Thermal conduction in a quantum system

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We numerically investigate thermal conduction in quantum dynamics. A one-dimensional quantum spin system is used as a model, which we can make integrable or nonintegrable by controlling parameter values. A different method to simulate heat reservoirs is introduced. Using this method, we perform numerical simulations of the spin chain in contact with two heat reservoirs at different temperatures. As a consequence, a flat temperature profile is observed in the integrable case, while a finite temperature gradient is found in a nonintegrable system. This result suggests that the Fourier heat law may be realized in nonintegrable systems and is consistent with the classical case reported in the literature. [S1063-651X(96)02409-9]

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The origin of diffusive behavior in thermal conduction, which is formulated in the Fourier heat law, is actively studied by many researchers. Unlike the equilibrium properties, such as the specific heat well described by Debye's theory, the Fourier heat law cannot be explained by the harmonic crystal, where the internal temperature gradient is not formed and the heat flux is proportional to the temperature difference rather than the temperature gradient [1]. Although few models have been proved analytically to satisfy the Fourier heat law [2], numerical studies have found a number of models exhibiting that behavior, e.g., diatomic Toda lattice [3,4], the model composed of free particles alternating with harmonically bound particles by Casati *et al.* [5] and its simplified variant by Prosen and Robnik [6], the Fermi-Pasta-Ulam model [7], and a kind of reversible cellular automata [8]. All of these models are classical one-dimensional lattice dynamical systems with strong nonlinearity. Thus, in the classical cases, it is understood that chaotic behavior originating from the nonlinearity or, more precisely, the nonintegrability is essential for the realization of the Fourier heat law. On the other hand, little is known about the relation between the Fourier heat law and quantum dynamics. Although the infinite thermal conductivity was derived for the quantum perfect harmonic crystal by a quantum Langevin approach [9], no models have been found to exhibit the Fourier heat law. In this paper we present a model that can be a candidate for such behavior.

We investigate energy transport in a quantum spin chain coupled with heat reservoirs. The use of spin systems has the advantage that they are numerically more tractable than oscillator systems because the Hilbert space is finite dimensional in the former case. Concerning equilibrium properties, Jensen and Shankar [10] studied realization of statistical behavior from quantum dynamics in relation to the number of degrees of freedom and the integrability. Their model is a one-dimensional Ising-type quantum spin chain subject to a magnetic field, which is described by the Hamiltonian

$$H_S=\alpha\sum_{i=1}^{N-1}\sigma_i^z\sigma_{i+1}^z+\xi\sum_{i=1}^{N}\sigma_i^x+\gamma\sum_{i=1}^{N}\sigma_i^z, \tag{1}$$

where σ_i^z and σ_i^x are Pauli matrices at site i, α denotes the Ising-type nearest-neighbor coupling constant, and ξ and γ are components of the magnetic field.

According to Jensen and Shankar, we call the system integrable when $\gamma=0$. This means that the system is then transformed into free fermions by a Jordan-Wigner transformation [11]. For example, under the periodic boundary condition we have

$$H_S=2\alpha\sum_k\left\{\left(\cos k+\frac{\xi}{\alpha}\right)^2+\sin^2 k\right\}^{1/2}(c_k^\dagger c_k-\tfrac{1}{2}), \tag{2}$$

where $c_k^\dagger$ and c_k are creation and annihilate operators of the fermion with wave number k, respectively. Thus the system with $\gamma=0$ is regarded as identical to a set of harmonic oscillators. In case of $\gamma\neq 0$, the system is nonintegrable in the sense that the system cannot be transformed into free fermions. This difference in integrability is reflected in the regularity of level spacing distributions in energy spectrum. We numerically calculate the level spacing distributions for the systems with size $N=9$ under the open boundary condition. Two cases of $\gamma=0$ and $\gamma=0.5$ with the other parameters fixed at $\alpha=0.5$ and $\xi=1.0$ are examined. Throughout the present paper, these parameter values are chosen to be used for the integrable and the nonintegrable cases. The distributions in the two cases are shown in Figs. 1(a) and 1(b). In the integrable case, the distribution has a peak at zero separation and the peak is shifted to a finite value in the nonintegrable case. This agrees with the common tendencies seen in quantum dynamical systems.

Jensen and Shankar carried out numerical simulations of the system with $N=7$ and found that the relaxation to equilibrium occurs and the equilibrium values of physical quan-

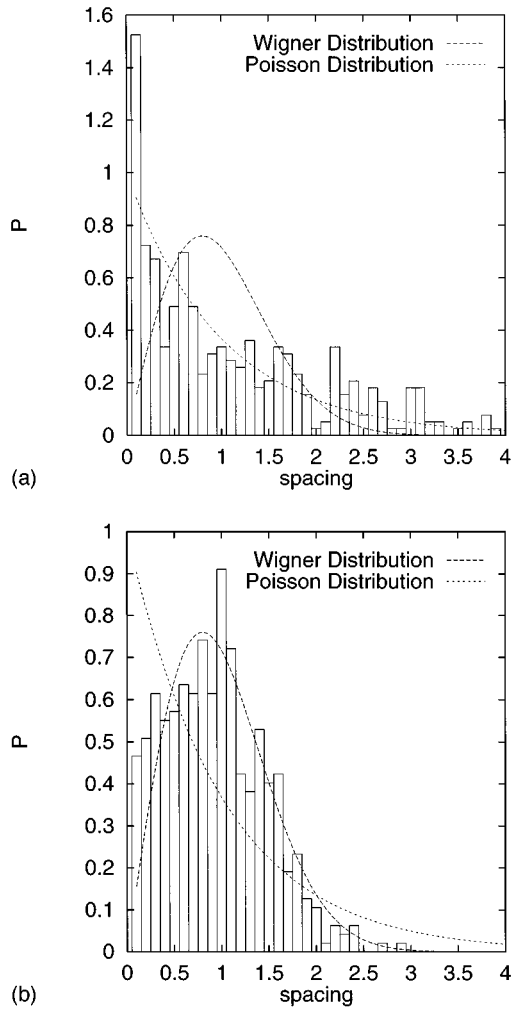

FIG. 1. Level spacing distributions for (a) the integrable system and (b) the nonintegrable system.

tities are successfully predicted by microcanonical ensembles, whether the system is integrable or nonintegrable. They concluded that for generic initial conditions both integrable and nonintegrable quantum systems with as few as seven degrees of freedom can exhibit statistical behavior. Their conclusions were reconfirmed by the present authors [12], where the system-size dependence of the statistical behavior was studied in detail and several definitions of temperature were examined. The lack of difference in equilibrium behavior between integrable and nonintegrable systems is not so surprising because it is frequently seen in classical systems also. For example, equilibrium thermodynamic behavior is observed commonly in a family of reversible cellular automata [13], though many of them do not support the Fourier heat law. Thus, as concerns nonequilibrium behavior, we can expect that the integrable and the nonintegrable systems show some differences.

We denote the reservoir Hamiltonian by H_R and the interaction between the system and the reservoir by $\lambda H_{\rm int}$, λ being the strength of the coupling. Thus the total Hamiltonian is given by

$$H_T = H_S + H_R + \lambda H_{\rm int}. \tag{3}$$

We suppose that the spins 1 and N are in contact with different heat reservoirs and the coupling between the spin chain and the reservoirs is assumed to be of Ising type,

$$H_{\rm int} = \overline{\sigma_1^z}\sigma_1^z + \sigma_N^z\overline{\sigma_N^z}, \tag{4}$$

where $\overline{\sigma_k^z}$ ($k=1$ or N) is the operator that belongs to the reservoir in contact with the kth spin. We do not specify the reservoir Hamiltonian H_R here, but instead later impose a certain condition on the correlation functions of the reservoir variables.

In [12] we showed that local temperatures can be defined by considering subsystems, each of which is composed of two consecutive spins and the bond in between. Let us define the following operators $\hat{a}(i)$ for convenience:

$$\hat{a}(2i-1) \equiv \xi\sigma_i^x + \gamma\sigma_i^z \quad \text{for } 1 \leqslant i \leqslant N,$$
$$\hat{a}(2i) \equiv \alpha\sigma_i^z\sigma_{i+1}^z \quad \text{for } 1 \leqslant i \leqslant N-1.$$

Then the Hamiltonian of the ith subsystem is written as

$$H_{\rm ss}(i) = \hat{a}(2i-1) + \hat{a}(2i) + \hat{a}(2i+1) \tag{5}$$

and the energy flux operators at the left and right ends of the ith subsystem are given by

$$J_L(i) = -i[\hat{a}(2i-1), \hat{a}(2i-2)] = -2\,\xi\alpha\sigma_{i-1}^z\sigma_i^y \tag{6}$$

and

$$J_R(i) = -i[\hat{a}(2i+2), \hat{a}(2i+1)] = 2\,\xi\alpha\sigma_{i+1}^y\sigma_{i+2}^z, \tag{7}$$

respectively. These three operators (5)–(7) are connected with the equation of continuity

$$\frac{\partial H_{\rm ss}(i,t)}{\partial t} = J_L(i) - J_R(i). \tag{8}$$

where $H_{\rm ss}(i,t)$ is the subsystem Hamiltonian in the Heisenberg picture. Note that the ith and $(i-1)$th subsystems share the ith spin.

Heat reservoirs are simulated in the following way. By the standard technique using projection operators and expansion in the coupling strength λ, the equation of motion for the density matrix of the system ρ is derived as

$$\frac{\partial\rho(t)}{\partial t} = -i[H_S, \rho(t)] - i\lambda[\langle\overline{\sigma_1^z}\rangle_1\sigma_1^z + \langle\overline{\sigma_N^z}\rangle_N\sigma_N^z, \rho(t)] + \lambda^2\{[\sigma_1^z, f_1(t) - f_1^\dagger(t)] + [\sigma_N^z, f_N(t) - f_N^\dagger(t)]\}, \tag{9}$$

to $O(\lambda^2)$, where $\langle\ \rangle_k$ ($k=1$ and N) means averaging with respect to the Gibbs state of the reservoir with inverse temperature β_k, operator $f_k(t)$ is defined as

$$f_k(t) = \int_0^t h_k(s) e^{-iH_S s}\rho(t-s)\sigma_k^z e^{iH_S s} ds, \tag{10}$$

and $h_k(s)$ is the autocorrelation functions of variables in the reservoirs

$$h_k(s) = \langle\Delta\overline{\sigma_k^z}\Delta\overline{\sigma_k^z}(s)\rangle_k, \tag{11}$$

where $\Delta\overline{\sigma_k^z}=\overline{\sigma_k^z}-\langle\overline{\sigma_k^z}\rangle_k$ and $\Delta\overline{\sigma_k^z}(s)=e^{iH_R s}\Delta\overline{\sigma_k^z}e^{-iH_R s}$.

Equation (9) is the second-order equation for the reduced density matrix [14]. In this equation, the autocorrelation function $h_k(s)$ is the most important because it includes all reservoir information relevant to the time evolution of the system. This type of equation is sometimes approximated into a Markovian by replacing $\rho(t-s)$ with $\rho(t)$. However, here we attempt to integrate the equation as rigorously as possible, assuming the following form for $h_k(s)$:

$$h_k(s)\simeq h_k(0)\exp\left(-\frac{|s|}{\tau_k}+i\omega_k s\right). \tag{12}$$

In fact, the autocorrelation function in the spin system (1) itself can be well fitted by the above function at least in a short time region. The couple of parameters (τ_k,ω_k) characterizes the dynamical structure of heat reservoir as well as its temperature. We control the values of (τ_k,ω_k) so that the system goes to the equilibrium state at the temperature we want.

Due to the non-Markovian character of Eq. (9), it is very difficult to solve it even numerically. However, the above functional form for $h_k(s)$ provides us with a method for numerical integration of Eq. (9). Consider a difference approximation with time step Δt for Eq. (10). Defining $g_k(t)=h_k(t)/h_k(0)$, we can write

$$f_k(t)\simeq h_k(0)\sum_{n=0}^{t/\Delta t} g_k(n\Delta t)e^{-iH_S n\Delta t}\rho(t-n\Delta t)\sigma_k^z e^{iH_S n\Delta t}\Delta t. \tag{13}$$

Then the next step value of $f_k(t)$ is calculated as

$$f_k(t+\Delta t)=h_k(0)\sum_{n=0}^{t/\Delta t+1} g_k(n\Delta t)e^{-iH_S n\Delta t}\rho(t-(n-1)\Delta t)\sigma_k^z e^{iH_S n\Delta t}\Delta t \tag{14}$$

$$=h_k(0)\rho(t+\Delta t)\sigma_k^z\Delta t+h_k(0)g_k(\Delta t)e^{-iH_S\Delta t}\sum_{n=0}^{t/\Delta t} g_k(n\Delta t)e^{-iH_S n\Delta t}\rho(t-n\Delta t)\sigma_k^z e^{iH_S n\Delta t}e^{iH_S\Delta t}\Delta t \tag{15}$$

$$=h_k(0)\rho(t+\Delta t)\sigma_k^z\Delta t+g_k(\Delta t)e^{-iH_S\Delta t}f_k(t)e^{iH_S\Delta t}\Delta t, \tag{16}$$

where we have used that the relation

$$g_k(t_1+t_2)=g_k(t_1)g_k(t_2)$$

holds for arbitrary times t_1 and t_2. Thus $f_k(t+\Delta t)$ is represented in the iterative form. Because the non-Markovian character comes only through $f_k(t)$ in Eq. (9), this allows us to integrate Eq. (9) numerically.

A necessary condition for heat reservoirs is that the system coupled with a reservoir has to relax to an equilibrium state characterized by a canonical ensemble. It is shown that if the function $h_k(s)$ satisfies the Kubo-Martin-Schwinger (KMS) condition

$$\hat{h}_k(\omega)=e^{\beta\omega}\hat{h}_k(-\omega), \tag{17}$$

where $\hat{h}_k(\omega)$ denotes the Fourier transform of h_k, the right-hand side of Eq. (9) vanishes for a Gibbs state $\rho=\rho_{\mathrm{Gibbs}}$ and the stationarity of the Gibbs state is guaranteed. Although our $h_k(s)$ given by Eq. (12) does not satisfy the KMS condition, it is possible that the Gibbs state is a numerically stable solution of Eq. (9) [15]. Thus we numerically simulate the system coupled with a single reservoir until the system reaches a stationary state and evaluate the density matrix. The stationary energy distribution thus obtained is shown in Fig. 2, where the system size $N=4$, reservoir parameters are chosen to be $(\tau_1,\omega_1)=(1.0,\pi/0.7)$, the system is the nonintegrable one, and the coupling $\lambda=\alpha$. The solid line shows the canonical distribution at temperature 1.2 and dots represent the diagonal elements of the density matrix in the representation that diagonalizes H_S. This representation also diagonalizes the stationary density matrix. The agreement between the observed energy distribution and the prediction by a canonical ensemble shows that the system certainly reaches equilibrium states described by statistical mechanics. We have also confirmed that two reservoirs at the same temperature connected at both ends lead the system to almost the same state as the single reservoir case. For various values of (τ,ω), corresponding temperature values are estimated from the slopes of the energy distributions.

In the simulation of heat conduction, we couple the system with two reservoirs at different temperatures and inte-

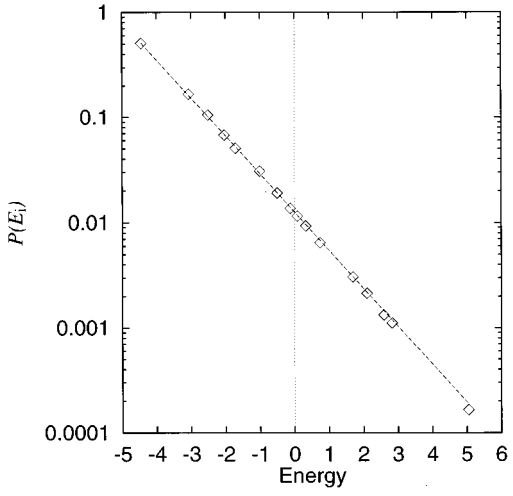

FIG. 2. Stationary energy distributions for the nonintegrable system coupled with a single reservoir.

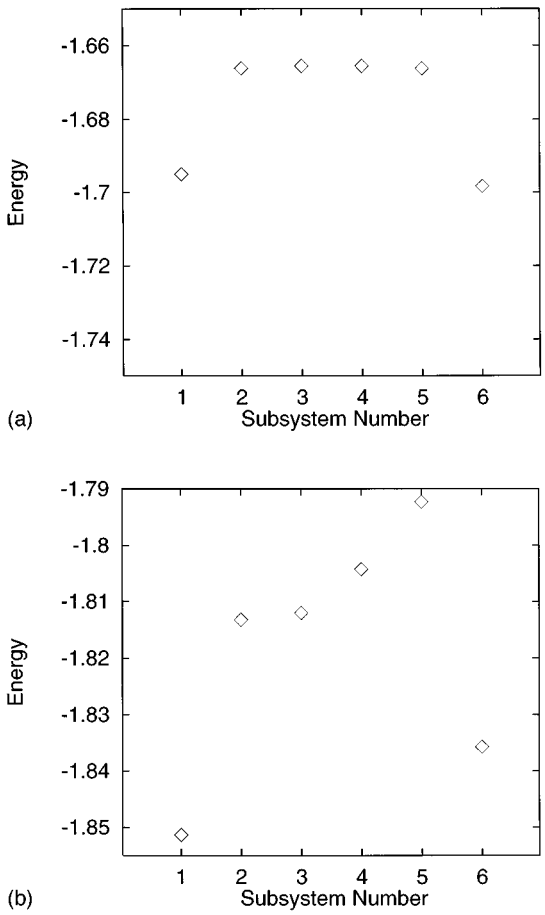

FIG. 3. Mean energies of the subsystems for (a) the integrable system and (b) the nonintegrable system.

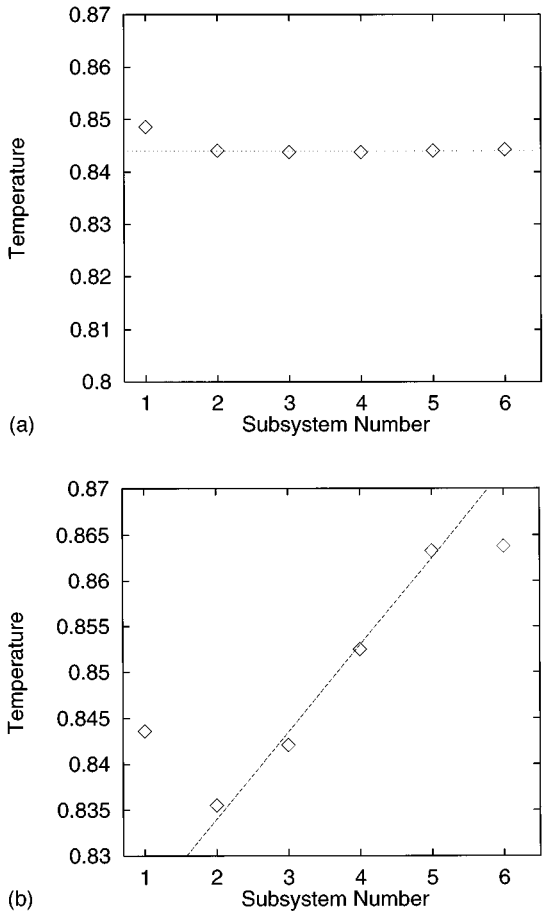

FIG. 4. Temperature profiles for (a) the integrable system and (b) the nonintegrable system.

grate Eq. (9) until the system reaches a stationary state. Thus we obtain the stationary density matrix. The mean energy of the ith subsystem is calculated in the stationary state and the results for the integrable and the nonintegrable cases are shown in Figs. 3(a) and 3(b), respectively. Here the system size is chosen to be $N=7$ and the coupling constant $\lambda=0.20$. The simulation has been executed with the fourth-order Runge-Kutta method with a time step of 0.005. The reservoir parameters are $(\tau_1,\omega_1)=(2.0,\pi/1.0)$ and $(\tau_N,\omega_N)=(1.0,\pi/0.5)$ for both systems, which correspond to temperatures 0.7 and 2.0, respectively.

The temperature of the ith subsystem is determined by comparing the observed ith local energy with its equilibrium expectational values

$$\langle \varepsilon_i(\beta)\rangle = \frac{\mathrm{Tr}\{H_{\mathrm{ss}}(i)e^{-\beta H_S'}\}}{\mathrm{Tr}\{e^{-\beta H_S'}\}}, \tag{18}$$

where

$$H_S' = H_S + \lambda(\langle\overline{\sigma_1^z}\rangle_1\sigma_1^z + \langle\overline{\sigma_N^z}\rangle_N\sigma_N^z). \tag{19}$$

The additional terms on the right-hand side are needed in order to take into account edge effects at the ends of the system and to eliminate the first-order terms in λ from the right-hand side of Eq. (9). Note that the energy-temperature relation thus obtained depends on subsystem location because of the lack of translational invariance. Thus the temperature distribution shows different behavior from the energy distribution.

The temperature profiles for the two types of the systems are shown in Figs. 4(a) and 4(b). In both cases, there are large temperature gaps between the lattice ends and the reservoirs and the region of temperature values narrows compared to the applied temperature gradient. The subsystems closest to the reservoirs show peculiar behavior, while a smooth curve is observed in the interior of the system. These behaviors are similar to those observed in the classical lattice dynamical systems, except that the temperature regions do not go to the middle of the applied temperatures but are shifted greatly toward the lower temperature value of the reservoirs. This is partly due to the finiteness of the time step Δt used in the simulations. We observe that varying Δt leads to quantitatively different results, though the qualitative behavior in the profile does not change. Further studies on the properties of the present approximation are planned for future. The temperature shift may have another origin because similar behavior is observed in the simulations with the use of cellular automata [16]. We have not reached a full understanding of this phenomenon.

Figure 4 also shows a difference in the integrable and nonintegrable systems. Namely, the internal temperature distribution has a finite slope in the nonintegrable case, which is in contrast with the flat temperature profile in the integrable case. Energy fluxes $J_L(i)$ and $J_R(i)$ take an identical mean value in the stationary state and are independent of i. In our nonintegrable case, the value of the stationary energy flux and the internal temperature gradient are about 0.0012 and 0.01, respectively. Thus the coefficient of thermal conductivity is estimated to be about 0.12.

The present study shows that, as in the classical systems, chaotic behavior generated from nonintegrability may play an essential role in nonequilibrium thermodynamic behavior. The present model shows a finite temperature gradient in the nonintegrable case. The formation of the temperature gradient is a necessary condition for the Fourier heat law, but, of course, not sufficient to say that the system obeys the Fourier heat law. To confirm the Fourier law, we have to check the system-size dependence of the heat flux. If the total heat flux does not depend on the system size the Fourier heat law is satisfied, but if it grows with system size it is not. In classical systems, both behaviors are observed, depending on the strength of the nonlinearity. Thus we cannot predict at present which is the case in our quantum spin model. If the Fourier heat law is satisfied, the Green-Kubo formula and the assumption of local equilibrium should also be checked. The present study is a first step and many problems are left for the future.

On the other hand, the present study has clarified that the integrable system does not obey the Fourier heat law. This is common behavior also seen in the classical harmonic crystal and various integrable systems. Because our system is expressed as free fermions, it corresponds to the harmonic crystal. There are other types of quantum integrable systems, that can be solved by the use of Bethe ansatz. They may correspond to nonlinear integrable systems in classical mechanics. It will be interesting to study heat conduction in such systems and to see whether there are any differences among theirs and the present one.

In quantum systems, nonintegrability affects the regularity in the energy spectrum. It can be used to characterize the degree of nonintegrability. Thus we hope to find a connection between the heat conduction behavior and some characteristics of the level statistics. Research in this direction is now in progress.

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