^{N_S} Q_k e^{-i\pi k}, \quad \text{for } u = -\frac{N_S}{2}.\quad (87)$$

The mode with $u \neq 0$ does not couple with $s = 0$ mode which couples with bath as mentioned in the preceding subsection II D. Equations of motion for $\tilde{Q}_s$ with $s \neq 0$ are independent of degrees of freedom in a bath and they are given by

$$M\ddot{\tilde{Q}}_u = -M\Omega_u^2 \tilde{Q}_u + \sqrt{N_S} f(t) \quad \text{for } s \neq 0 \text{ and } s = u \neq 0,\quad (89)$$

$$M\ddot{\tilde{Q}}_s = -M\Omega_s^2 \tilde{Q}_s \quad \text{for } s \neq 0 \text{ and } s \neq u \neq 0.\quad (90)$$

The response to applied force with $u \neq 0$ is given by

$$R(t) = \left(\frac{N_S g}{M}\right) \int_0^t \frac{\sin \Omega_u(t-t') f(t')}{\Omega_u} dt'.\quad (91)$$
which becomes for sinusoidal force [Eq. (76)],

\[
R(t) = \left( \frac{N_S g}{M} \right) \left( \frac{\tilde{\Omega}_u \sin \omega t - \omega \sin \tilde{\Omega}_u t}{\tilde{\Omega}_u (\tilde{\Omega}_u^2 - \omega^2)} \right).
\] (92)

In the limit of \( c = 0.0 \), \( R(t) \) is given by Eqs. (91) and (92) with \( \tilde{\Omega}_u = \Omega_u \). The effect of finite coupling is realized by a change in \( \tilde{\Omega}_u \) as given by Eq. (33). Note that the response to applied force with \( u = 0 \) has been studied in subsection II D [Eq. (72)].
We present model calculations for sinusoidal forces with $\omega = 0.5$ and $g = 1.0$ in Eq. (76) for $N_S = 12$, $N_B = 100$, $K = B = M = m = \omega_0 = 1.0$. Figure 5 shows $R(t)/N_S$ for isolated systems ($c_0 = 0.0$) with $u = 0.0$, $-2.0$, $-4.0$ and $-6.0$. Magnitudes of $R(t)/N_S$ become smaller for larger $|u|$. Figure 6(a) and 6(b) show $R(t)/N_S$ for uniform ($u = 0.0$) and staggered forces ($u = -6.0$), respectively, with couplings of $c_0 = 0.0$ (dashed curve), $5.0$ (chain curve) and $10.0$ (solid curve). Comparing Fig. 6(b) with Fig. 6(a), we notice that an effect of couplings for staggered forces is less effective than that for uniform forces.

B. Spatial correlation

Employing eigenfrequencies for $f(t) = 0$ obtained in subsection II C, we may calculate the spatial correlation between $Q_k$ and $Q_{k+m}$,

$$\Gamma_m \equiv \sum_{k=1}^{N_S} \langle Q_k Q_{k+m} \rangle,$$

$$= \sum_{s=-N_S/2}^{N_S/2-1} \langle \tilde{Q}_s^* \tilde{Q}_s \rangle e^{-i2\pi ms/N_S},$$

with $\langle \tilde{Q}_s^* \tilde{Q}_s \rangle$ evaluated by

$$\langle \tilde{Q}_s^* \tilde{Q}_s \rangle = -\left(\frac{1}{\beta M \tilde{\Omega}_s}\right) \frac{\partial \ln Z_S}{\partial \tilde{\Omega}_s},$$

where the bracket $\langle \rangle$ denotes the average over $H$ and $Z_S$ is given by Eq. (46). $\Gamma_m$ with $m = 0$ expresses a (summed) variance of $Q_k$: $\Gamma_0 = \sum_{k=1}^{N_S} \langle Q_k^2 \rangle$. After some manipulations with the use of the diagonalized Hamiltonian given by Eq. (38), we obtain

$$\langle \tilde{Q}_s^* \tilde{Q}_s \rangle = \frac{\hbar}{2M \tilde{\Omega}_s} \coth \left(\frac{\beta \hbar \tilde{\Omega}_s}{2}\right)$$

for $s \neq 0$, (96)

$$= \frac{\hbar}{2M \tilde{\Omega}_0} \sum_{i=1}^{2} \coth \left(\frac{\beta \hbar \phi_i}{2}\right) \left(\frac{\partial \phi_i}{\partial \tilde{\Omega}_0}\right)$$

for $s = 0$, (97)

with

$$\frac{\partial \phi_1}{\partial \tilde{\Omega}_0} = \frac{\tilde{\Omega}_0}{2\phi_1} \left[ 1 + \frac{\tilde{\Omega}_0^2 - \omega_0^2}{\sqrt{(\tilde{\Omega}_0^2 - \omega_0^2)^2 + 4N_SN_Bc^2/Mm}} \right],$$

(98)

$$\frac{\partial \phi_2}{\partial \tilde{\Omega}_0} = \frac{\tilde{\Omega}_0}{2\phi_2} \left[ 1 - \frac{\tilde{\Omega}_0^2 - \omega_0^2}{\sqrt{(\tilde{\Omega}_0^2 - \omega_0^2)^2 + 4N_SN_Bc^2/Mm}} \right],$$

(99)
where \( \phi_1 \) and \( \phi_2 \) are given by Eqs. (10) and (11). Substituting Eqs. (96) and (97) into Eq. (??), we obtain \( \Gamma_m \),

\[
\Gamma_m = \sum_{s=-N_S/2}^{N_S/2-1} \frac{\hbar}{2M\Omega_s} \coth \left( \frac{\beta \hbar \Omega_s}{2} \right) e^{-i2\pi ms/N_s}
\]

\[
+ \frac{\hbar}{2M\Omega_0} \left[ 2 \sum_{i=1}^{2} \coth \left( \frac{\beta \hbar \phi_i}{2} \right) \left( \frac{\partial \phi_i}{\partial \Omega_i} \right) - \coth \left( \frac{\beta \hbar \Omega_0}{2} \right) \right].
\]

(100)

For \( T = 0 \) and \( T \to \infty \), \( \Gamma_m \) becomes

\[
\Gamma_m = \sum_{s=-N_S/2}^{N_S/2-1} \left( \frac{\hbar}{2M\Omega_s} \right) e^{-i2\pi ms/N_s} + \frac{\hbar}{2M\Omega_0} \left[ 2 \sum_{i=1}^{2} \left( \frac{\partial \phi_i}{\partial \Omega_i} \right) - 1 \right]
\]

(101)

\[
= \sum_{s=-N_S/2}^{N_S/2-1} \left( \frac{k_B T}{M\Omega_s^2} \right) e^{-i2\pi ms/N_s} + \frac{k_B T}{M\Omega_0} \left[ 2 \sum_{i=1}^{2} \frac{\partial \ln \phi_i}{\partial \Omega_i} - \frac{1}{\Omega_0} \right]
\]

(102)

for \( T \to \infty \).

In the case of uncoupled, isolated system with \( K = 0.0 \) and \( c = 0.0 \), \( \Gamma_m \) is given by

\[
\Gamma_m = \delta_{m0} \left( \frac{N_S \hbar}{2M\Omega_0} \right) \coth \left( \frac{\beta \hbar \Omega_0}{2} \right)
\]

(103)

which is proportional to \( N_S \) and which vanishes for \( m \geq 1 \). It is, however, not the case for \( K \neq 0.0 \) or \( c \neq 0.0 \). Indeed in the case of \( K \neq 0.0 \), \( \Gamma_m \) is finite for \( m \geq 1 \) because of direct particle-particle couplings of \( K \) and indirect couplings of \(-c_\ell e_\ell / m\bar{\omega}_m^2\) in the second term of Eq. (100). Even when \( K = 0.0 \), \( \Gamma_m \) with \( c \neq 0.0 \) remains finite with a small negative value.

Figure 7 shows the temperature dependence of \( \Gamma_m(T)/N_S \) for \( m = 0 \) (solid curve), 1 (dashed curve) and 2 (chain curve) of HO systems with \( N_S = 10, N_B = 100, K = D = M = m = \omega_0 = 1.0 \) and \( c_0 = 10.0 \). \( \Gamma_m(T) \) is finite at \( T = 0 \), and at \( T \to \infty \) it is proportional to temperature, as Eqs. (101) and (102) show. Magnitude of \( \Gamma_m \) is smaller for a larger \( m \). The dotted curve expresses \( C_0 \) \((= \langle \hat{Q}_s^2 \hat{Q}_0 \rangle)\) which is larger than \( \Gamma_0 \) because \( \Omega_0 < \Omega_s \) with \( s \neq 0 \).

\( N_S \) dependences of \( \Gamma_0(T)/N_S \) at \( k_B T/\hbar\omega_0 = 0.0 \) and 10.0 are shown in Fig. 8(a) and 8(b), respectively, for \( c_0 = 0.0 \) (open circles), 1.0 (filled square) and 10.0 (filled circles). For \( c_0 = 0.0 \), \( \Gamma_0(0) \) is proportional to \( N_S \) as expected. However, when the system-bath coupling is introduced, \( \Gamma_0 \) is not proportional to \( N_S \) as shown in Fig. 8. This is realized not only at zero temperature but also at high temperature.

Even when external forces are applied, the spatial correlation is not modified, which is the characteristics of the open system with the linear system-bath coupling. In the open system with the nonlinear system-bath coupling, the spatial correlation is modified by an applied force 26.
IV. CONCLUSION

Responses of open small quantum systems described by the \((N_S + N_B)\) model \[13, 14\] have been studied. By using double canonical transformations mentioned in subsections II B and II C, we obtain the diagonalized Hamiltonian, from which the response to applied forces is obtained with the use of Husimi’s method for a driven quantum HO \[21\]. The response to a uniform force given by Eq. (4) is generally not proportional to \(N_S\) against our implicit expectation. This nonlinear response is consistent with the system specific heat in open small quantum systems previously discussed in Ref. \[14\], and it is realized also in spatial correlation \(\Gamma_m\) not only at low temperatures but also at high temperatures. These facts show an importance of taking account of finite \(N_S\) in discussing open quantum and classical systems. It would be interesting to examine the obtained non-linearly by experiments for open small systems.
FIG. 8: (Color online) The $N_S$ dependence of $\Gamma_0(T)/N_S$ at (a) $k_B T/\hbar \omega_0 = 0.0$ and (b) $k_B T/\hbar \omega_0 = 10.0$ for $c_0 = 0.0$ (dashed curve), 1.0 (chain curve) and 10.0 (solid curve) of a HO system ($N_S = 10$, $N_B = 100$, $K = D = M = m = \omega_0 = 1.0$).
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[25] We may take into account the interaction in baths, adopting the bath Hamiltonian: \( H_B = \sum_{n=1}^{N_B} \left[ \frac{p_n^2}{2m} + \frac{k}{2}(q_n - q_{n+1})^2 \right] \) where \( k \) denotes a force constant between neighboring particles [14].

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