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Thermal conductivity in one-dimensional quasi-periodic Toda lattices

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Abstract. We investigate the thermal conductivity in one-dimensional quasi-periodic Toda lattice by means of the molecular dynamics technique. The lattice consists of two kinds of atom with different masses which are arranged according to the Fibonacci sequence. The temperature profile exhibits exponential behaviour as does the diatomic Toda lattice presented in our previous paper. The thermal conductivity is evaluated by separating the ballistically propagating part from the total heat flow. Heat conduction in the Toda lattice with quasi-periodic mass distribution is found to obey Fourier's law. The resultant thermal conductivity is inversely proportional to local temperature and the magnitude is reduced remarkably in comparison with that of the diatomic Toda lattice.

1. Introduction

Heat transport phenomena have been described phenomenologically in terms of Fourier's law. It is known that heat is carried by lattice vibrations in an electrically insulating material. Many attempts to derive Fourier's law from first principles have been performed using molecular dynamics techniques [1–9]. However, most attempts have failed to present the normal thermal conductivity without external disturbances except in some special cases, e.g. a ding-a-ling model [7]. In 1983, Mokross and Büttner [10] suggested that a one-dimensional diatomic Toda lattice could offer the normal thermal conductivity. More recently, Jackson and Mistriotis [11] investigated the heat conduction for a larger diatomic Toda lattice and confirmed the existence of Fourier's law by means of a similar method.

Although they seemed to present successfully the normal thermal conductivity, analyses of the thermal conductivity in terms of molecular dynamics so far could not be justified on account of at least two points. First, the temperature profile has been assumed to be linear to evaluate thermal conductivity and always approximated to a straight profile. However, the temperature profiles obtained numerically are rather exponential [5, 10, 11]. Second, another important point is that heat is transported not only through the diffusive process but also through the non-diffusive or ballistic process [5, 11]. The non-diffusive part cannot give a finite thermal conductivity. Therefore, we have to separate the ballistic heat current from the total heat currents in numerical experiments to evaluate the thermal conductivity.

In a previous paper [12], taking account of the two important points mentioned above which had been overlooked so far, we investigated the existence of Fourier's law in the one- and two-dimensional diatomic Toda lattices by means of the molecular

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dynamics technique. We found that the bending temperature profile reflects the temperature dependence of the thermal conductivity and confirmed the existence of Fourier's law by excluding the ballistic component of heat current. The resultant thermal conductivity is inversely proportional to the local temperature for both the one- and the two-dimensional lattices as well as the three-dimensional solids in the temperature region above the peak of thermal conductivity.

Quasi-periodic systems have attracted much attention recently and have been studied theoretically and experimentally since the discovery of the quasi-crystalline phases in Al–Mn alloys [13]. The lattice vibrational properties of the quasi-periodic systems have been investigated numerically and theoretically [14, 15], which are expected to reflect the self-similarity of the lattice structure. Machida and Fujita [15] investigated a harmonic one-dimensional Fibonacci lattice and found that there is some specific vibrational state referred to as a critical state whose properties are intermediate between a localized and extended state as well as an electronic system. The corresponding frequency spectrum exhibits spiky structures. On the other hand, phonon transmission through quasi-periodic superlattices [16] is known to be affected by the quasi-periodic lattice structures. The transmission rate exhibits a spiky structure in the quasi-periodic superlattice where two kinds of layers (GaAs and AlAs) are stacked following the Fibonacci sequence. Thus, the characteristic features in the phonon transmission rate are expected to cause the vital phenomena in thermal conductivity. At very low temperatures where the phonon picture still survives, the thermal conductivity will be affected drastically by the critical states. At high temperatures, the anharmonic interatomic interaction couples the critical states and might give considerable changes in the thermal conductivity. The question is whether the effect of quasi-periodicity on the thermal conductivity at high temperatures is enhanced or reduced . Little is known about the effect of the anharmonic potential on the lattice vibrational states in the quasi-periodic system.

In this paper, we study the thermal conductivity of a one-dimensional quasi-periodic lattice with Toda potential using the molecular dynamics technique.

The plan of this paper is as follows: in section 2, we describe the model to be studied and mention the method of numerical simulation. We discuss the local rate of divergence of trajectories in the phase space to clarify the temperature region where the normal thermal conductivity is expected. In section 3, the temperature dependence of thermal conductivity is discussed from the temperature profiles and the thermal conductivity is estimated by excluding the ballistic heat current from the total current. We compare the results with those of the diatomic Toda lattice. Summary and discussions are presented in section 4.

2. One-dimensional Fibonacci Toda lattices

We consider a one-dimensional Toda lattice whose mass distribution is governed by the Fibonacci rule, i.e. an arrangement of two kinds of atom, A and B, which follows the Fibonacci sequence given by the rule $F_n = F_{n-1}F_{n-2}$ starting with $F_1 = \mathrm{A}$ and $F_2 = \mathrm{AB}$. We refer to this lattice as the Fibonacci Toda lattice hereafter. The masses of atoms A and B are m_A and m_B, respectively. The total energy of the lattice is

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \tfrac{1}{2} \sum_{i(\neq j)}^{N} \sum_{j}^{N} V(u_i - u_j) \tag{1}$$

where p_i and u_i are the momentum and displacement, respectively, of the ith atom. N is total number of atoms. The interatomic potential $V(r)$ is a Toda potential defined by

$$V(r) = (b/a)\ \exp(-ar) + br - b/a \tag{2}$$

where r is the relative displacement and a and b are the potential parameters which are all set to unity in our paper. Figure 1 shows the mass configuration for the Fibonacci Toda lattice. To avoid the deformation of temperature profiles near the heat baths due to thermal boundary resistence, the specimen lattice is sandwiched with two buffer areas of monatomic Toda lattices with ten atoms. As the monatomic Toda lattice is integrable [17], there is no temperature gradient in the buffer areas. On the other hand, the mass arrangement of the specimen lattice following the Fibonacci sequence breaks the integrability and a finite temperature gradient is expected to appear as well as the diatomic lattice with the Toda potential.

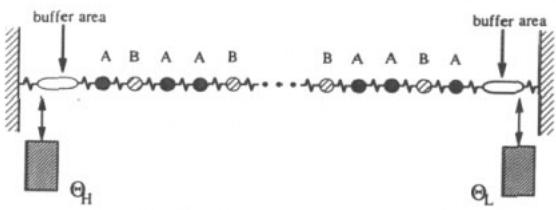

Figure 1. Model and experimental situation for the one-dimensional Fibonacci Toda lattice. Circles with label A or B denote the atoms with masses m_A and m_B of specimen lattice, respectively. The magnitude of m_A and m_B are set to be 1.0 and 0.5, respectively, in the numerical experiments. There are buffer areas at both ends of the specimen lattice in order to avoid deformation of the temperature profile. The buffer areas are monatomic Toda lattices whose masses are also set to unity here. All particles are connected with Toda potentials. The lattice is heated by the elastic collision of atoms between the lattice ends and the heat reservoirs whose temperatures are Θ_H and Θ_L.

The end atoms are linked to the fixed walls with the Toda potential and interact impulsively with atoms of heat baths with prescribed temperatures Θ_H and Θ_L. The elastic collision between the end atoms and gas particles in the heat baths provides the energy exchange between the specimen lattice and the heat baths. The gas particles are assumed to have the Maxwell distribution in velocity of the form

$$N(v,\Theta) = \sqrt{\frac{M}{2\pi k_B \Theta}}\ \exp\left(-\frac{Mv^2}{2k_B\Theta}\right) \tag{3}$$

where M is the mass of the gas particles, Θ is the temperature of the heat bath and k_B is the Boltzmann constant which is set to unity hereafter.

The equation of motion is solved numerically by means of Runge–Kutta–Gill method. In this work, we set $m_A = 1, m_B = 0.5$. The masses of buffer areas and gas particles are also set to unity. The time fraction interval of the simulations is taken suitably, so that the energy conservation in the non-equilibrium state will hold within the error of 0.1%.

As is well known, stochastic behaviour is closely related to the irreversibility of the phenomena. Therefore, the investigation of the divergence of trajectories starting

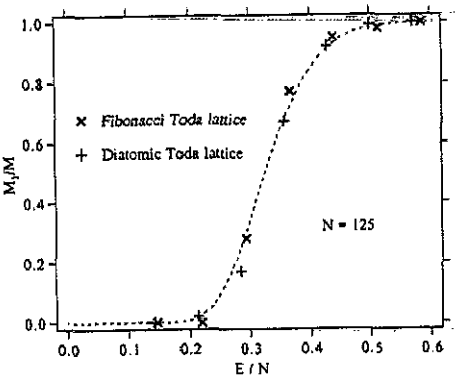

Figure 2. The probability in the phase space that the system exhibits the stochastic behaviour versus the energy per atom for both the Fibonacci and the diatomic lattices with $N = 125$. The characteristic time interval is $T_s = 96$ for both cases.

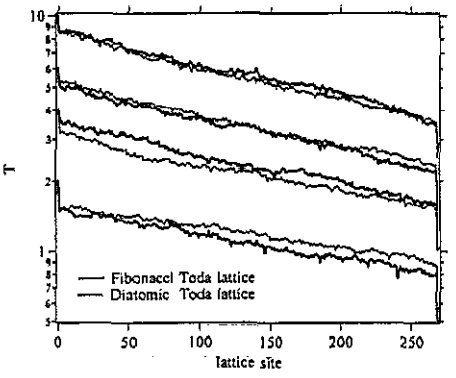

Figure 3. Temperature profiles for one-dimensional inhomogeneous Toda lattices. The length of specimen lattices is 250 atoms. The bold full curves denote those for the Fibonacci lattices, and the thin full curves those for the diatomic lattices. The temperatures of the heat baths are $(\Theta_H = 10, \Theta_L = 2.5), (\Theta_H = 6, \Theta_L = 1.5), (\Theta_H = 4, \Theta_L = 1)$ and $(\Theta_H = 2, \Theta_L = 0.5)$ from the top, respectively (all in Kelvin).

from two points close to each other in phase space has been performed to check the global thermal equilibrium. However, in the non-equilibrium state, as denoted by Jackson and Mistriotis [11], the dynamical behaviour must become stochastic within a short time interval whilst the incoming pulses still stay in the system, for the normal thermal conductivity.

Whether the system exhibits irreversibility or not in the non-equilibrium state depends on the strength of non-linearity of the system, and the strength will change critically with temperature. We therefore investigate the divergence of trajectories in a short time interval with varying total energy for the one-dimensional Fibonacci Toda lattice with $N = 125$ excluding buffer areas. The sound transit time interval is estimated to be $T_s = 96$ from the pulse and wave propagation experiments. The time interval is equal to that of the one-dimensional diatomic lattices. The type of divergence of trajectories is judged from the value of the quantity $\mu(T_s)$ defined by

$$\mu(T_s) = \int_0^{T_s} \mathrm{d}t \, \{|d(t) - A(q_\Gamma, p_\Gamma, T_s) \exp[k(q_\Gamma, p_\Gamma, T_s)t]|^2 - |d(t) - B(q_\Gamma, p_\Gamma, T_s)t - C(q_\Gamma, p_\Gamma, T_s)|^2\}. \tag{4}$$

Here $d(t)$ is the distance between two trajectories starting in the neighbourhood of a point in the phase space which is approximated for $0 < t < T_s$ by a function of the form $A(q_\Gamma, p_\Gamma, T_s) \exp[k(q_\Gamma, p_\Gamma, T_s)t]$ and also by a linear function of the form $B(q_\Gamma, p_\Gamma, T_s)t + C(q_\Gamma, p_\Gamma, T_s)$ using the least-squares method. Therefore, the negative μ denotes that the divergence of trajectories is close to exponential behaviour and that the irreversibility can be expected. We calculated the local rate of divergence 100 times at every value of energy per atom. This test was performed numerically and the ratios of the number M_1 of the exponential development to the total trials M were obtained for the energy per atom, namely E/N.

Figure 2 exhibits the resultant probability that the system offers the stochastic behaviour for both the Fibonacci and the diatomic Toda lattices with 125 atoms. The dynamical behaviour for the Fibonacci Toda lattice becomes stochastic above $E/N = 0.3$ and saturates at around $E/N = 0.5$. The dependence of the probability on the energy per atom is almost the same as that of the diatomic Toda lattices. The critical value of the energy per atom is reduced with increasing system size. As the energy per atom is almost equivalent to the temperature of the system, the normal thermal conductivity is expected in the region $T > 0.5$ at least.

3. Thermal conductivity

The local temperature is defined to be twice the averaged local kinetic energy as follows:

$$T_i = 2\langle p_i^2/2m_i \rangle. \tag{5}$$

Here the angular brackets denote the time average. We investigate the Fibonacci Toda lattices with $N = 250$, 350 and 450. Each system has the buffer areas with ten atoms at both ends. The temperature profiles are investigated by varying the temperatures of the heat baths, whilst keeping their ratio $\Theta_H/\Theta_L = 4$. Figure 3 exhibits the resultant temperature profiles of the system with $N = 250$ together with those of the diatomic Toda lattice of the same length. There clearly exist sharp drops in the temperature profiles at both ends of the lattices, which exhibit a thermal boundary resistance (Kapitza resistance) because of the existence of the acoustic mismatching. We can easily see that the temperature profiles vary exponentially with respect to the distance in the same way as for the diatomic Toda lattices. This is true for the other cases with 350 and 450 atoms. We can empirically approximate the temperature profiles by an exponential function of the form

$$T(x) = T_H(T_L/T_H)^{x/N} \tag{6}$$

where T_H and T_L are the temperatures at the ends of the specimen lattice and x measures the distance from the interface between the buffer area and the specimen lattice. The temperature profile (6) yields the temperature gradient as

$$(\mathrm{d}T/\mathrm{d}x) = -(1/N)\ \log\ (T_L/T_H)\ T. \tag{7}$$

The absolute values of temperature gradients of the Fibonacci Toda lattices become larger than those of the diatomic Toda lattices as the temperatures of the heat baths decrease. This means that the Fibonacci lattice has a smaller thermal conductivity, which will be confirmed below.

The heat current J can be represented in terms of the local energy conservation law as

$$J(i+1,i) - J(i,i-1) + \partial\epsilon_i/\partial t = Q_H\delta_{i,1} + Q_L\delta_{i,N}. \tag{8}$$

Q_H and Q_L are the energies per unit time exchanged with the heat baths of high and low temperatures, respectively. At the steady non-equilibrium state, summing equation (8) from the heat bath with Θ_H, the time-averaged heat current yields

$$\langle J(i+1,i)\rangle = \langle Q_H\rangle \tag{9}$$

because the time-dependent term vanishes. As can be seen from equation (9), the heat current no longer depends on the lattice position. We have used this as a criterion of the establishment of the steady non-equilibrium state in the numerical experiments.

As we pointed out in the previous paper and also noted in section 1, the heat current consists of the two kinds of heat flow. One is the normal or the diffusive current J_N and the other is the ballistic or non-diffusive current J_B:

$$J = J_N + J_B. \tag{10}$$

Here the normal heat current J_N is expected to obey Fourier's law:

$$J_N = -\kappa \, dT/dx. \tag{11}$$

On the other hand, the non-diffusive current J_B is considered to depend on the temperature difference $T_{B,H} - T_{B,L}$ between the two heat baths and on the system size N. It should be noted that T_H is not equal to $T_{B,H}$, and T_L to $T_{B,L}$, because of the existence of the thermal boundary resistance.

Substituting equations (7) and (11) into (10), we have

$$J = \kappa(1/N) \log(T_H/T_L) \, T + J_B(T_{B,H} - T_{B,L}, N). \tag{12}$$

Although the local temperature varies with the lattice position exponentially, the heat current is constant through the lattice in the steady non-equilibrium state. Therefore, the thermal conductivity κ has to be inversely proportional to the local temperature in order to cancel the temperature dependence of the first term of the right-hand side of (12) as

$$\kappa = \xi/T. \tag{13}$$

Here ξ is a parameter to be determined from the data in the numerical experiment. In order to confirm the validity of Fourier's law, the constant ξ should be independent of the system size. In order to determine the parameter ξ, we rewrite the equation as follows:

$$JN/\log(T_H/T_L) = \xi + J_B(T_{B,H} - T_{B,L}, N)N/\log(T_H/T_L). \tag{14}$$

Figure 4(*a*) exhibits the results of the one-dimensional Fibonacci Toda lattice. It should be noted that the data are independent of the lattice size. As the temperature difference $T_{B,H} - T_{B,L}$ decreases, the magnitude of $JN/\log(T_H/T_L)$ decreases monotonically and seems to achieve a finite value at zero temperature difference. Figure 4(*b*) shows the details at the small temperature differences together with the data for diatomic cases. Extrapolating the data to the origin, we have the finite values of ξ to be 15.9 and 36.8 for the Fibonacci and diatomic Toda lattices, respectively.

4. Summary and discussion

We have investigated the heat transport phenomena of the one-dimensional Fibonacci Toda lattice in terms of the molecular dynamics technique. We checked the local rate

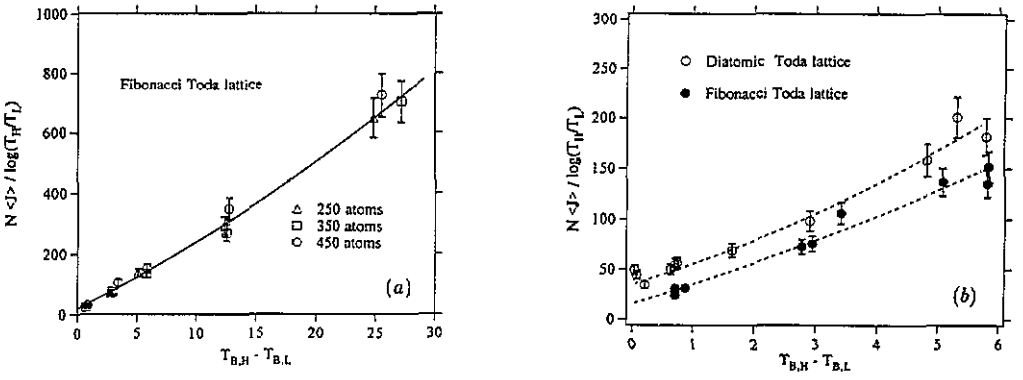

Figure 4. (*a*) The heat current per unit length per $\log(T_H/T_L)$ versus the temperature difference of the buffer areas for the one-dimensional Fibonacci Toda lattices. The open triangles, open squares and open circles denote the data for the lattices with N = 250, 350 and 450, respectively. The full curve is drawn using the least-square method. (*b*) The heat current per unit length per $\log(T_H/T_L)$ versus temperature difference of the buffer areas for the one-dimensional Fibonacci and diatomic Toda lattices at small temperature differences. The full circles denote the one-dimensional Fibonacci Toda lattices. There is no distinction between the data with respect to the lattice size for legibility. The open circles denote the diatomic lattices. The broken curves are drawn using the least-squares method to exhibit the extrapolation of the data to zero temperature difference. The extrapolated magnitude of ξ becomes 15.9 for the Fibonacci Toda lattice. The magnitude of the diatomic Toda lattice is 36.8.

of divergence of trajectories in a phase space and found that the system exhibits stochastic behaviour in a short time interval above some critical temperature. The resultant temperature profiles are empirically expressed by an exponential function, as are those of the diatomic Toda lattices. The derivative of the temperature profiles is proportional to the local temperature. This requires that the thermal conductivity is inversely proportional to the local temperature. The heat current consists of diffusive and non-diffusive components. By excluding the non-diffusive part, the coefficient ξ of thermal conductivity is determined from the experimental results and yields ξ = 15.9 for the Fibonacci lattice. This is about 43% of that of the corresponding diatomic Toda lattices (ξ = 36.8). The parameter is also identified to be independent of the lattice size. This gives evidence that the present Fibonacci Toda lattice can give the normal thermal conductivity.

In this paper, we anticipated some novel phenomena in the thermal conductivity due to the possible existence of the critical states of the lattice vibration in the quasi-periodic structure. Comparing the results with those of the diatomic Toda lattice, as far as thermal conductivity is concerned, there is no qualitative difference between the Fibonacci and diatomic Toda lattices except the magnitude of thermal conductivity. As is well understood, the anharmonic potential couples vibrational modes and smears the fine structure in the frequency spectrum. At the temperatures where the normal thermal conductivity is expected, the anharmonicity is so strong that the dynamical behaviour of the lattice vibrations becomes stochastic. The characteristic features of normal modes in the quasi-periodic system are mainly due to the interference between the reflected waves in the system. In general, the stochastic behaviour breaks the coherence. This is the reason why there is no essential difference in the heat conduction between the Fibonacci and diatomic Toda lattice.

Now we give a qualitative explanation why the thermal conductivity of the Fibonacci Toda lattice is more reduced than that of the diatomic Toda lattice. As was seen in figure 3, the difference between the temperature profiles of the Fibonacci and the diatomic Toda lattices with the same heat baths is small. The logarithm of the ratio T_H/T_L of the Fibonacci Toda lattices is almost equal to that of the diatomic lattices. Therefore, the reduction in the thermal conductivity is attributed to the decrease in the heat flow in the Fibonacci Toda lattices.

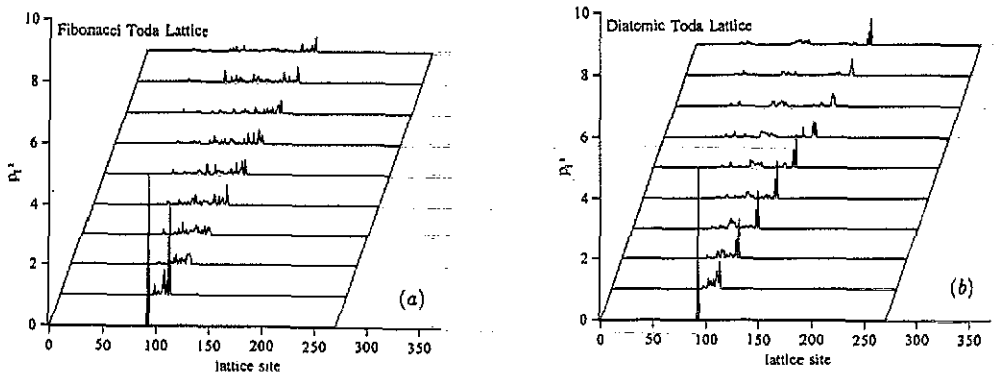

Figure 5. The propagation and attenuation of an initial velocity impulse, where the ordinate is the squared momentum of the atoms: (*a*) the Fibonacci Toda lattice; (*b*) the diatomic Toda lattice.

The collisions between pulses are known to be important to the energy sharing between the particles in the lattice [11]. In this respect, we investigate the decay of a velocity pulse in the Fibonacci and diatomic Toda lattice. Figures 5(*a*) and 5(*b*) exhibit the decay of the pulse followed by the emission of a train of small pulses for the Fibonacci and diatomic Toda lattices, respectively. The emission of the small pulses and the decay of the main pulse are more marked in the Fibonacci Toda lattice than in the diatomic lattice. In order to investigate quantitatively the time evolution of the energy distribution in the lattice, we evaluate the time-dependent participation ratio $P(t)$ defined by

$$P(t) = \langle \epsilon_i(t) \rangle^2 / \langle \epsilon_i(t)^2 \rangle \tag{15}$$

where ϵ_i is the local energy of the ith atom and the angular brackets denote the site averaging. The participation ratio takes the value of unity when the vibrational energy is shared equally to all atoms. On the other hand, it has the value of $1/N$ when the energy is concentrated on one atom, where N is the total number of atoms. Figure 6 confirms that the collapse of the primary pulse is more rapid in the Fibonacci Toda lattice than in the diatomic lattice. As the collision between the primary pulses plays a dominant role in the energy-sharing mechanism, the rapid decay of the primary pulse may lead to the reduction in the diffusive part of the heat currents, namely the reduction in the normal thermal conductivity in the Fibonacci Toda lattices.

According to the present results, the thermal conductivity for the quasi-crystalline solids is expected to differ considerably in magnitude from that of crystals. The experiment to measure the thermal conductivity of the insulating quasi-crystalline solids is rather difficult since it is hard to prepare a large enough specimen for the

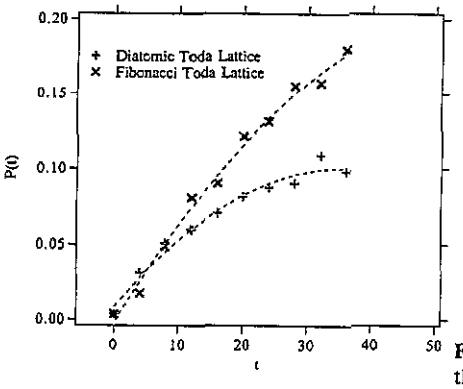

Figure 6. The time evolution of the participation ratio for the Fibonacci Toda lattice and the diatomic lattice.

heat conduction experiment. This is the main reason why we undertook a numerical simulation of the heat conduction in the one-dimensional quasi-periodic model solid.

In higher dimensions, the quasi-periodic structure is modelled with the Penrose lattice in two dimensions and icosahedral structure in three dimensions. Therefore, it would be worthwhile to investigate the thermal conductivity by means of the molecular dynamics technique in these aperiodic structures.

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