Energy Transport in the Integrable System in Contact with Various Types of Phonon Reservoirs

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(June 5, 2018)

We study how energy transport in an integrable system is affected by the spectral densities of heat reservoirs. The model investigated here is the quantum harmonic chain whose both ends are in contact with two heat reservoirs at different temperatures. The master equation for the reduced density matrix is derived on the assumption that the reservoirs are composed of an infinite number of independent harmonic oscillators. We evaluate temperature profile and energy flux in the stationary state for the master equation and discuss how they depend on the types of spectral densities. When we attach the reservoirs of the same type of spectral density, we find that the temperature profile is independent of the types. On the other hand, when the two reservoirs have different types of spectral densities, the energy profile near the ends of the chain depends on the types. When the coupling is finite, the temperature profile near the ends shows wide variation of behavior dependent on spectral densities and temperatures of reservoirs. This dependence is discussed with the Fokker-Planck equations obtained in the classical limit.

05.60.+w,05.30.-d,05.70.Ln

I. INTRODUCTION

Generally integrable systems show abnormal energy transport, namely the Fourier heat law is not realized there. This attributes to the lack of scattering between modes, which should be induced by nonintegrability. Two typical characteristics are seen in the energy transport in integrable systems. One is energy flux per unit volume independent of the system size. The other is a flat temperature profile with no global temperature gradient.

The harmonic chain is a typical integrable system which shows these characteristics [3–7]. Rieder, Lebowitz and Lieb (RLL) investigated the classical harmonic chain whose ends are in contact with heat reservoirs at different temperatures [3]. They exactly evaluated the covariance matrix of the variables in the stationary state using the Langevin equation, and they proved these characteristics. That is, they found that energy flux per volume is proportional to only temperature difference and is independent of the system size, and no global temperature gradient is formed. Although the temperature profile is flat in the internal region, they found the peculiar behavior in the vicinity of the ends of the chain. Namely, the local temperature is higher than the bulk value near the colder reservoir, and lower near the hotter reservoir.

Zürcher and Talkner (ZT) [4] investigated a quantum model corresponding to that of RLL with use of the quantum Langevin equation [5]. As for the bulk behavior, they found the same features as in the classical case. That is, no global temperature gradient is formed and energy flux is independent of system size. In the high temperature limit, the quantum Langevin equation is reduced to the Langevin equation with the Gaussian white noise and all the characteristics obtained in [3] are reproduced. However, temperature profile in the vicinity of the ends of the system shows some variety depending on temperature and a damping constant.

The reservoir employed in these studies is only the Ohmic type, which is one of the possible three types of heat reservoirs: sub-Ohmic, Ohmic, and super-Ohmic. Because integrable systems have no scattering between modes, their nonequilibrium behavior will be easily affected by the types of reservoirs at the boundary. Thus in this paper, we investigate how nonequilibrium nature in the harmonic chain depends on the types of reservoirs. Here we derive
the master equation for the reduced density matrix through the projection operator method on assumption that the
reservoir is composed of an infinite number of independent harmonic oscillators. This method is valid in the weak
coupling limit and for slow motion of the system because it treats the second order perturbation with respect to a
coupling constant and the Markovian approximation [3].

We investigate the effect of the spectral density on the temperature profile and energy flux in the quantum harmonic
chain in contact with two reservoirs applying the master equation for reduced density matrix. At the weak
coupling limit, the stationary state can be obtained analytically, and it is found that when the two reservoirs have the same
type of spectral density, the temperature profile is independent of it, and the profile is the same as the result previously
reported [9]. On the other hand, when the spectral densities are of different types, the temperature profile depends
on the types. Even in the classical limit, the internal temperature deviates from the mean value of the temperature of
the reservoirs and we observe a deviation of temperatures around ends from the temperature of internal region. The
direction of deviation is determined by frequency dependence of the spectral density near \( \omega = 0 \)

We also investigate the reduced density matrix with finite values of the coupling constant numerically. Although it
is derived in the perturbation of the coupling constant and it is only valid in the weak coupling limit, we dare regard
the master equation with a finite coupling constant as a model for a time evolution with a dissipation. In other words,
we assume that the time evolution qualitatively represents a kind of real phenomena in nature, where the coupling
constant represents the strength of the dissipative mechanism. We study qualitatively the dependence of temperature
profile on the types of reservoirs. It even has been reported in some cases that the reduced density matrix with a
finite coupling can produce a good long time behavior of the system in comparison with the exact path-integral result
not only qualitatively but also quantitatively [10].

Temperature profile at the ends of the chain is found to depend on the spectral density and the temperatures of
the reservoirs even when reservoirs at both ends have same type of spectral density. The dependence on the types of
the reservoirs is discussed in the Fokker-Planck equations in the classical limit.

This paper is organized as follows. In Sec. II, we derive the master equation for the reduced density matrix of
a general many body system in contact with a phonon reservoir. Sec. III is devoted to the investigation on energy
transport in the harmonic chain coupled to the phonon reservoirs at weak coupling limit. In Sec. VI, we consider the
case of finite coupling and investigate corresponding Fokker-Planck equations. Summary and discussions are given in
Sec. V.

II. THE PHONON RESERVOIR

A. Master equation for reduced density matrix

In this subsection, we derive the master equation for the reduced density matrix of a system in contact with a
phonon reservoir. Let us consider the following total Hamiltonian \( H_{\text{tot}} \),

\[
H_{\text{tot}} = H + H_{\text{int}} + H_R,
\]

where \( H \) denotes the Hamiltonian for the system of interest, \( H_R \) denotes the Hamiltonian for the reservoir, and \( H_{\text{int}} \)
describes the interaction between the system and the reservoir. We assume that the reservoir consists of an infinite
number of mutually independent harmonic oscillators [11–13], that is,

\[
H_R = \sum_\alpha \frac{p_\alpha^2}{2m_\alpha} + \frac{m_\alpha \omega_\alpha^2 x_\alpha^2}{2} = \sum_\alpha \hbar \omega_\alpha \left( b_\alpha^\dagger b_\alpha + \frac{1}{2} \right),
\]

where \( b_\alpha^\dagger \) and \( b_\alpha \) are the creation and annihilation operators for the \( \alpha \)th mode. We assume a linear coupling between
a Hermitian operator of the system \( X \) and reservoir’s operators in the form.

\[
H_{\text{int}} = \sum_\alpha \lambda \left( \frac{m_\alpha \omega_\alpha}{2} \right)^{1/2} \gamma_\alpha x_\alpha X + \lambda' \sum_\alpha \frac{\gamma_\alpha^2}{4\omega_\alpha} X^2
\]

\[
= \lambda \sqrt{N} \sum_\alpha \gamma_\alpha \left( b_\alpha^\dagger + b_\alpha \right) X + \lambda' \sum_\alpha \frac{\gamma_\alpha^2}{4\omega_\alpha} X^2 \quad (\lambda' \geq \lambda),
\]

where \( \lambda \) is a coupling constant and \( \gamma_\alpha \)'s and \( \lambda' \) are some constants. We put the second term in the right hand side in
order to make the total Hamiltonian to be bounded [14]. This term is regarded as a part of \( H' \):
\[ H \rightarrow H + X^2 \sum_{\alpha} \frac{\gamma^2_{\alpha}}{4\omega_{\alpha}} X. \]  

(2.4)

In this section, we do not make any assumption for the system, though we consider a harmonic chain for the system in the next section.

We derive the master equation for the reduced density matrix following the standard method \[9\]. We start from the quantum Liouville equation for the total system

\[
\frac{\partial \rho_{\text{tot}}(t)}{\partial t} = \frac{1}{i\hbar} [H_{\text{tot}}, \rho_{\text{tot}}(t)],
\]

(2.5)

where \( \rho_{\text{tot}}(t) \) is the density matrix for the total system. Under the condition that the reservoir is initially in the equilibrium state at inverse temperature \( \beta \), the degrees of freedom of the reservoir are traced out with the aid of projection operators. In order to obtain an equation which can be solved practically, we usually expand it up to the second order with respect to \( \lambda \) and also adopt the Markovian approximation, which is valid when correlations between reservoir’s variables are short-lived. As the result we obtain an equation for the reduced density matrix \( \rho(t) = \text{Tr}_R \rho_{\text{tot}}(t) \) (\( \text{Tr}_R \) means the trace concerning the reservoir’s degrees of freedom) of the form

\[
\frac{\partial}{\partial t} \rho(t) = \frac{1}{i\hbar} [H, \rho(t)] - \lambda^2 \Gamma \rho(t),
\]

(2.6)

where \( \Gamma \rho(t) \) is given by

\[
\Gamma \rho(t) = \frac{1}{\hbar^2} \int_0^\infty dt' \int_{-\infty}^{\infty} d\omega e^{i\omega t'} \Phi(\omega) \left\{ XX(-t')\rho(t) - e^{\beta \hbar \omega} X(t)X(-t')\rho(t)X - X(-t')\rho(t)X \right\}.
\]

(2.7)

In Eq. (2.7), \( X(-t') \) means the Heisenberg operator at time \(-t'\)

\[
X(-t') = e^{-iHt'/\hbar} X e^{iHt'/\hbar},
\]

(2.8)

and the function \( \Phi(\omega) \) denotes the Fourier transform of the two-point function of the reservoir’s operators coupling to \( X \), namely,

\[
\Phi(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} \Phi(t)dt,
\]

(2.9)

where \( \Phi(t) \) is given by

\[
\Phi(t) = \text{Tr}_R \left[ \sum_{\alpha,\alpha'} \frac{\gamma^2_{\alpha,\alpha'}}{2} \gamma_{\alpha,\alpha'}(0)X\alpha(t)e^{-\beta H_R} \right] / \text{Tr}_R e^{-\beta H_R} = \hbar \sum_{\alpha} \gamma^2_{\alpha} e^{i\omega_{\alpha} t} + \frac{e^{\beta \hbar \omega_{\alpha}} e^{-i\omega_{\alpha} t}}{e^{\beta \hbar \omega_{\alpha}} - 1}.
\]

(2.10)

Hence, denoting the reservoir’s density of states with respect to frequency \( \omega \) by \( D(\omega) \), we can write \( \Phi(\omega) \) as

\[
\Phi(\omega) = \hbar \gamma(\omega) \frac{D(\omega) - D(-\omega)}{e^{\beta \hbar \omega} - 1},
\]

(2.11)

where we introduced a smooth function \( \gamma(\omega) \) that satisfies \( \gamma(\pm \omega_{\alpha}) = \gamma_{\alpha} \). Here we define the spectral density \( I(\omega) \) as

\[
I(\omega) = \gamma(\omega)^2 D(\omega).
\]

(2.12)

The following form for the spectral density is considered in the literature,

\[
I(\omega) = I_0 \omega^n \theta(\omega),
\]

(2.13)

where \( \theta(\omega) \) is the step function: \( \theta(\omega) = 1 \) for \( \omega \geq 0 \) and \( \theta(\omega) = 0 \) for \( \omega < 0 \). The reservoir is called Ohmic if \( \alpha = 1 \), sub-Ohmic if \( \alpha < 1 \), and super-Ohmic if \( \alpha > 1 \).
In the following we rewrite Eq. (2.6) in a form convenient for later use. Let us consider the matrix components of operator $\Gamma \rho(t)$, $\langle k | \Gamma \rho(t) | n \rangle$, where $| k \rangle$ and $| n \rangle$ are eigenstates for the system Hamiltonian $H$ with energy eigenvalues $E_k$ and $E_n$, respectively. For the integral with respect to $t'$, we use the mathematical formula

$$\int_0^\infty e^{i\nu t'} dt' = \pi \delta(\nu) + \mathcal{P} \frac{i}{\nu}, \quad (2.14)$$

neglecting the principal value and the Kubo-Martin-Schwing er (KMS) condition $\Phi(\omega)e^{\beta \omega} = \Phi(-\omega)$. Then, the matrix components of operator $\Gamma \rho(t)$ is written as

$$\langle k | \Gamma \rho(t) | n \rangle = \frac{i}{\hbar} \sum_{l,m} \left[ X_{k,l}X_{l,m} \Phi \left( \frac{E_l - E_m}{\hbar} \right) \rho_{m,n}(t) - X_{k,l} \rho_{l,m}(t) X_{n,m}^* \Phi \left( \frac{E_n - E_m}{\hbar} \right) + \rho_{k,l} X_{m,l}^* \Phi \left( \frac{E_m - E_l}{\hbar} \right) X_{n,m} - \rho_{l,m}(t) X_{n,m} \right]. \quad (2.15)$$

Now we introduce the operator $R$ whose matrix elements are

$$\langle l | R | m \rangle = \frac{1}{\hbar} X_{l,m} \Phi \left( \frac{E_l - E_m}{\hbar} \right) = \frac{1}{\hbar} X_{l,m} \frac{I(E_l - E_m)}{e^{\beta(E_l - E_m)} - 1}. \quad (2.16)$$

Then $\Gamma \rho(t)$ is written in the following compact form,

$$\Gamma \rho(t) = \frac{i}{\hbar} \left( XR\rho(t) - R\rho(t)X - X\rho(t)R^\dagger + \rho(t)R^\dagger X \right) \quad (2.17)$$

Thus we arrive at the master equation of the form

$$\frac{\partial \rho(t)}{\partial t} = \frac{1}{i\hbar}[H, \rho(t)] - \frac{\pi \lambda^2}{\hbar} \left( [X, R\rho(t)] + [X, \rho(t)]^\dagger \right). \quad (2.18)$$

This is a generalized Lindblad form treating general many body system with the coupling form (2.3). When the system has many body interaction, the noncommutabilities cause the operator $R$ to contain all degrees of freedom of the system even if $H_{\text{int}}$ is a part of the system. Thus, in general $R$ has a complicated form with all degrees freedom of the system. Nevertheless, Eq. (2.16) gives the explicit and compact form of $R$ for the general systems when the reservoir is given by (2.2). Thus we can expect that the master equation (2.18) is widely applicable for the concrete studies of many body systems.

In the present study this master equation is used as a basic equation for a system coupled with the phonon reservoir. It is readily checked that Eq. (2.13) satisfies at least a necessary condition for the master equation, i.e., the canonical distribution $e^{-\beta H}/\text{Tr}(e^{-\beta H})$ into $\rho$ in Eq. (2.18) gives a stationary solution. We also expect the stability of the stationary solution at least when $\lambda$ is small enough.

**B. Comparison with the Quantum Langevin dynamics**

Here we briefly review another type of equation representing quantum dynamics with a thermal environment that is called a quantum Langevin equation which was used in previous studies and compare it with the master equation for reduced density matrix (2.18) (see also for other types of quantum Langevin equations we no not explain here).

The quantum Langevin equation was introduced by Ford, Kac, and Mazur. They considered the following coupled oscillators composed of $(2N + 1)$ particles,

$$H = \frac{1}{2} \sum_{n=-N}^{N} p_n^2 + \frac{1}{2} \sum_{m,n=-N}^{N} q_m A_{m,n} q_n, \quad (2.19)$$

where $q_n$ and $p_n$ are the $n$th canonical coordinate and momentum variable, respectively. The matrix $A = (A_{m,n})$ is a $(2N + 1) \times (2N + 1)$ symmetric matrix whose elements are
\[
A_{m,n} = \frac{1}{2N+1} \sum_{k=-N}^{N} \omega_k^2 \exp \left[ i \frac{2\pi k}{2N+1} (m-n) \right].
\] (2.20)

It should be noted that the eigenvalues of this matrix are \( \omega_s^2 \) \( (s = -N, -N+1, \cdots, N-1, N) \). The authors assumed that the initial state of the system \((2.19)\) is in equilibrium at a temperature, and examined under what condition the behavior of particle 0 can be described by a Langevin equation. They found the following. If the eigen-frequencies of the whole system, \( \omega_s \), have the special form
\[
\omega_s^2 = f^2 \tan^2 \left( \frac{\pi s}{2N+1} \right),
\] (2.21)
the motion of a particle of the system in the equilibrium state is described by
\[
\frac{\partial q_0(t)}{\partial t} = p_0, \quad (2.22a)
\]
\[
\frac{\partial p_0(t)}{\partial t} = -fp_0 + E(t), \quad (2.22b)
\]
where \( q_0, p_0 \) and \( E(t) \) are operators in the Heisenberg picture. The operator \( E(t) \) is described by operators of particles. In the equilibrium state, \( E(t) \) behaves like the Gaussian random force with vanishing mean \( \langle E(t) \rangle = 0 \), where \( \langle ... \rangle \) means \( \text{Tr} \{ \exp(-\beta H(\{q_i(0)\}, \{p_i(0)\})) \} / Z \). It also satisfies the commutation relation
\[
[E(t), E(s)] = 2i\hbar f \frac{\partial}{\partial t} \delta(t-s) \quad (2.23)
\]
and has the symmetrized correlation
\[
\frac{1}{2} \langle E(t)E(t+\tau) + E(t+\tau)E(t) \rangle = \frac{\hbar f}{\pi} \int_0^\infty \omega \coth \left( \frac{\beta \hbar \omega}{2} \right) \cos(\omega \tau) d\omega. \quad (2.24)
\]
This dynamics yields a classical Langevin equation with Gaussian white noise in the classical limit \( \hbar \rightarrow 0 \).

This dynamics has been applied to the quantum harmonic chain and investigated some quantum effects in energy transport phenomena \([4,7]\). However strictly speaking this quantum Langevin equation is the dynamics for a simple particle system in an equilibrium state. Therefore this dynamics is not consistent with a nonequilibrium dynamics for many body system in principle. The master equation for reduced density matrix \((2.18)\) is derived for general many body system on the assumption that only the reservoir is in equilibrium. Thus the master equation \((2.18)\) is more suitable in this context.

### III. ENERGY TRANSPORT IN THE QUANTUM HARMONIC CHAIN AT THE WEAK COUPLING LIMIT

In this section, we investigate energy transport in the quantum harmonic chain in contact with two phonon reservoirs at different temperatures with various types of spectral density of the thermal reservoir and examine what is common with and what is different from the results in the classical case \([3]\) and also the quantum case \([4]\) with the Ohmic spectral density. We first discuss the case of weak coupling limit.

#### A. System

Here we take the one-dimensional quantum harmonic chain,
\[
H = \sum_{n=1}^{N} \frac{p_n^2}{2m} + \sum_{n=0}^{N} m\omega_0^2 (x_{n+1} - x_n)^2,
\] (3.1)
as the system. This Hamiltonian should be considered to be the renormalized Hamiltonian including the second term in \((2.3)\). As in \([3]\), we impose the fixed boundary condition, \( x_0 = x_{N+1} = 0 \). By Fourier transformation:
and \( \lambda \) is coupled only to one reservoir. Even when the two different reservoirs are contact with the system, the decoupled respectively. Here operators \( u_k \) and \( v_k \) satisfy the commutation relations for canonical variables

\[
[u_k, v_{k'}] = i\hbar \delta_{k,k'} \quad \text{and} \quad [u_k, u_{k'}] = [v_k, v_{k'}] = 0, \tag{3.4}
\]

and introducing the creation and annihilation operators \( a_k^\dagger \) and \( a_k \) in the ordinary manner:

\[
a_k = \sqrt{\frac{m\omega_0 \sin(k/2)}{\hbar}} \left( u_k + \frac{iv_k}{2m\omega_0 \sin(k/2)} \right) \quad \text{and} \quad a_k^\dagger = \sqrt{\frac{m\omega_0 \sin(k/2)}{\hbar}} \left( u_k - \frac{iv_k}{2m\omega_0 \sin(k/2)} \right),
\]

we obtain

\[
H = \sum_k \hbar \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right). \tag{3.5}
\]

B. Equation of Motion of the System which Contacts with Two Different Reservoirs

In order to describe the system whose ends are attached to phonon reservoirs at different temperatures, we set dynamical model where the contacts with thermal baths are taking into account by the dissipation terms of the forms in Eq.(2.18). That is, variables at the left-end and right-end points \( x_1 \) and \( x_N \) are linearly coupled with one phonon reservoir at inverse temperature \( \beta_L \) and \( \beta_R \), respectively.

We assume that the coupling strength \( \lambda \) and the form of the coupling \( \gamma_\alpha \) in Eq. (2.3) are common for both the reservoirs. Then the master equation for the reduced density matrix is written as

\[
\frac{\partial}{\partial t} \rho(t) = \frac{1}{i\hbar} [H, \rho(t)] - \mu \Gamma_L \rho(t) - \mu \Gamma_R \rho(t), \tag{3.6}
\]

where \( \mu = \lambda^2 \). In principle the form of the dissipation terms of Eq. (2.18) is derived in the condition where the system is coupled only to one reservoir. Even when the two different reservoirs are contact with the system, the decoupled form of the dissipation term in (3.6) is valid in the order of \( \lambda^2 \). From (2.18) the damping terms \( \Gamma_L \rho(t) \) and \( \Gamma_R \rho(t) \) are

\[
\Gamma_L \rho(t) = \frac{\pi}{\hbar} \left\{ [x_1, R_L \rho(t)] + [x_1, R_L \rho(t)]^\dagger \right\} \quad \text{and} \quad \Gamma_R \rho(t) = \frac{\pi}{\hbar} \left\{ [x_N, R_R \rho(t)] + [x_N, R_R \rho(t)]^\dagger \right\},
\]

respectively. Here operators \( R_L \) and \( R_R \) are defined through the matrix elements

\[
|l \rangle R_L |m \rangle = \frac{I_L(E_l - E_m)}{e^{\beta_L(E_l - E_m)} - 1} |l \rangle |x_1 \rangle m \rangle, \tag{3.8a}
\]

\[
|l \rangle R_R |m \rangle = \frac{I_R(E_l - E_m)}{e^{\beta_R(E_l - E_m)} - 1} |l \rangle |x_N \rangle m \rangle, \tag{3.8b}
\]

and \( E_l \) denotes the energy eigenvalue for state \( |l \rangle \). \( I_L \) and \( I_R \) are the spectral density of the left and the right reservoir, respectively.

To solve this equation, we need to express the operators \( R_L \) and \( R_R \) in terms of \( a_k \) and \( a_k^\dagger \). The operators \( x_1 \) and \( x_N \) are written as

\[
x_1 = \sqrt{\frac{\hbar}{2(N+1)m\omega_0}} \sum_k \frac{\sin k}{\sqrt{\sin(k/2)}} \left( a_k + a_k^\dagger \right) \tag{3.9}
\]
and

\[ x_N = \sqrt{\frac{\hbar}{2(N+1)m\omega_0}} \sum_k \frac{\sin(Nk)}{\sin(k/2)} (a_k + a_k^\dagger). \]  \tag{3.10}

Let \( |n_k\rangle \) denote the eigenstate for the number operator \( a_k^\dagger a_k \) with the eigenvalue \( n_k \), namely \( a_k^\dagger a_k |n_k\rangle = n_k |n_k\rangle \). The eigenstates for the system Hamiltonian \( (3.5) \) are given by the direct product of number states \( |n_k\rangle \) as \( \{n_k\} = \prod_k |n_k\rangle \), whose energy eigenvalue is \( E(\{n_k\}) = \sum_k (n_k + \frac{1}{2}) \hbar \omega_k \).

The matrix elements of \( R_L \) are given in terms of the eigenstates \( \{n_k\} \) as,

\[
\langle \{n_{k'}\}|R_L|\{m_{k'}\} \rangle = \sqrt{\frac{\hbar}{2(N+1)m\omega_0}} \sum_k \frac{\sin k}{\sin(k/2)} \frac{I_L(E(\{n_{k'}\}) - E(\{m_{k'}\}))}{\exp \beta_L[E(\{n_{k'}\}) - E(\{m_{k'}\})] - 1} \times \left[ \langle \{n_{k'}\}|a_k|\{m_{k'}\} \rangle + \langle \{n_{k'}\}|a_k^\dagger|\{m_{k'}\} \rangle \right]. \tag{3.11}
\]

Now we note that

\[
\langle \{n_{k'}\}|a_k|\{m_{k'}\} \rangle \neq 0 \quad \text{only if} \quad n_{k'} = m_{k'} - \delta_{k',k} \quad \text{for} \quad \forall k', \tag{3.12}
\]

\[
\langle \{n_{k'}\}|a_k^\dagger|\{m_{k'}\} \rangle \neq 0 \quad \text{only if} \quad n_{k'} = m_{k'} + \delta_{k',k} \quad \text{for} \quad \forall k'. \tag{3.13}
\]

and \( I(\omega) = 0 \) for \( \omega < 0 \). Then Eq. (3.11) is transformed into

\[
\langle \{n_{k'}\}|R_L|\{m_{k'}\} \rangle = \sqrt{\frac{\hbar}{8(N+1)m\omega_0}} \sum_k \frac{\sin k}{\sin(k/2)} \frac{I_L(\omega_k)}{\sin(\beta_L \hbar \omega_k/2)} \left( e^{\beta_L \hbar \omega_k/2} a_k + e^{-\beta_L \hbar \omega_k/2} a_k^\dagger \right) \langle \{n_{k'}\}|a_k|\{m_{k'}\} \rangle. \tag{3.14}
\]

Thus the operator \( R_L \) can be represented as

\[
R_L = \sqrt{\frac{\hbar}{8(N+1)m\omega_0}} \sum_k \frac{\sin k}{\sin(k/2)} \frac{I_L(\omega_k)}{\sin(\beta_L \hbar \omega_k/2)} \left( e^{\beta_L \hbar \omega_k/2} a_k + e^{-\beta_L \hbar \omega_k/2} a_k^\dagger \right). \tag{3.15}
\]

In the same manner, the operator \( R_R \) is represented as

\[
R_R = \sqrt{\frac{\hbar}{8(N+1)m\omega_0}} \sum_k \frac{\sin(Nk)}{\sin(k/2)} \frac{I_R(\omega_k)}{\sin(\beta_R \hbar \omega_k/2)} \left( e^{\beta_R \hbar \omega_k/2} a_k + e^{-\beta_R \hbar \omega_k/2} a_k^\dagger \right). \tag{3.16}
\]

C. Moments in the Stationary State

As will be shown later, to evaluate mean kinetic energy of a particle and energy flux in the stationary state, we have only to calculate the second moments

\[
\langle a_k a_{k'} \rangle = \text{Tr}(a_k a_{k'} \rho_{\text{st}}) \tag{3.17}
\]

and

\[
\langle a_k^\dagger a_{k'} \rangle = \text{Tr}(a_k^\dagger a_{k'} \rho_{\text{st}}), \tag{3.18}
\]

where \( \rho_{\text{st}} \) denotes the stationary solution of Eq. (3.6). First, we consider Eq. (3.17). Because the left hand side of Eq. (3.6) vanishes in the stationary state, we obtain

\[
\frac{1}{\hbar} \text{Tr} (a_k a_{k'} [H, \rho]) - \frac{\pi \mu}{\hbar} \left[ \text{Tr} (a_k a_{k'} [x_1, R_L \rho_{\text{st}}]) + \text{Tr} \left( a_k a_{k'} [x_1, R_L \rho_{\text{st}}]^\dagger \right) \right] - \frac{\pi \mu}{\hbar} \left[ \text{Tr} (a_k a_{k'} [x_N, R_R \rho]) + \text{Tr} \left( a_k a_{k'} [x_N, R_R \rho]^\dagger \right) \right] = 0. \tag{3.19}
\]
This equation is rewritten as follows after tedious but straightforward calculations,

\[
i(\omega_k + \omega_{k'})\langle a_k a_{k'} \rangle + \frac{\pi \mu}{4(N+1)m_\omega} \sum_{k_1} \frac{\sin k_1}{\sqrt{\sin(k_1/2) \sinh(\beta_r \hbar \omega_{k_1}/2)}} I_L(\omega_{k_1}) \\
\times \left\{ \frac{\sin k'}{\sqrt{\sin(k'/2)}} \left[ e^{\beta_l \hbar \omega_{k_1}/2}(\langle a_k a_{k_1} \rangle - \langle a_{k_1} a_k \rangle) + e^{-\beta_l \hbar \omega_{k_1}/2}(\langle a_{k_1} a_k \rangle - \langle a_k a_{k_1} \rangle) \right] \\
+ \frac{\sin k}{\sqrt{\sin(k/2)}} \left[ e^{\beta_l \hbar \omega_{k_1}/2}(\langle a_{k_1} a_{k'} \rangle - \langle a_{k'} a_{k_1} \rangle) + e^{-\beta_l \hbar \omega_{k_1}/2}(\langle a_{k} a_{k'} \rangle - \langle a_{k'} a_k \rangle) \right] \right\} \\
+ \frac{\pi \mu}{4(N+1)m_\omega} \sum_{k_1} \frac{\sin(Nk_1)}{\sqrt{\sin(k_1/2) \sinh(\beta_R \hbar \omega_{k_1}/2)}} I_R(\omega_{k_1}) \\
\times \left\{ \frac{\sin(Nk')}{\sqrt{\sin(k'/2)}} \left[ e^{\beta_l \hbar \omega_{k_1}/2}(\langle a_k a_{k_1} \rangle - \langle a_{k_1} a_k \rangle) + e^{-\beta_l \hbar \omega_{k_1}/2}(\langle a_{k_1} a_k \rangle - \langle a_k a_{k_1} \rangle) \right] \\
+ \frac{\sin(Nk)}{\sqrt{\sin(k/2)}} \left[ e^{\beta_l \hbar \omega_{k_1}/2}(\langle a_{k_1} a_{k'} \rangle - \langle a_{k'} a_{k_1} \rangle) + e^{-\beta_l \hbar \omega_{k_1}/2}(\langle a_{k} a_{k'} \rangle - \langle a_{k'} a_k \rangle) \right] \right\} \\
= 0.
\] (3.20)

In the same way, Eq. (3.18) is also transformed into

\[
i(\omega_{k'} - \omega_k)\langle a_{k'} a_k \rangle + \frac{\pi \mu}{4(N+1)m_\omega} \sum_{k_1} \frac{\sin k_1}{\sqrt{\sin(k_1/2) \sinh(\beta_l \hbar \omega_{k_1}/2)}} I_L(\omega_{k_1}) \\
\times \left\{ \frac{\sin k}{\sqrt{\sin(k/2)}} \left[ e^{\beta_l \hbar \omega_{k_1}/2}(\langle a_k a_{k_{1'}} \rangle - \langle a_{k_{1'}} a_k \rangle) + e^{-\beta_l \hbar \omega_{k_1}/2}(\langle a_{k} a_{k_{1'}} \rangle - \langle a_{k_{1'}} a_k \rangle) \right] \\
+ \frac{\sin k'}{\sqrt{\sin(k'/2)}} \left[ e^{\beta_l \hbar \omega_{k_1}/2}(\langle a_{k_{1'}} a_k \rangle - \langle a_k a_{k_{1'}} \rangle) + e^{-\beta_l \hbar \omega_{k_1}/2}(\langle a_{k_{1'}} a_k \rangle - \langle a_k a_{k_{1'}} \rangle) \right] \right\} \\
+ \frac{\pi \mu}{4(N+1)m_\omega} \sum_{k_1} \frac{\sin(Nk_1)}{\sqrt{\sin(k_1/2) \sinh(\beta_R \hbar \omega_{k_1}/2)}} I_R(\omega_{k_1}) \\
\times \left\{ \frac{\sin(Nk')}{\sqrt{\sin(k'/2)}} \left[ e^{\beta_l \hbar \omega_{k_1}/2}(\langle a_k a_{k_{1'}} \rangle - \langle a_{k_{1'}} a_k \rangle) + e^{-\beta_l \hbar \omega_{k_1}/2}(\langle a_{k} a_{k_{1'}} \rangle - \langle a_{k_{1'}} a_k \rangle) \right] \\
+ \frac{\sin(Nk)}{\sqrt{\sin(k/2)}} \left[ e^{\beta_l \hbar \omega_{k_1}/2}(\langle a_{k_{1'}} a_k \rangle - \langle a_k a_{k_{1'}} \rangle) + e^{-\beta_l \hbar \omega_{k_1}/2}(\langle a_{k_{1'}} a_k \rangle - \langle a_k a_{k_{1'}} \rangle) \right] \right\} \\
= 0.
\] (3.21)

### D. Total Energy $E_{\text{tot}}$

We will solve these equations by perturbation. Expanding $\langle a_k a_{k'} \rangle$ and $\langle a_{k'} a_k \rangle$ with respect to $\mu$,

\[
\langle a_k a_{k'} \rangle = \langle a_k a_{k'} \rangle_0 + \mu \langle a_k a_{k'} \rangle_1 + \mu^2 \langle a_k a_{k'} \rangle_2 + \cdots,
\]

\[
\langle a_{k'} a_k \rangle = \langle a_{k'} a_k \rangle_0 + \mu \langle a_{k'} a_k \rangle_1 + \mu^2 \langle a_{k'} a_k \rangle_2 + \cdots,
\]

\[
\langle a_k a_{k'} \rangle = \langle a_k a_{k'} \rangle_0 + \mu \langle a_k a_{k'} \rangle_1 + \mu^2 \langle a_k a_{k'} \rangle_2 + \cdots,
\]

\[
\langle a_{k'} a_k \rangle = \langle a_{k'} a_k \rangle_0 + \mu \langle a_{k'} a_k \rangle_1 + \mu^2 \langle a_{k'} a_k \rangle_2 + \cdots.
\]

We consider the relation of each order of $\mu$. Using the commutation relations,

\[
\langle a_k a_{k'} \rangle_n = \langle a_{k'} a_k \rangle_n,
\]

\[
\langle a_{k'} a_k \rangle_n = \langle a_k a_{k'} \rangle_n + \delta_{n,0}\delta_{k,k'}.
\]

(3.26)
we obtain the following relations at the zeroth order,
\[(\omega_k + \omega_{k'})\langle a_k a_{k'}^\dagger\rangle_0 = 0 \quad \text{and} \quad (\omega_{k'} - \omega_k)\langle a_k^\dagger a_{k'}\rangle_0 = 0. \tag{3.27}\]
Accordingly we have for all \(k\) and \(k'\)
\[\langle a_k a_{k'}\rangle_0 = 0, \tag{3.28}\]
and for \(k \neq k'\)
\[\langle a_k^\dagger a_{k'}\rangle_0 = 0. \tag{3.29}\]
Putting \(k = k'\) in the first order equation of \(\mu\), we have
\[
\frac{\sin^2 k I_L(\omega_k)}{\sinh(\beta_L \hbar \omega_k/2)} \left( e^{\beta_L \hbar \omega_k/2} \langle a_k^\dagger a_k\rangle_0 - e^{-\beta_L \hbar \omega_k/2} \langle a_k a_k^\dagger\rangle_0 \right) \\
+ \frac{\sin^2(Nk) I_R(\omega_k)}{\sinh(\beta_R \hbar \omega_k/2)} \left( e^{\beta_R \hbar \omega_k/2} \langle a_k^\dagger a_k\rangle_0 - e^{-\beta_R \hbar \omega_k/2} \langle a_k a_k^\dagger\rangle_0 \right) = 0. \tag{3.30}\]
Since \(\sin^2 k = \sin^2(Nk) \neq 0\), Eq. (3.30) leads to
\[\langle a_k^\dagger a_k\rangle_0 = \frac{1}{I_L(\omega_k) + I_R(\omega_k)} \left[ \frac{I_L(\omega_k)}{e^{\beta_L \hbar \omega_k} - 1} + \frac{I_R(\omega_k)}{e^{\beta_R \hbar \omega_k} - 1} \right]. \tag{3.31}\]
Here the energy of the system is,
\[E_{st} = \text{Tr} (H \rho_{st}) = \sum_k \frac{\hbar \omega_k}{I_L(\omega_k) + I_R(\omega_k)} \left[ \frac{I_L(\omega_k)}{e^{\beta_L \hbar \omega_k} - 1} + \frac{I_R(\omega_k)}{e^{\beta_R \hbar \omega_k} - 1} \right]. \tag{3.32}\]
In particular, when \(I_L(\omega_k) = I_R(\omega_k)\), we find that \(E_{st}\) is the arithmetic mean between equilibrium energy at inverse temperature \(\beta_L\) and at \(\beta_R\) regardless of the types of the spectral density, i.e.
\[E_{st} = \frac{1}{2} \left[ \frac{\text{Tr} (He^{-\beta_L H})}{\text{Tr} e^{-\beta_L H}} + \frac{\text{Tr} (He^{-\beta_R H})}{\text{Tr} e^{-\beta_R H}} \right]. \tag{3.33}\]

**E. Kinetic Energy of a Particle and Energy Flux**

Here we compute mean kinetic energy of each particle and energy flux up to the first order with respect to \(\mu\). The mean kinetic energy of the \(n\)th particle, \(\varepsilon_n\) is defined by
\[\varepsilon_n = \left\langle \frac{\vec{p}_n^2}{2m} \right\rangle = \text{Tr} \left( \frac{\vec{p}_n^2}{2m} \rho_{st} \right), \tag{3.34}\]
which is expressed in terms of the creation and annihilation operators as
\[\varepsilon_n = \frac{-\hbar \omega_0}{N + 1} \sum_{k,k'} \sqrt{\sin(k/2) \sin(k'/2) \sin(kn) \sin(k'n)} \\
\times \left( \langle a_k a_{k'}\rangle - \langle a_k^\dagger a_{k'}\rangle - \langle a_k a_{k'}^\dagger\rangle + \langle a_k^\dagger a_{k'}\rangle \right). \tag{3.35}\]
Substituting the results obtained in the last subsection into the above equation, we have
\[\varepsilon_n = \frac{-\hbar \omega_0}{N + 1} \sum_k \sin(k/2) \sin^2 (kn) \left( 2\langle a_k^\dagger a_k\rangle_0 + 1 \right) \\
= \frac{-\hbar \omega_0}{N + 1} \sum_k \sin(k/2) \sin^2 (kn) \left[ \frac{2}{I_L(\omega_k) + I_R(\omega_k)} \left( \frac{I_L(\omega_k)}{e^{\beta_L \hbar \omega_k} - 1} + \frac{I_R(\omega_k)}{e^{\beta_R \hbar \omega_k} - 1} \right) + 1 \right]. \tag{3.36}\]
In the classical limit, Eq. (3.36) becomes
\[
2\varepsilon_n = \frac{2T_L}{\pi} \int_0^{\pi} dk \sin^2(kn) \frac{I_L(\omega_k)}{I_L(\omega_k) + I_R(\omega_k)} + \frac{2T_R}{\pi} \int_0^{\pi} dk \sin^2(kn) \frac{I_R(\omega_k)}{I_L(\omega_k) + I_R(\omega_k)},
\] (3.37)
where \(T_L = \beta_L^{-1}\) and \(T_R = \beta_R^{-1}\) are the temperature values of the left reservoir and the right reservoir, respectively. In the classical limit, \(2\varepsilon_n\) can be interpreted as the temperature at site \(n\). Especially when both the reservoirs are of the same type, namely, \(I_L(\omega_k) = I_R(\omega_k)\), we have \(2\varepsilon_n = \frac{T_L + T_R}{2}\) regardless of the types of the spectral density. This means completely flat temperature profile, which was originally found by RLL when the both reservoirs are of the Ohmic type \[\text{[3]}\]. On the other hand, Eq. (3.37) shows that the temperature profile in integrable systems can be easily changed by controlling the combination of the types of spectral density of reservoirs, so that in the case of \(I_L(\omega_k) \neq I_R(\omega_k)\), the internal temperature deviates from \(\frac{T_L + T_R}{2}\) in the classical limit.

We numerically estimate (3.36) to investigate the general feature of temperature profile for various combinations of spectral densities. We present typical temperature profiles in Fig.1. In Fig.1(a) we take the sub-Ohmic type reservoir \(I_L = \omega^{0.5}\) for left side, and the super-Ohmic one \(I_R = \omega^{1.5}\) for the right side. In Fig.1(b), the converse case, namely, \(I_L = \omega^{1.5}\) and \(I_R = \omega^{0.5}\) is considered. In both the cases, parameters are set to \(m = \hbar = \omega_0 = 1.0,\) and \(T_L = 200.0, T_R = 50.0\). As is known from these figures, temperature deviates from the internal temperature value in the same direction in the vicinity of both the ends. As the result the deviated temperature values become close to the temperature of the reservoir whose spectral density has larger power. We numerically confirmed this dependence for many sets of spectral densities \((I_L, I_R)\) and temperatures \((T_L, T_R)\) including low temperatures.

Energy flux is defined via the equation of continuity. From the master equation (3.6), time derivative for the energy of the system satisfies
\[
\frac{\partial}{\partial t} \text{Tr} (H \rho(t)) = -\text{Tr} (\mu HT_L \rho(t)) - \text{Tr} (\mu HT_R \rho(t)).
\] (3.38)
The first term in the right-hand side is regarded as incoming energy flux from the left reservoir and the second term incoming energy flux from the right reservoir. We call the former \(J_L^t\) and the latter \(J_R^t\). In the stationary state, of course \(J_L^t + J_R^t = 0\) must hold. We can calculate \(J_L^t\) as follows,
\[
J_L^t = -\frac{\pi \hbar \mu}{m} \text{Tr} \left( H [x_1, R_L \rho] + H [x_1, R_L \rho]^\dagger \right) = \frac{\pi \hbar \mu}{(N + 1)m} \sum_k \frac{I_L(\omega_k)I_R(\omega_k)}{I_L(\omega_k) + I_R(\omega_k)} \left( \frac{1}{e^{\beta_L \hbar \omega_k} - 1} - \frac{1}{e^{\beta_R \hbar \omega_k} - 1} \right).
\] (3.39)
If \(N \gg 1\), we can replace the summation by an integral and obtain
\[
J_L^t = \frac{\hbar \mu}{m} \int_0^{\pi} \frac{I_L(\omega_k)I_R(\omega_k)}{I_L(\omega_k) + I_R(\omega_k)} \sin^2 k \left( \frac{1}{e^{\beta_L \hbar \omega_k} - 1} - \frac{1}{e^{\beta_R \hbar \omega_k} - 1} \right) dk.
\] (3.40)
In the classical limit \((h \rightarrow 0)\), \(J_L^t\) goes to
\[
J_L^c = \mu C (T_L - T_R),
\] (3.41)
where
\[
C = \frac{1}{m \omega_0} \int_0^{\pi} \sin^2 k \frac{I_L(2\omega_0 \sin(k/2))I_R(2\omega_0 \sin(k/2))}{\sin(k/2) I_L(2\omega_0 \sin(k/2)) + I_R(2\omega_0 \sin(k/2))} dk.
\] (3.42)
Thus in the classical limit, energy flux is proportional to the temperature difference and independent of the system size regardless of the types and the combinations of the spectral densities of reservoirs.

**IV. Finite Coupling**

The master equation (2.18) is justified only in \(O(\mu)\). However when we study the model with a finite coupling constant, the quantitative effect of a finite coupling inevitably deviates from those of the original model. Nevertheless, time evolution of the reduced density matrix has been regarded as describing a variety of relaxation processes, and it successfully explained a variety of interesting phenomena in real systems \[\text{[7,19]}\]. This shows that the master equation
can well approximate the dynamics in real dissipative system at least qualitatively. In some case the time evolution of reduced density matrix with a finite coupling reproduces quantitatively correct results even for long time \([10]\).

Thus we investigate here the effect of finite coupling which is a small but finite value, and discuss the behavior of temperature profile qualitatively. In this section, we confine ourselves to the case of the same spectral density at both ends, namely

\[ I_L = I_R = I. \]  

(A. Temperature Profile)

We evaluate contributions from higher-order terms and find deviations from the flat temperature profile near the ends of the chain. We first calculate the first-order coefficients. From the first-order equations in \((3.20)\) and \((3.21)\), we have for all \(k\) and \(k'\)

\[
\langle a_L a_{k'} \rangle_1 = \frac{i\pi [\sin k \sin k' - \sin(Nk) \sin(Nk')]}{4(N+1)m\omega_0(\omega_k + \omega_{k'}) \sin(k/2) \sin(k'/2)} \times [I(\omega_k) (n_L(\omega_k) - n_R(\omega_k)) + I(\omega_{k'}) (n_L(\omega_{k'}) - n_R(\omega_{k'}))],
\]

and for \(k \neq k'\)

\[
\langle a_L^\dagger a_{k'} \rangle_1 = \frac{i\pi [\sin k \sin k' - \sin(Nk) \sin(Nk')]}{4(N+1)m\omega_0(\omega_k - \omega_{k'}) \sin(k/2) \sin(k'/2)} \times [I(\omega_k) (n_L(\omega_k) - n_R(\omega_k)) + I(\omega_{k'}) (n_L(\omega_{k'}) - n_R(\omega_{k'}))],
\]

where \(n_L(\omega)\) is the Bose-Einstein distribution functions at an inverse temperature \(\beta_L\)

\[
n_L(\omega) = \frac{1}{e^{\beta_L \hbar \omega} - 1},
\]

and \(n_R(\omega)\) is that at \(\beta_R\)

\[
n_R(\omega) = \frac{1}{e^{\beta_R \hbar \omega} - 1}.
\]

Equations \((3.20)\) and \((3.21)\) imply that the first-order coefficients must be pure imaginary. On the other hand, \(\langle a_L^\dagger a_{k'} \rangle_1\) must be real at the same time. Thus, we have

\[
\langle a_L^\dagger a_{k'} \rangle_1 = 0.
\]

From Eqs. \((3.20)\) and \((3.21)\), it turns out that if \(n \geq 1\) the \((n+1)\)st-order terms are computed via the following equations from the \(n\)th order terms; For all \(k\) and \(k'\),

\[
\langle a_k a_{k'} \rangle_{n+1} = \frac{i\pi}{2(N+1)m\omega_0(\omega_k + \omega_{k'})} \sum_{k_1} I(\omega_{k_1}) \times \left[ \frac{\sin k_1 \sin k + \sin(Nk_1) \sin(Nk')}{\sin(k_1/2) \sin(k'/2)} \left( \langle a_k a_{k_1} \rangle_n - \langle a_k^\dagger a_{k_1} \rangle_n \right) + \frac{\sin k_1 \sin k - \sin(Nk_1) \sin(Nk)}{\sin(k_1/2) \sin(k/2)} \left( \langle a_{k'} a_{k_1} \rangle_n - \langle a_{k'}^\dagger a_{k_1} \rangle_n \right) \right].
\]

If \(k \neq k'\),

\[
\langle a_k^\dagger a_{k'} \rangle_{n+1} = \frac{i\pi}{2(N+1)m\omega_0(\omega_k - \omega_{k'})} \sum_{k_1} I(\omega_{k_1}) \times \left[ \frac{\sin k_1 \sin k' + \sin(Nk_1) \sin(Nk')}{\sin(k_1/2) \sin(k'/2)} \left( \langle a_k^\dagger a_{k_1} \rangle_n - \langle a_k a_{k_1} \rangle_n^* \right) + \frac{\sin k_1 \sin k - \sin(Nk_1) \sin(Nk)}{\sin(k_1/2) \sin(k/2)} \left( \langle a_{k'}^\dagger a_{k_1} \rangle_n - \langle a_{k'} a_{k_1} \rangle_n \right) \right],
\]

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and \( \langle a_k^\dagger a_k \rangle_{n+1} \) is computed through the other coefficients of the same order as

\[
\langle a_k^\dagger a_k \rangle_{n+1} = \frac{1}{2} \left( \langle a_k a_k \rangle_{n+1} + \langle a_k a_k \rangle_{n+1}^* \right)
- \frac{\sqrt{\sin(k/2)}}{4I(\omega_k) \sin^2 k} \sum_{k' \neq k} \frac{\sin(k' \sin k + \sin(Nk') \sin(Nk))}{\sqrt{\sin(k'/2)}} I(\omega_{k'})
\times \left( \langle a_k^\dagger a_k \rangle_{n+1} + \langle a_k^\dagger a_k \rangle_{n+1}^* - \langle a_k a_k \rangle_{n+1} + \langle a_k a_k \rangle_{n+1}^* \right).
\]

(4.9)

Because the above equations contain the spectral density, we have to specify its functional form. As has given in [2, 13], we employ the following form for the spectral density

\[
I(\omega) = I_0 \omega^\alpha.
\]

(4.10)

For \( \alpha = 1.0 \) and \( \alpha = 1.5 \), we have computed mean kinetic energy of the \( n \)th particle \( \varepsilon_n \) up to the 20th order, where quantities [3.23, 1.23] seem to converge. For each \( \alpha \), the following sets of temperatures of for the reservoirs are chosen: (a) \( T_L = 200.0 \) and \( T_R = 50.0 \), (b) \( T_L = 10.0 \) and \( T_R = 0.1 \) and (c) \( T_L = 0.1 \) and \( T_R = 0.02 \). These choices of parameters are the same as used in [4] by ZT. Other parameters are commonly set as \( m = \omega_0 = \hbar = 1.0 \), \( \mu = 0.1 \), and \( I_0 = 1/\pi \). In the equilibrium state at inverse temperature \( \beta \), \( \varepsilon_n \) is given by

\[
\varepsilon_n = \phi_n(\beta) = \frac{\hbar \omega_0}{N+1} \sum_{l=1}^{N} \sin \frac{\pi l}{2(N+1)} \sin^2 \frac{\pi n}{N+1} \coth \left( \beta \hbar \omega_0 \sin \frac{\pi l}{2(N+1)} \right),
\]

(4.11)

and thus the local temperatures \( T_n \) is defined by the above function, i.e. \( T_n = 1/\phi_n^{-1}(\varepsilon_n) \).

In fig.2 and 3, \( \{T_n\} \) are plotted for \( \alpha = 1.0 \) and 1.5, respectively. All the figures show that higher-order contributions are small except near the ends of the chain. In other words, the bulk behavior is unchanged, where the temperature profile near the ends of the chain exhibits various dependencies on the details of the parameters \( (T_L, T_R, \alpha) \). When the reservoirs are Ohmic, the temperature profile near the ends are similar to those obtained by ZT with the quantum Langevin approach.

When the reservoirs are Ohmic and temperature is high (Fig. 2(a)), temperature drops near the left end which contacts with the hotter reservoir and rises near the other end contacting with the colder reservoir. This is the same paradoxical behavior as found by RLL and also observed by ZT. Such behavior disappear when the reservoirs are super-Ohmic (Fig. 3(a)). The second particles from the ends shows monotonic temperature variation. Figure 2 (c) and Fig. 3 (c) exhibit temperature profile when the temperatures are low where quantum effects are important. These two figures almost coincide. In both cases, temperatures near the ends are high which should be due to the quantum fluctuations. We may say that differences in the spectral densities does not affect the temperature profile at low temperatures. In the medium temperature cases, Fig. 2 (b) and Fig. 3 (b), mixed behavior of the classical and quantum features are observed. (See also the figures in reference [3]).

For \( T_L = 200.0 \) and \( T_R = 50.0 \), temperature deviations of the particle 2 and the particle \( (N-1) \) from the mean internal temperature are plotted in Fig. 4 for various \( \alpha \). There we find that the peculiarity, i.e. inversion of temperature near the ends, is observed in the sub-Ohmic and Ohmic cases, while it disappears when \( \alpha \geq \alpha_c (\approx 1.04) \).

**B. Fokker-Planck Equation in the Classical Limit**

In the previous subsection, the temperature profiles is found to depend on values of \( \alpha \). In particular, the peculiarity found by RLL [3] disappears in the super-Ohmic regime. Since the differences are seen at high temperatures, some characteristics depending to the values \( \alpha \) must appear in the Fokker-Planck equation obtained from the master equation in the classical limit. Actually, we will find that the diffusion term in the Fokker-Planck equation takes a different form from that derived from the Langevin equation except the Ohmic case. In order to study the difference in relaxation at the contacting point, we investigate the Fokker-Planck equation for a system with a single reservoir.

When a heat reservoir is attached to the left end of the chain, the classical Langevin equations for canonical variables \( x_n(t) \) and \( p_n(t) \), \( n = 1, 2, ..., N \) are

\[
\frac{\partial x_n}{\partial t} = \{x_n, H\}
\]

(4.12)

\[
\frac{\partial p_n}{\partial t} = \{p_n, H\} - \delta_{n,1} \nu p_n + \delta_{n,1} \xi(t)
\]

(4.13)
where $\{-,\}$ means the Poisson bracket. The correlation function of the Gaussian white random force $\xi(t)$ is connected with the damping constant $\nu$ and the temperature at the first particle $\beta$ via the fluctuation-dissipation theorem as

$$\langle \xi(t)\xi(t') \rangle = \frac{2\nu}{\beta}\delta(t-t').$$  \hfill (4.14)

As is well known, the Langevin equations are equivalent to the Fokker-Planck equation

$$\frac{\partial P(t)}{\partial t} = \{H, P(t)\} + \nu \frac{\partial}{\partial p_1} \left( p_1 \frac{1}{m} + \beta^{-1} \frac{\partial}{\partial p_1} \right) P(t),$$  \hfill (4.15)

where $P(t)$ is the distribution function on the phase space.

We now turn to our master equation. Inserting the representation for operator $R_L$ into the master equation $[3.15]$, we have

$$\frac{\partial \rho(t)}{\partial t} = \frac{1}{i\hbar}[H, \rho(t)] - \frac{\pi \mu}{\sqrt{8(N+1)m\hbar\omega_0}} \sum_k \frac{\sin k}{\sin(k/2) \sinh(\beta\hbar\omega_k/2)} I(\omega_k)$$

$$\times \left\{ [x_1, (e^{\beta\hbar\omega_k/2}a_k + e^{-\beta\hbar\omega_k/2}a_k^\dagger) \rho(t)] - [x_1, \rho(t)] \left( e^{\beta\hbar\omega_k/2}a_k^\dagger + e^{-\beta\hbar\omega_k/2}a_k \right) \right\},$$

where we omitted suffix L. Expressing the creation and annihilation operators by the position and momentum operators,

$$\frac{\partial \rho(t)}{\partial t} = \frac{1}{i\hbar}[H, \rho(t)]$$

$$- \frac{\pi \mu}{(N+1)\hbar} \sum_{k,n} I(\omega_k) \sin k \sin(kn) \left\{ \coth \left( \frac{\beta\hbar\omega_k}{2} \right) [x_n, [x_1, \rho(t)]] \right\}$$

$$+ \frac{i}{2m\omega_0 \sin(k/2)} \left( p_n [x_1, \rho(t)] + [x_1, \rho(t)] p_n + 2[x_1, p_n, \rho(t)] \right).$$  \hfill (4.17)

In the classical limit, the density matrix $\rho(t)$ is replaced by the distribution function $P(t)$ Therefore, Eq. (4.17) is transformed into

$$\frac{\partial P(t)}{\partial t} = \{H, P(t)\} + \sum_{n=1}^N C_n \frac{\partial}{\partial p_n} \left( \frac{p_n}{m} + \beta^{-1} \frac{\partial}{\partial p_n} \right) P(t),$$  \hfill (4.18)

where

$$C_n = \frac{2\mu}{\omega_0} \int_0^\pi I(2\omega_0 \sin(k/2)) \cos(k/2) \sin(kn) dk,$$  \hfill (4.19)

The time-evolution equation for the covariance matrix derived from Eq. (4.18) is also confirmed to agree with the classical limit of the corresponding quantum equation.

When the reservoir is Ohmic, namely $I(\omega) = I_0\omega$, the coefficients $C_n$ are evaluated as

$$C_n = \pi \mu I_0 \delta_{n,1},$$  \hfill (4.20)

and Eq. (4.18) agrees with the Fokker-Planck equation derived from the Langevin equation (4.13). In this case, the two-point function (2.11) tends to the delta function in the classical limit

$$\lim_{h \to 0} \Phi(t) = \frac{2\pi I_0}{\beta} \delta(t).$$  \hfill (4.21)

Therefore, we find that the correlation function of the noise is white in the Ohmic case, which is consistent with the Langevin equation (4.13).

If the reservoir is sub-Ohmic or super-Ohmic, however, $C_n$ does not vanish for $n \geq 2$. Figure 5 shows $C_n$ as a function of $n$ for various values of $\alpha$. The sign of $C_n$ ($n \geq 2$) is positive in the sub-Ohmic regime and negative in the super-Ohmic regime. The difference in temperature profiles discussed in the previous subsection should be explained by this $\alpha$-dependence of the coefficients $C_n$. 

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V. SUMMARY AND DISCUSSION

We investigated the effect of the types of reservoirs on the thermal conduction in the harmonic chain. We derived the master equation for general many body system in contact with phonon reservoirs. In many body system, the dissipation term is different from one of one-particle system due to the noncommutability of many body interaction, so that the dissipation term has rather complicated form. However we have the explicit form for the dissipation term \[2.16\] and \[2.18\]. We used it as the basic equation to study behavior of the system. The equation generally satisfies the necessary condition for the master equation that the canonical distribution must be a stationary solution when the reservoirs are at the same temperature.

In Sec. 3, we have applied the master equation to energy transport in the quantum harmonic chain. We attached a phonon reservoir at one end and another at the other end. At weak coupling limit \((\lambda \rightarrow 0)\), we obtained explicit form of internal energy and energy flux. We rigorously proved that when the spectral densities of the reservoirs are of same type, the total energy of the system takes the arithmetic mean of the equilibrium energies at \(T_L\) and \(T_R\) regardless of the type of the spectral density. This result leads to the classical temperature \(T_L + T_R\) which is originally found by RLL using the Ohmic type of reservoir. On the other hand, when the types of spectral densities are different, the internal temperature is a function of the both densities, so that the temperature does not converge to \(T_L + T_R\) in the classical limit. The difference of spectral densities induces the deviation of temperatures around the both edges from the internal value. The temperature in the vicinity of both ends become close to the temperature of the reservoir whose spectral density has larger power. We numerically confirmed that this feature is general when the reservoirs are of different types.

We numerically investigated the effect of finite coupling. We considered only the case of the same spectral densities of the reservoirs. Finite coupling contributes to the temperature profile only near the ends of the chain and bulk behavior is the same as that of weak coupling limit. We found that the profile near the ends depends on the spectral density for the reservoirs. When the reservoir temperature is sufficiently low where quantum fluctuations are dominant, temperature growth near both the ends was observed in every case. When the reservoir temperatures are high enough and the reservoir is sub-Ohmic or Ohmic, the same peculiar behavior, i.e., nonmonotonic change of the temperature, is observed as found in [3]. However, in the case of super-Ohmic reservoir, the peculiarity disappears.

In order to understand the dependence on the spectral density, we derived Fokker-Planck equations from the master equation in the classical limit. If the reservoir is Ohmic the Fokker-Planck equation agrees with the standard one derived from the Langevin equation. When the reservoir is non-Ohmic, however, there appears difference in the diffusion term, i.e., form of second derivative. The coefficients of the diffusion terms were calculated from the spectral density. This difference causes different temperature profiles near the ends of the chain.

We expect that the master equation derived here can be used for other systems such as spin systems for which the Langevin approach is practically difficult. In the case of the harmonic chain, operator \(R\) was written in a simple form by using some system operators. Thus we were able to analyze the master equation systematically. This can be done because the harmonic chain is integrable. Thus, similar procedure can be developed for other integrable systems, e.g. the XY model [20].

In this paper we have confined ourselves to the integrable system. However the master equation derived here is generally applicable to any system because the matrix element of \(R\) is explicitly given. Thus it would be an interesting future problem to study the thermal conductivity in nonintegrable system where the Fourier heat law is realized [2].

ACKNOWLEDGMENT

We gratefully acknowledge partial financial support from Grant-in-Aid for Scientific Research from the Ministry of Education, Science and Culture.

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FIG. 1. Temperature profile along the chain for $T_L = 200.0, T_R = 50.0$: (a) $I_L(\omega) = \omega^{0.5}$ and $I_R(\omega) = \omega^{1.5}$; (b) $I_L(\omega) = \omega^{1.5}$ and $I_R(\omega) = \omega^{0.5}$. The system size is $N = 150$.

FIG. 2. Temperature profile along the chain for $\alpha = 1.0$: (a) $T_L = 200.0, T_R = 50.0$; (b) $T_L = 10.0, T_R = 0.1$; (c) $T_L = 0.1, T_R = 0.02$. The system size is $N = 150$.

FIG. 3. Temperature profile along the chain for $\alpha = 1.5$: (a) $T_L = 200.0, T_R = 50.0$; (b) $T_L = 10.0, T_R = 0.1$; (c) $T_L = 0.1, T_R = 0.02$. The system size is $N = 150$.

FIG. 4. Deviations of the temperature at particle 2 and particle $(N - 1)$ from the mean internal temperature $T_{av}$. The temperatures of the reservoirs are $T_L = 200.0$ and $T_R = 50.0$. Thus, $T_{av} = 125.0$.

FIG. 5. Coefficients $C_n$ as a function of $n$ for various values of $\alpha$. 
Fig. 1, K. Saito, S. Takesue, S. Miyashita
Fig. 2, K. Saito, S. Takesue, S. Miyashita
Fig. 3, K. Saito, S. Takesue, S. Miyashita
Fig. 4, K. Saito, S. Takesue, S. Miyashita
Fig. 5, K. Saito, S. Takesue, S. Miyashita