Energy transport in the integrable system in contact with various types of phonon reservoirs

K. Saito
Department of Applied Physics, School of Engineering, University of Tokyo, Bunkyo-ku, Tokyo 113–8656, Japan

S. Takesue
Faculty of Integrated Human Studies, Kyoto University, Kyoto 606–8501, Japan

S. Miyashita
Department of Applied Physics, School of Engineering, University of Tokyo, Bunkyo-ku, Tokyo 113–8656, Japan
(Received 8 October 1999; revised manuscript received 30 June 1999)

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 with both ends 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 a 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.

PACS number(s): 05.60.−k, 05.30.−d, 05.70.Ln

I. INTRODUCTION

Generally integrable systems show abnormal energy transport, namely, the Fourier heat law is not realized there [1,2]. 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 [8]. 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 Ref. [3] are reproduced. However, the 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 the 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 [9].

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 [3,4]. 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].

The 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 the 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. Section 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 $H_{\rm tot}$:

$$H_{\rm tot}=H+H_{\rm int}+H_{\rm R}, \tag{2.1}$$

where H denotes the Hamiltonian for the system of interest, $H_{\rm R}$ denotes the Hamiltonian for the reservoir, and $H_{\rm int}$ describes the interaction between the system and the reservoir. We assume that the reservoir consists of an infinite number of mutually independent harmonic oscillators [11–14], that is,

$$H_{\rm R}=\sum_\alpha \frac{p_\alpha^2}{2m_\alpha}+\frac{m_\alpha\omega_\alpha^2x_\alpha^2}{2}=\sum_\alpha \hbar\omega_\alpha\left(b_\alpha^\dagger b_\alpha+\frac{1}{2}\right), \tag{2.2}$$

where $b_\alpha^\dagger$ and b_α are the creation and annihilation operators for the αth mode. We assume a linear coupling between a Hermitian operator of the system X and reservoir's operators in the form

$$H_{\rm int}=\sum_\alpha \lambda\left(\frac{m_\alpha\omega_\alpha}{2}\right)^{1/2}\gamma_\alpha x_\alpha X+\lambda'^2\sum_\alpha\frac{\gamma_\alpha^2}{4\omega_\alpha}X^2$$
$$=\lambda\sqrt{\hbar}\sum_\alpha \gamma_\alpha(b_\alpha^\dagger+b_\alpha)X+\lambda'^2\sum_\alpha\frac{\gamma_\alpha^2}{4\omega_\alpha}X^2 \quad (\lambda'\geqslant\lambda), \tag{2.3}$$

where λ is a coupling constant and γ_αs and λ' are some constants. We put the second term in the right hand side in order to make the total Hamiltonian to be bounded [15]. This term is regarded as a part of H:

$$H\rightarrow H+\lambda'^2\sum_\alpha\frac{\gamma_\alpha^2}{4\omega_\alpha}X^2. \tag{2.4}$$

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

$$\frac{\partial\rho_{\rm tot}(t)}{\partial t}=\frac{1}{i\hbar}[H_{\rm tot},\rho_{\rm tot}(t)], \tag{2.5}$$

where $\rho_{\rm tot}(t)$ is the density matrix for the total system. Under the condition that the reservoir is initially in the equilibrium state at inverse temperature β, 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 second order with respect to λ and also adopt the Markovian approximation, which is valid when correlations between the reservoir's variables are short-lived. As a result we obtain an equation for the reduced density matrix $\rho(t)=\mathrm{Tr}_R\,\rho_{\rm tot}(t)$ (Tr_R means the trace concerning the reservoir's degrees of freedom) of the form

$$\frac{\partial}{\partial t}\rho(t)=\frac{1}{i\hbar}[H,\rho(t)]-\lambda^2\Gamma\rho(t), \tag{2.6}$$

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

$$\Gamma\rho(t)=\frac{1}{\hbar^2}\int_0^\infty dt'\int_{-\infty}^\infty d\omega e^{i\omega t'}\Phi(\omega)$$
$$\times\{XX(-t')\rho(t)-e^{\beta\hbar\omega}X\rho(t)X(-t')$$
$$+e^{\beta\hbar\omega}\rho(t)X(-t')X-X(-t')\rho(t)X\}. \tag{2.7}$$

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

$$X(-t')=e^{-iHt'/\hbar}Xe^{iHt'/\hbar}, \tag{2.8}$$

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

$$\Phi(\omega)=\frac{1}{2\pi}\int_{-\infty}^\infty e^{-i\omega t}\Phi(t)dt, \tag{2.9}$$

where $\Phi(t)$ is given by

$$\Phi(t)=\mathrm{Tr}_R\left[\sum_{\alpha,\alpha'}\left(\frac{m_\alpha\omega_\alpha}{2}\right)^{1/2}\left(\frac{m_{\alpha'}\omega_{\alpha'}}{2}\right)^{1/2}\times\gamma_\alpha\gamma_{\alpha'}x_\alpha(0)x_{\alpha'}(t)e^{-\beta H_R}\right]\Big/\mathrm{Tr}_R\,e^{-\beta H_R}$$

$$=\hbar\sum_\alpha\ \gamma_\alpha^2\frac{e^{i\omega_\alpha t}+e^{\beta\hbar\omega_\alpha}e^{-i\omega_\alpha t}}{e^{\beta\hbar\omega_\alpha}-1}. \tag{2.10}$$

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

$$\Phi(\omega)=\hbar\,\gamma(\omega)^2\frac{D(\omega)-D(-\omega)}{e^{\beta\hbar\omega}-1}, \tag{2.11}$$

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

$$I(\omega)=\gamma(\omega)^2D(\omega). \tag{2.12}$$

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

$$I(\omega)=I_0\omega^\alpha\theta(\omega), \tag{2.13}$$

where $\theta(\omega)$ is the step function: $\theta(\omega)=1$ for $\omega\geqslant 0$ and $\theta(\omega)=0$ for $\omega<0$. The reservoir is called Ohmic if $\alpha=1$, sub-Ohmic if $\alpha<1$, and super-Ohmic if $\alpha>1$ [13].

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

$$\int_0^\infty e^{i\nu t}dt=\pi\delta(\nu)+\mathcal{P}\frac{i}{\nu}, \tag{2.14}$$

neglecting the principal value [9,18,19] and the Kubo-Martin-Schwinger (KMS) condition $\Phi(\omega)e^{\beta\hbar\omega}=\Phi(-\omega)$. Then, the matrix components of operator $\Gamma\rho(t)$ is written as

$$\langle k|\Gamma\rho(t)|n\rangle=\frac{\pi}{\hbar^2}\sum_{l,m}\left[X_{k,l}X_{l,m}\Phi\left(\frac{E_l-E_m}{\hbar}\right)\rho_{m,n}(t)-X_{k,l}\rho_{l,m}(t)X^*_{n,m}\Phi\left(\frac{E_n-E_m}{\hbar}\right)+\rho_{k,l}(t)X^*_{m,l}\Phi\left(\frac{E_m-E_l}{\hbar}\right)X_{m,n}-X_{k,l}\Phi\left(\frac{E_k-E_l}{\hbar}\right)\rho_{l,m}(t)X_{m,n}\right]. \tag{2.15}$$

Now we introduce the operator R whose matrix elements are

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

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

$$\Gamma\rho(t)=\frac{\pi}{\hbar}[XR\rho(t)-R\rho(t)X-X\rho(t)R^\dagger+\rho(t)R^\dagger X]=\frac{\pi}{\hbar}\{[X,R\rho(t)]+[X,R\rho(t)]^\dagger\}. \tag{2.17}$$

Thus we arrive at the master equation of the form

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

This is a generalized Lindblad form [16,17] treating general many body system with the coupling form (2.3). When the system has many body interactions, the noncommutabilities cause the operator R to contain all degrees of freedom of the system even if H_{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 Eq. (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. (2.18) satisfies at least a necessary condition for the master equation, i.e., the canonical distribution $e^{-\beta H}/\mathrm{Tr}(e^{-\beta H})$ into ρ in Eq. (2.18) gives a stationary solution. We also expect the stability of the stationary solution at least when λ 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 [4] and compare it with the master equation for reduced density matrix (2.18) (see also Ref. [15] for other types of quantum Langevin equations we no not explain here).

The quantum Langevin equation was introduced by Ford, Kac, and Mazur [8]. They considered the following coupled oscillators composed of $2N+1$ particles:

$$H=\frac{1}{2}\sum_{n=-N}^{N}p_n^2+\frac{1}{2}\sum_{m,n=-N}^{N}q_mA_{m,n}q_n, \tag{2.19}$$

where q_n and p_n are the ith canonical coordinate and momentum variable, respectively. The matrix $\mathbf{A}=(A_{m,n})$ is a $(2N+1)\times(2N+1)$ symmetric matrix whose elements are

$$A_{m,n}=\frac{1}{2N+1}\sum_{k=-N}^{N}\omega_k^2\exp\left[i\frac{2\pi k}{2N+1}(m-n)\right]. \tag{2.20}$$

It should be noted that the eigenvalues of this matrix are ω_s^2 $(s=-N,-N+1,\ldots,N-1,N)$. 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 eigenfrequencies of the whole system ω_s, have the special form

$$\omega_s^2=f^2\tan^2\left(\frac{\pi s}{2N+1}\right), \tag{2.21}$$

the motion of a particle of the system in the equilibrium state is described by

$$\frac{\partial q_0(t)}{\partial t}=p_0, \tag{2.22a}$$

$$\frac{\partial p_0(t)}{\partial t}=-fp_0+E(t), \tag{2.22b}$$

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 as the Gaussian random force with vanishing mean $\langle E(t)\rangle=0$, where $\langle\cdots\rangle$ means $\mathrm{Tr}(\exp[-\beta H(\{q_i(0)\},\{p_i(0)\})]\ldots)/Z$. It also satisfies the commutation relation

$$[E(t),E(s)]=2i\hbar f\frac{\partial}{\partial t}\delta(t-s) \tag{2.23}$$

and has the symmetrized correlation

$$\frac{1}{2}\langle E(t)E(t+\tau)+E(t+\tau)E(t)\rangle=\frac{\hbar f}{\pi}\int_0^\infty\omega\coth\left[\frac{\beta\hbar\omega}{2}\right]\cos(\omega\tau)d\omega. \tag{2.24}$$

This dynamics yields a classical Langevin equation with Gaussian white noise in the classical limit $\hbar\to 0$.

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 a 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

$$H=\sum_{n=1}^{N}\frac{p_n^2}{2m}+\sum_{n=0}^{N}\frac{m\omega_0^2}{2}(x_{n+1}-x_n)^2 \tag{3.1}$$

as the system. This Hamiltonian should be considered to be the renormalized Hamiltonian including the second term in Eq. (2.3). As in Ref. [3], we impose the fixed boundary condition, $x_0=x_{N+1}=0$. By Fourier transformation

$$x_n=\sqrt{\frac{2}{N+1}}\sum_k u_k\sin(kn),$$

$$p_n=\sqrt{\frac{2}{N+1}}\sum_k v_k\sin(kn), \tag{3.2}$$

the Hamiltonian is decoupled into the normal modes as

$$H=\sum_k\frac{v_k^2}{2m}+\frac{m\omega_k^2u_k^2}{2} \tag{3.3}$$

where $\omega_k=2\omega_0\sin(k/2)$. The wave number k runs through the values $k=\pi\ell/(N+1)$ $(\ell=1,2,\ldots,N-1,N)$. It is easily found that 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

$$a_k=\sqrt{\frac{m\omega_0\sin(k/2)}{\hbar}}\left(u_k+\frac{iv_k}{2m\omega_0\sin(k/2)}\right)$$

and

$$a_k^\dagger=\sqrt{\frac{m\omega_0\sin(k/2)}{\hbar}}\left(u_k-\frac{iv_k}{2m\omega_0\sin(k/2)}\right),$$

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 β_L and β_R, respectively.

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

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

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 Eq. (3.6) is valid in the order of λ^2. From Eq. (2.18) the damping terms $\Gamma_L\rho(t)$ and $\Gamma_R\rho(t)$ are

$$\Gamma_L\rho(t)=\frac{\pi}{\hbar}\{[x_1,R_L\rho(t)]+[x_1,R_L\rho(t)]^\dagger\}$$

and (3.7)

$$\Gamma_R\rho(t)=\frac{\pi}{\hbar}\{[x_N,R_R\rho(t)]+[x_N,R_R\rho(t)]^\dagger\},$$

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

$$\langle l|R_L|m\rangle=\frac{I_L\left(\frac{E_l-E_m}{\hbar}\right)-I_L\left(-\frac{E_l-E_m}{\hbar}\right)}{e^{\beta_L(E_l-E_m)}-1}\langle l|x_1|m\rangle, \quad (3.8a)$$

$$\langle l|R_R|m\rangle=\frac{I_R\left(\frac{E_l-E_m}{\hbar}\right)-I_R\left(-\frac{E_l-E_m}{\hbar}\right)}{e^{\beta_R(E_l-E_m)}-1}\langle l|x_N|m\rangle, \quad (3.8b)$$

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

$$x_1=\sqrt{\frac{\hbar}{2(N+1)m\omega_0}}\sum_k\frac{\sin k}{\sqrt{\sin(k/2)}}(a_k+a_k^\dagger) \quad (3.9)$$

and

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

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 $|\{n_k\}\rangle=\Pi_k|n_k\rangle$, whose energy eigenvalue is $E(\{n_k\})=\Sigma_k(n_k+\frac{1}{2})\hbar\omega_k$.

The matrix elements of R_L are given in terms of the eigenstates $|\{n_k\}\rangle$ as

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

Now we note that

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

$$\langle\{n_{k'}\}|a_k^\dagger|\{m_{k'}\}\rangle\neq 0 \quad \text{only if} \quad n_{k'}=m_{k'}+\delta_{k',k} \quad \text{for} \quad \forall k', \quad (3.13)$$

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

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

Thus the operator R_L can be represented as

$$R_L=\sqrt{\frac{\hbar}{8(N+1)m\omega_0}}\sum_k\frac{\sin k}{\sqrt{\sin(k/2)}}\frac{I_L(\omega_k)}{\sinh(\beta_L\hbar\omega_k/2)}(e^{\beta_L\hbar\omega_k/2}a_k+e^{-\beta_L\hbar\omega_k/2}a_k^\dagger). \quad (3.15)$$

In the same manner, the operator R_R is represented as

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

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

$$\langle a_k a_{k'}\rangle=\mathrm{Tr}(a_k a_{k'}\rho_{\mathrm{st}}) \tag{3.17}$$

and

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

where ρ_{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

$$\begin{aligned}&\frac{1}{i\hbar}\mathrm{Tr}(a_k a_{k'}[H,\rho])-\frac{\pi\mu}{\hbar}[\mathrm{Tr}(a_k a_{k'}[x_1,R_L\rho_{\mathrm{st}}])+\mathrm{Tr}(a_k a_{k'}[x_1,R_L\rho_{\mathrm{st}}]^\dagger)]\\&\quad-\frac{\pi\mu}{\hbar}[\mathrm{Tr}(a_k a_{k'}[x_N,R_R\rho])+\mathrm{Tr}(a_k a_{k'}[x_N,R_R\rho]^\dagger)]=0.\end{aligned} \tag{3.19}$$

This equation is rewritten as follows after tedious but straightforward calculations:

$$\begin{aligned}&i(\omega_k+\omega_{k'})\langle a_k a_{k'}\rangle+\frac{\pi\mu}{4(N+1)m\omega_0}\sum_{k_1}\frac{\sin k_1}{\sqrt{\sin(k_1/2)}}\frac{I_L(\omega_{k_1})}{\sinh(\beta_L\hbar\omega_{k_1}/2)}\\&\times\left\{\frac{\sin k'}{\sqrt{\sin(k'/2)}}[e^{\beta_L\hbar\omega_{k_1}/2}(\langle a_k a_{k_1}\rangle-\langle a_{k_1}^\dagger a_k\rangle)+e^{-\beta_L\hbar\omega_{k_1}/2}(\langle a_k a_{k_1}^\dagger\rangle-\langle a_{k_1}a_k\rangle)]\right.\\&\left.+\frac{\sin k}{\sqrt{\sin(k/2)}}[e^{\beta_L\hbar\omega_{k_1}/2}(\langle a_{k'}a_{k_1}\rangle-\langle a_{k_1}^\dagger a_{k'}\rangle)+e^{-\beta_L\hbar\omega_{k_1}/2}(\langle a_{k'}a_{k_1}^\dagger\rangle-\langle a_{k_1}a_{k'}\rangle)]\right\}\\&+\frac{\pi\mu}{4(N+1)m\omega_0}\sum_{k_1}\frac{\sin(Nk_1)}{\sqrt{\sin(k_1/2)}}\frac{I_R(\omega_{k_1})}{\sinh(\beta_R\hbar\omega_{k_1}/2)}\\&\times\left\{\frac{\sin(Nk')}{\sqrt{\sin(k'/2)}}[e^{\beta_R\hbar\omega_{k_1}/2}(\langle a_k a_{k_1}\rangle-\langle a_{k_1}^\dagger a_k\rangle)+e^{-\beta_R\hbar\omega_{k_1}/2}(\langle a_k a_{k_1}^\dagger\rangle-\langle a_{k_1}a_k\rangle)]\right.\\&\left.+\frac{\sin(Nk)}{\sqrt{\sin(k/2)}}[e^{\beta_R\hbar\omega_{k_1}/2}(\langle a_{k'}a_{k_1}\rangle-\langle a_{k_1}^\dagger a_{k'}\rangle)+e^{-\beta_R\hbar\omega_{k_1}/2}(\langle a_{k'}a_{k_1}^\dagger\rangle-\langle a_{k_1}a_{k'}\rangle)]\right\}=0.\end{aligned} \tag{3.20}$$

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

$$\begin{aligned}&i(\omega_{k'}-\omega_k)\langle a_k^\dagger a_{k'}\rangle+\frac{\pi\mu}{4(N+1)m\omega_0}\sum_{k_1}\frac{\sin k_1}{\sqrt{\sin(k_1/2)}}\frac{I_L(\omega_{k_1})}{\sinh(\beta_L\hbar\omega_{k_1}/2)}\\&\times\left\{\frac{\sin k}{\sqrt{\sin(k/2)}}[e^{\beta_L\hbar\omega_{k_1}/2}(\langle a_{k_1}^\dagger a_{k'}\rangle-\langle a_{k'}a_{k_1}\rangle)+e^{-\beta_L\hbar\omega_{k_1}/2}(\langle a_{k_1}a_{k'}\rangle-\langle a_{k'}a_{k_1}^\dagger\rangle)]\right.\\&\left.+\frac{\sin k'}{\sqrt{\sin(k'/2)}}[e^{\beta_L\hbar\omega_{k_1}/2}(\langle a_k^\dagger a_{k_1}\rangle-\langle a_{k_1}^\dagger a_k^\dagger\rangle)+e^{-\beta_L\hbar\omega_{k_1}/2}(\langle a_k^\dagger a_{k_1}^\dagger\rangle-\langle a_{k_1}a_k^\dagger\rangle)]\right\}\\&+\frac{\pi\mu}{4(N+1)m\omega_0}\sum_{k_1}\frac{\sin(Nk_1)}{\sqrt{\sin(k_1/2)}}\frac{I_R(\omega_{k_1})}{\sinh(\beta_R\hbar\omega_{k_1}/2)}\end{aligned}$$

$$\times\left\{\frac{\sin(Nk)}{\sqrt{\sin(k/2)}}[e^{\beta_R\hbar\omega_{k_1}/2}(\langle a_{k_1}^\dagger a_{k'}\rangle-\langle a_{k'}a_{k_1}\rangle)+e^{-\beta_R\hbar\omega_{k_1}/2}(\langle a_{k_1}a_{k'}\rangle-\langle a_{k'}a_{k_1}^\dagger\rangle)]\right.$$

$$\left.+\frac{\sin(Nk')}{\sqrt{\sin(k'/2)}}[e^{\beta_R\hbar\omega_{k_1}/2}(\langle a_k^\dagger a_{k_1}\rangle-\langle a_{k_1}^\dagger a_k^\dagger\rangle)+e^{-\beta_R\hbar\omega_{k_1}/2}(\langle a_k^\dagger a_{k_1}^\dagger\rangle-\langle a_{k_1}a_k^\dagger\rangle)]\right\}=0. \quad (3.21)$$

D. Total energy $E_{\rm st}$

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

$$\langle a_k a_{k'}\rangle=\langle a_k a_{k'}\rangle_0+\mu\langle a_k a_{k'}\rangle_1+\mu^2\langle a_k a_{k'}\rangle_2+\cdots, \quad (3.22)$$

$$\langle a_k^\dagger a_{k'}^\dagger\rangle=\langle a_k^\dagger a_{k'}^\dagger\rangle_0+\mu\langle a_k^\dagger a_{k'}^\dagger\rangle_1+\mu^2\langle a_k^\dagger a_{k'}^\dagger\rangle_2+\cdots, \quad (3.23)$$

$$\langle a_k^\dagger a_{k'}\rangle=\langle a_k^\dagger a_{k'}\rangle_0+\mu\langle a_k^\dagger a_{k'}\rangle_1+\mu^2\langle a_k^\dagger a_{k'}\rangle_2+\cdots, \quad (3.24)$$

$$\langle a_k a_{k'}^\dagger\rangle=\langle a_k a_{k'}^\dagger\rangle_0+\mu\langle a_k a_{k'}^\dagger\rangle_1+\mu^2\langle a_k a_{k'}^\dagger\rangle_2+\cdots, \quad (3.25)$$

we consider the relation of each order of μ. Using the commutation relations

$$\langle a_k a_{k'}\rangle_n=\langle a_{k'}a_k\rangle_n,$$

$$\langle a_k^\dagger a_{k'}^\dagger\rangle_n=\langle a_{k'}^\dagger a_k^\dagger\rangle_n,$$

$$\langle a_k a_{k'}^\dagger\rangle_n=\langle a_{k'}^\dagger a_k\rangle_n+\delta_{n,0}\delta_{k,k'}, \quad (3.26)$$

we obtain the following relations at the zeroth order:

$$(\omega_k+\omega_{k'})\langle a_k a_{k'}\rangle_0=0 \quad \text{and} \quad (\omega_{k'}-\omega_k)\langle a_k^\dagger a_{k'}\rangle_0=0. \quad (3.27)$$

Accordingly we have for all k and k'

$$\langle a_k a_{k'}\rangle_0=0, \quad (3.28)$$

and for $k\neq k'$

$$\langle a_k^\dagger a_{k'}\rangle_0=0. \quad (3.29)$$

Putting $k=k'$ in the first order equation of μ, we have

$$\frac{\sin^2 kI_L(\omega_k)}{\sinh(\beta_L\hbar\omega_k/2)}(e^{\beta_L\hbar\omega_k/2}\langle a_k^\dagger a_k\rangle_0-e^{-\beta_L\hbar\omega_k/2}\langle a_k a_k^\dagger\rangle_0)$$

$$+\frac{\sin^2(Nk)I_R(\omega_k)}{\sinh(\beta_R\hbar\omega_k/2)}(e^{\beta_R\hbar\omega_k/2}\langle a_k^\dagger a_k\rangle_0$$

$$-e^{-\beta_R\hbar\omega_k/2}\langle a_k a_k^\dagger\rangle_0)=0. \quad (3.30)$$

Since $\sin^2 k=\sin^2(Nk)\neq 0$, Eq. (3.30) leads to

$$\langle a_k^\dagger a_k\rangle_0=\frac{1}{I_L(\omega_k)+I_R(\omega_k)}\left[\frac{I_L(\omega_k)}{e^{\beta_L\hbar\omega_k}-1}+\frac{I_R(\omega_k)}{e^{\beta_R\hbar\omega_k}-1}\right]. \quad (3.31)$$

Here the energy of the system is

$$E_{\rm st}=\mathrm{Tr}(H\rho_{\rm st})=\sum_k\frac{\hbar\omega_k}{I_L(\omega_k)+I_R(\omega_k)}\times\left[\frac{I_L(\omega_k)}{e^{\beta_L\hbar\omega_k}-1}+\frac{I_R(\omega_k)}{e^{\beta_R\hbar\omega_k}-1}\right]. \quad (3.32)$$

In particular, when $I_L(\omega_k)=I_R(\omega_k)$, we find that $E_{\rm st}$ is the arithmetic mean between equilibrium energy at inverse temperature β_L and at β_R regardless of the types of the spectral density, i.e.,

$$E_{\rm st}=\frac{1}{2}\left[\frac{\mathrm{Tr}(He^{-\beta_L H})}{\mathrm{Tr}\,e^{-\beta_L H}}+\frac{\mathrm{Tr}(He^{-\beta_R H})}{\mathrm{Tr}\,e^{-\beta_R H}}\right]. \quad (3.33)$$

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 μ. The mean kinetic energy of the nth particle ε_n is defined by

$$\varepsilon_n=\left\langle\frac{p_n^2}{2m}\right\rangle=\mathrm{Tr}\left(\frac{p_n^2}{2m}\rho_{\rm st}\right), \quad (3.34)$$

which is expressed in terms of the creation and annihilation operators as

$$\varepsilon_n=\frac{-\hbar\omega_0}{N+1}\sum_{k,k'}\sqrt{\sin(k/2)\sin(k'/2)}\sin(kn)\sin(k'n)\times(\langle a_k a_{k'}\rangle-\langle a_k a_{k'}^\dagger\rangle-\langle a_k^\dagger a_{k'}\rangle+\langle a_k^\dagger a_{k'}^\dagger\rangle). \quad (3.35)$$

Substituting the results obtained in the last subsection into the above equation, we have

$$\varepsilon_n=\frac{\hbar\omega_0}{N+1}\sum_k\sin(k/2)\sin^2(kn)(2\langle a_k^\dagger a_k\rangle_0+1)$$

$$=\frac{\hbar\omega_0}{N+1}\sum_k\sin(k/2)\sin^2(kn)\left[\frac{2}{I_L(\omega_k)+I_R(\omega_k)}\times\left(\frac{I_L(\omega_k)}{e^{\beta_L\hbar\omega_k}-1}+\frac{I_R(\omega_k)}{e^{\beta_R\hbar\omega_k}-1}\right)+1\right]. \quad (3.36)$$

In the classical limit, Eq. (3.36) becomes

$$2\varepsilon_n=\frac{2T_L}{\pi}\int_0^\pi dk\sin^2(kn)\frac{I_L(\omega_k)}{I_L(\omega_k)+I_R(\omega_k)}+\frac{2T_R}{\pi}\int_0^\pi dk\sin^2(kn)\frac{I_R(\omega_k)}{I_L(\omega_k)+I_R(\omega_k)}, \quad (3.37)$$

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

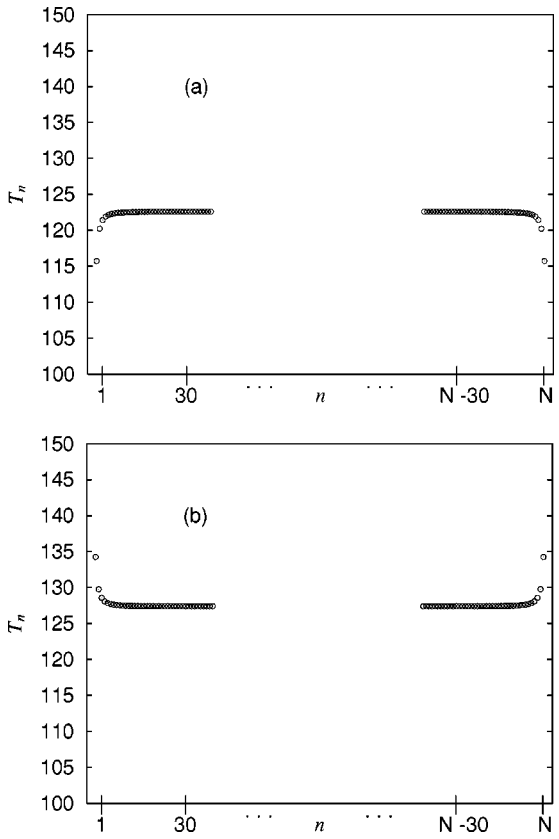

FIG. 1. Temperature profile along the chain for $T_L=200.0$, $T_R=50.0$: (a) $I_L(\omega)=\omega^{0.5}$ and $I_R(\omega)=\omega^{1.5}$, (b) $I_L(\omega)=\omega^{1.5}$ and $I_R(\omega)=\omega^{0.5}$. The system size is $N=150$.

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 $2\varepsilon_n=(T_L+T_R)/2$ 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 [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 $(T_L+T_R)/2$ in the classical limit.

We numerically estimate Eq. (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), the time derivative for the energy of the system satisfies

$$\frac{\partial}{\partial t}\mathrm{Tr}[H\rho(t)]=-\mathrm{Tr}[\mu H\Gamma_L\rho(t)]-\mathrm{Tr}[\mu H\Gamma_R\rho(t)]. \quad (3.38)$$

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 and the latter J_R. In the stationary state, of course $J_L^{\mathrm{st}}+J_R^{\mathrm{st}}=0$ must hold. We can calculate J_L^{st} as follows:

$$\begin{aligned}J_{\mathrm{L}}^{\mathrm{st}}&=-\frac{\pi\mu}{\hbar}\mathrm{Tr}(H[x_1,R_L\rho]+H[x_1,R_L\rho]^{\dagger})\\&=\frac{\pi\hbar\mu}{(N+1)m}\sum_k\frac{I_L(\omega_k)I_R(\omega_k)}{I_L(\omega_k)+I_R(\omega_k)}\\&\quad\times\left(\frac{1}{e^{\beta_L\hbar\omega_k}-1}-\frac{1}{e^{\beta_R\hbar\omega_k}-1}\right). \quad (3.39)\end{aligned}$$

If $N\gg 1$, we can replace the summation by an integral and obtain

$$\begin{aligned}J_L^{\mathrm{st}}&=\frac{\hbar\mu}{m}\int_0^{\pi}\frac{I_L(\omega_k)I_R(\omega_k)}{I_L(\omega_k)+I_R(\omega_k)}\\&\quad\times\sin^2 k\left(\frac{1}{e^{\beta_L\hbar\omega_k}-1}-\frac{1}{e^{\beta_R\hbar\omega_k}-1}\right)dk. \quad (3.40)\end{aligned}$$

In the classical limit $(\hbar\to 0)$, $J_{\mathrm{L}}^{\mathrm{st}}$ goes to

$$J_L^{\mathrm{st}}=\mu C(T_L-T_R), \quad (3.41)$$

where

$$\begin{aligned}C&=\frac{1}{m\omega_0}\int_0^{\pi}\frac{\sin^2 k}{\sin(k/2)}\\&\quad\times\frac{I_L(2\omega_0\sin(k/2))I_R(2\omega_0\sin(k/2))}{I_L(2\omega_0\sin(k/2))+I_R(2\omega_0\sin(k/2))}dk. \quad (3.42)\end{aligned}$$

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 [18,20]. This shows that the master equation can well approximate the dynamics in real dissipative system at least qualitatively. In some cases the time evolution of the reduced density matrix with a finite coupling reproduces quantitatively correct results even for long times [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,

$$I_L = I_R = I. \tag{4.1}$$

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 Eqs. (3.20) and (3.21), we have for all k and k'

$$\langle a_k a_{k'} \rangle_1 = \frac{i\pi[\sin k \sin k' - \sin(Nk)\sin(Nk')]}{4(N+1)m\omega_0(\omega_k+\omega_{k'})\sqrt{\sin(k/2)\sin(k'/2)}} \times \{I(\omega_k)[n_L(\omega_k)-n_R(\omega_k)] + I(\omega_{k'})[n_L(\omega_{k'})-n_R(\omega_{k'})]\}, \tag{4.2}$$

and for $k \neq k'$

$$\langle a_k^\dagger a_{k'} \rangle_1 = \frac{i\pi[\sin k \sin k' - \sin(Nk)\sin(Nk')]}{4(N+1)m\omega_0(\omega_k-\omega_{k'})\sqrt{\sin(k/2)\sin(k'/2)}} \times \{I(\omega_k)[n_L(\omega_k)-n_R(\omega_k)] + I(\omega_{k'})[n_L(\omega_{k'})-n_R(\omega_{k'})]\}, \tag{4.3}$$

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

$$n_L(\omega) = \frac{1}{e^{\beta_L \hbar\omega}-1}, \tag{4.4}$$

and $n_R(\omega)$ is that at β_R

$$n_R(\omega) = \frac{1}{e^{\beta_R \hbar\omega}-1}. \tag{4.5}$$

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

$$\langle a_k^\dagger a_k \rangle_1 = 0. \tag{4.6}$$

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

$$\langle a_k a_{k'} \rangle_{n+1} = \frac{i\pi}{2(N+1)m\omega_0(\omega_k+\omega_{k'})} \sum_{k_1} I(\omega_{k_1}) \times \left[\frac{\sin k_1 \sin k' + \sin(Nk_1)\sin(Nk')}{\sqrt{\sin(k_1/2)\sin(k'/2)}} \times (\langle a_k a_{k_1} \rangle_n - \langle a_{k_1}^\dagger a_k \rangle_n) + \frac{\sin k_1 \sin k + \sin(Nk_1)\sin(Nk)}{\sqrt{\sin(k_1/2)\sin(k/2)}} \times \langle a_{k'} a_{k_1} \rangle_n - (\langle a_{k_1}^\dagger a_{k'} \rangle_n) \right]. \tag{4.7}$$

If $k = k'$,

$$\langle a_k^\dagger a_{k'} \rangle_{n+1} = \frac{i\pi}{2(N+1)m\omega_0(\omega_{k'}-\omega_k)} \sum_{k_1} I(\omega_{k_1}) \times \left[\frac{\sin k_1 \sin k' + \sin(Nk_1)\sin(Nk')}{\sqrt{\sin(k_1/2)\sin(k'/2)}} \times (\langle a_k^\dagger a_{k_1} \rangle_n - \langle a_k a_{k_1} \rangle_n^*) + \frac{\sin k_1 \sin k + \sin(Nk_1)\sin(Nk)}{\sqrt{\sin(k_1/2)\sin(k/2)}} \times (\langle a_{k_1}^\dagger a_{k'} \rangle_n - \langle a_{k'} a_{k_1} \rangle_n) \right] \tag{4.8}$$

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

$$\langle a_k^\dagger a_k \rangle_{n+1} = \frac{1}{2}(\langle a_k a_k \rangle_{n+1} + \langle a_k a_k \rangle_{n+1}^*) - \frac{\sqrt{\sin(k/2)}}{4I(\omega_k)\sin^2 k} \times \sum_{k' \neq k} \frac{\sin k' \sin k + \sin(Nk')\sin(Nk)}{\sqrt{\sin(k'/2)}} I(\omega_{k'}) \times (\langle a_{k'}^\dagger a_k \rangle_{n+1} + \langle a_k^\dagger a_{k'} \rangle_{n+1} - \langle a_k a_{k'} \rangle_{n+1} - \langle a_k a_{k'} \rangle_{n+1}^*). \tag{4.9}$$

Because the above equations contain the spectral density, we have to specify its functional form. As has given in Eq. (2.13), we employ the following form for the spectral density:

$$I(\omega) = I_0 \omega^\alpha. \tag{4.10}$$

For $\alpha = 1.0$ and $\alpha = 1.5$, we have computed mean kinetic energy of the nth particle ε_n up to the 20th order, where quantities (3.22)–(3.25) seem to converge. For each α, 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 Ref. [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 β, ε_n is given by

$$\varepsilon_n = \phi_n(\beta) = \frac{\hbar\omega_0}{N+1} \sum_{l=1}^{N} \sin\frac{\pi l}{2(N+1)} \times \sin^2\frac{\pi l n}{N+1} \coth\left[\beta\hbar\omega_0 \sin\frac{\pi l}{2(N+1)}\right], \tag{4.11}$$

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

In Figs. 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 de-

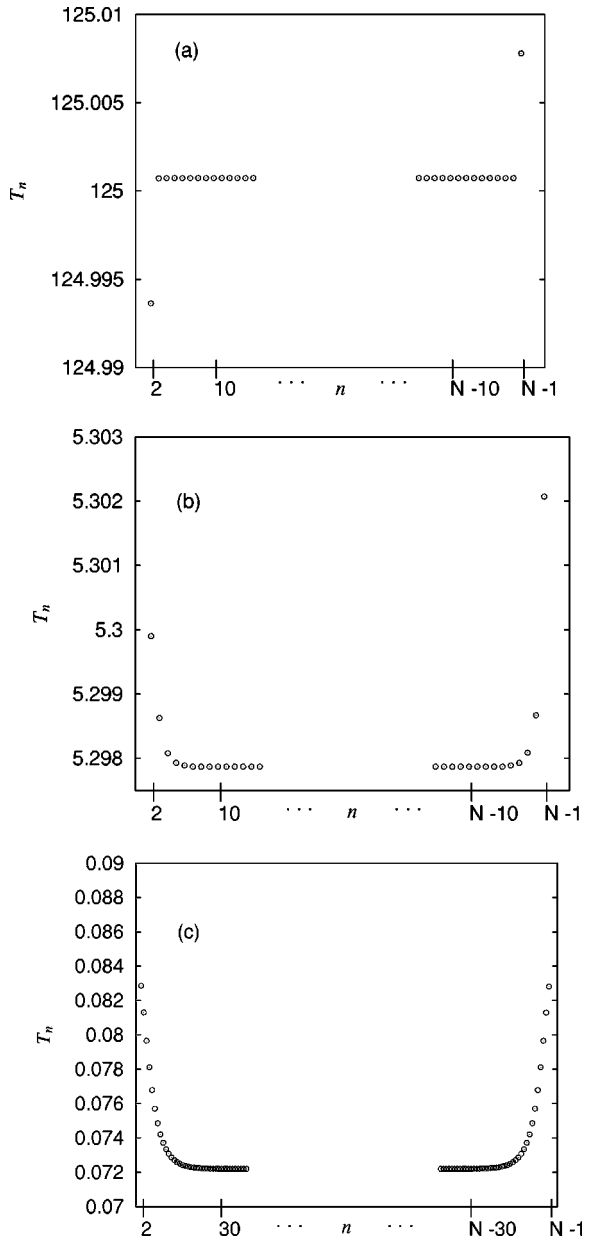

FIG. 2. Temperature profile along the chain for $\alpha=1.0$: (a) $T_L=200.0$, $T_R=50.0$; (b) $T_L=10.0$, $T_R=0.1$; (c) $T_L=0.1$, $T_R=0.02$. The system size is $N=150$.

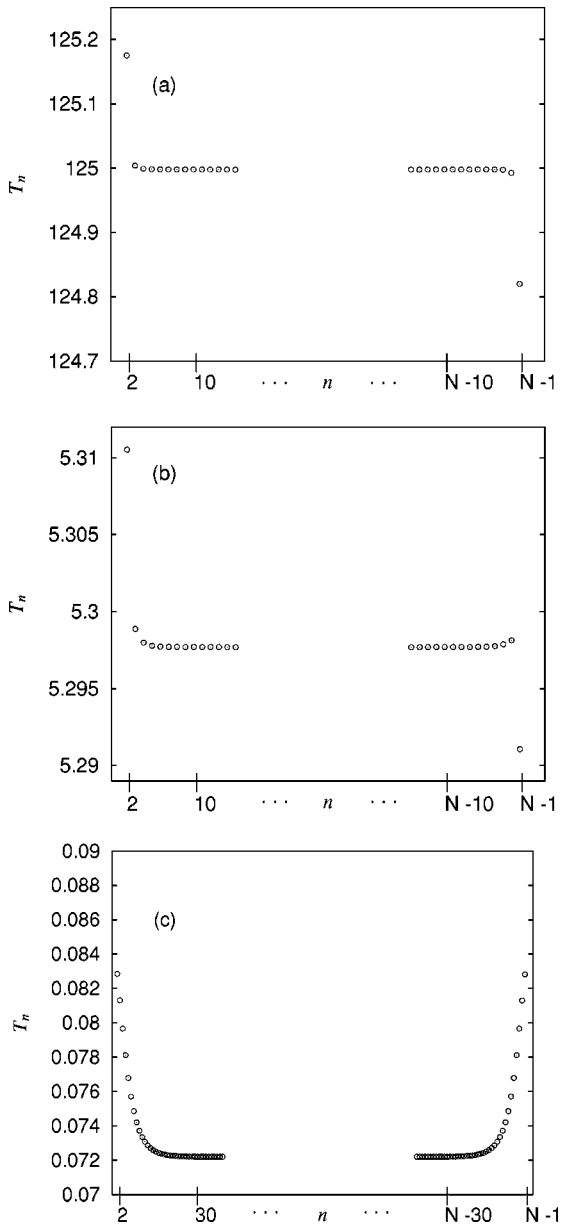

FIG. 3. Temperature profile along the chain for $\alpha=1.5$: (a) $T_L=200.0$, $T_R=50.0$; (b) $T_L=10.0$, $T_R=0.1$; (c) $T_L=0.1$, $T_R=0.02$. The system size is $N=150$.

pendencies on the details of the parameters (T_L, T_R, α). 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 disappears when the reservoirs are super-Ohmic [Fig. 3(a)]. The second particles from the ends show monotonic temperature variation.

Figures 2(c) and 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, Figs. 2(b) and 3(b), mixed behavior of the classical and quantum features are observed. (See also the figures in Ref. [4].)

For $T_L=200.0$ and $T_R=50.0$, temperature deviations of particles 2 and $(N-1)$ from the mean internal temperature are plotted in Fig. 4 for various α. 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 $\alpha \geqslant \alpha_c (\simeq 1.04)$.

B. Fokker-Planck equation in the classical limit

In the previous subsection, the temperature profiles is found to depend on values of α. In particular, the peculiarity found by RLL [3] disappears in the super-Ohmic regime.

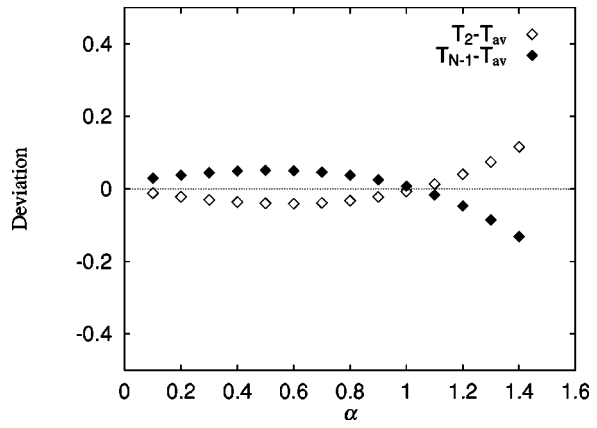

FIG. 4. Deviations of the temperature at particle 2 and particle $(N-1)$ from the mean internal temperature T_{av}. The temperatures of the reservoirs are $T_L=200.0$ and $T_R=50.0$. Thus, $T_{\mathrm{av}}=125.0$.

Since the differences are seen at high temperatures, some characteristics depending on the values α 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 in 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 $p_n(t)$, $n=1,2,\ldots,N$ are

$$\frac{\partial x_n}{\partial t}=\{x_n,H\}, \tag{4.12}$$

$$\frac{\partial p_n}{\partial t}=\{p_n,H\}-\delta_{n,1}\nu\frac{p_n}{m}+\delta_{n,1}\xi(t). \tag{4.13}$$

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

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

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

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

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 (3.15) into the master equation (2.6), we have

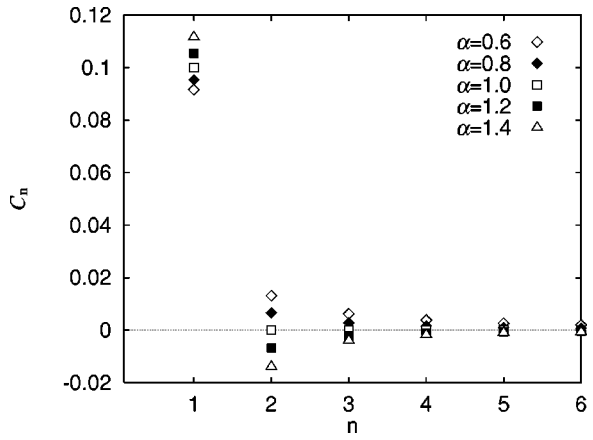

FIG. 5. Coefficients C_n as a function of n for various values of α.

$$\begin{aligned}\frac{\partial\rho(t)}{\partial t}=&\frac{1}{i\hbar}[H,\rho(t)]-\frac{\pi\mu}{\sqrt{8(N+1)m\hbar\omega_0}}\\&\times\sum_k\frac{\sin k}{\sqrt{\sin(k/2)}}\frac{I(\omega_k)}{\sinh(\beta\hbar\omega_k/2)}\\&\times\{[x_1,(e^{\beta\hbar\omega_k/2}a_k+e^{-\beta\hbar\omega_k/2}a_k^\dagger)\rho(t)]\\&-[x_1,\rho(t)(e^{\beta\hbar\omega_k/2}a_k^\dagger+e^{-\beta\hbar\omega_k/2}a_k)]\},\end{aligned} \tag{4.16}$$

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

$$\begin{aligned}\frac{\partial\rho(t)}{\partial t}=&\frac{1}{i\hbar}[H,\rho(t)]-\frac{\pi\mu}{(N+1)\hbar}\sum_{k,n}I(\omega_k)\sin k\sin(kn)\\&\times\left\{\coth\left(\frac{\beta\hbar\omega_k}{2}\right)[x_n,[x_1,\rho(t)]]\right.\\&+\frac{i}{2m\omega_0\sin(k/2)}\{p_n[x_1,\rho(t)]\\&\left.+[x_1,\rho(t)]p_n+2[x_1,p_n]\rho(t)\}\right\}.\end{aligned} \tag{4.17}$$

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

$$\frac{\partial P(t)}{\partial t}=\{H,P(t)\}+\sum_{n=1}^{N}C_n\frac{\partial}{\partial p_1}\left(\frac{p_n}{m}+\beta^{-1}\frac{\partial}{\partial p_n}\right)P(t), \tag{4.18}$$

where

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

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

$$C_n=\pi\mu I_0\delta_{n,1}, \tag{4.20}$$

and Eq. (4.18) agrees with the Fokker-Planck equation derived from the Langevin equation (4.15). In this case, the two-point function (2.10) tends to the delta function in the classical limit

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

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 $n\geqslant 2$. Figure 5 shows C_n as a function of n for various values of α. The sign of C_n $(n\geqslant 2)$ 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 α dependence of the coefficients C_n.

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 a general many body system in contact with phonon reservoirs. In a 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 terms (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. III, 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 ($\lambda\to 0$), 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 $(T_L+T_R)/2$ 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 $(T_L+T_R)/2$ 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 Ref. [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., the form of the 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 [21].

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].

ACKNOWLEDGMENTS

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

[1] R.E. Peierls, *Quantum Theory of Solids* (Oxford University Press, London, 1955).

[2] K. Saito, S. Takesue, and S. Miyashita, Phys. Rev. E **54**, 2404 (1996).

[3] Z. Rieder, J.L. Lebowitz, and E. Lieb, J. Math. Phys. **8**, 1073 (1967).

[4] U. Zürcher and P. Talkner, Phys. Rev. A **42**, 3267 (1990); **42**, 3278 (1990).

[5] K. Ishii and H. Matsuda, Prog. Theor. Phys. Suppl. **45**, 56 (1970).

[6] W.M. Visscher, Prog. Theor. Phys. **46**, 729 (1971).

[7] W.M. Visscher and M. Rich, Phys. Rev. A **12**, 675 (1975).

[8] G.W. Ford, M. Kac, and P. Mazur, J. Math. Phys. **6**, 504 (1965).
[9] R. Kubo, M. Toda, and N. Hashitsume, *Statistical Physics II* (Springer-Verlag, New York, 1985).
[10] S. Kohler, T. Dittrich, and P. Hänggi, Phys. Rev. E **55**, 300 (1997).
[11] A.O. Caldeira and A.J. Leggett, Ann. Phys. (N.Y.) **149**, 374 (1983); Physica A **121**, 587 (1983).
[12] B.L. Hu, J. Paz, and Y. Zhang, Phys. Rev. D **45**, 2843 (1992); **47**, 1576 (1993).
[13] H. Grabert, P. Schramn, and G. Ingold, Phys. Rep. **3**, 115 (1988).
[14] D.P. Visco, Jr. and S. Sen, Phys. Rev. E **57**, 224 (1998).
[15] G.W. Ford, J.T. Lewis, and R.F. O'Connell, Phys. Rev. A **37**, 4419 (1988).
[16] G. Lindblad, Commun. Math. Phys. **48**, 119 (1976).
[17] R. Karrlein and H. Grabert, Phys. Rev. E **55**, 153 (1997).
[18] W.H. Louisell, *Quantum Statistical Properties of Radiation* (Wiley, New York, 1973).
[19] W. Weidlich and F. Haake, Z. Phys. **185**, 30 (1965).
[20] S. Miyashita, H. Ezaki, and E. Hanamura, Phys. Rev. A **57**, 2046 (1998).
[21] K. Saito, S. Miyashita, and S. Takesue (unpublished).