Energy transport between two attractors connected by a Fermi–Pasta–Ulam chain

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Abstract.   We numerically study the time evolution of a system which consists of two attractors connected by a one-dimensional Fermi–Pasta–Ulam (FPU) chain. It is found that there exists a self-consistent large-scale structure in the system even after a sufficiently long time. The wavelet transform is envoked to separate the modes of different scales. We discover that the existence of a nonlinear long-wavelength mode in the system assists the energy transport, which leads to the violation of the Fourier heat law in a one-dimensional FPU model as observed by other authors.

1. Introduction

The finding of Fermi *et al* [1] (hereafter referred to as FPU) in 1955, i.e. the absence of energy equipartition in a system of coupled nonlinear oscillators, became a cornerstone in modern statistical mechanics [2, 3]. It stimulated the study of nonlinear dynamics and chaos.

Since the first numerical experiment of FPU, many works have been done on one-dimensional (1D) anharmonic oscillators to study various problems related to irreversiblie statistical mechanics [2]. In addition to studies of the relation between the stochastic motions and thermodynamics properties [4, 5], the FPU model has recently been used to study another important problem in nonequilibrium systems, namely, the heat conduction in a 1D chain [6, 7].

Kaburaki and Machida [6] studied the thermal conductivity of different 1D FPU chains (mono-atomic and diatomic) by coupling the chain of N particles to thermal reservoirs which is realized by numerical random generators. They found that the thermal conductivity κ diverges as $N^{1/2}$ approximately for the mono-atomic FPU chain. Whereas for the diatomic FPU chain, the thermal conductivity is only constant when the mass ratio becomes much larger (or smaller) than 1. As the mass ratio becomes approximately unity the diatomic FPU model is reduced to the mono-atomic FPU model, and the thermal conductivity diverges.

Most recently, Lepri *et al* [7] (hereafter referred to as LLP), revisited this problem by using a different method of realizing the thermal reservoir. In LLP's study, two Nosé–Hoover 'thermostats' [8, 9] were put on the first and last particles of the FPU-β model (FPU model with quartic potential). The two reservoirs are kept at constant temperatures T_+ and T_-, respectively. The two ends of the chain are fixed. After a certain transient time, the nonequilibrium stationary state sets in and the temperature profile becomes nonlinear

shaped. Their results confirm the finding of Kaburaki and Machida, i.e. the Fourier heat law is not justified in the FPU model.

We would like to point out that the divergence behaviour of thermal conductivity in the 1D FPU model does not depend on the choice of the reservoirs' temperature T_+ and T_-. For example, in the early work, Kaburaki and Machida [6] used $T_+ = 100$ and $T_- = 10$, while in LLP's work $T_+ = 152$, $T_- = 24$. More recently, we have also investigated this model at very low temperatures such as $T_+ = 0.3$, $T_- = 0.2$ [10]. In all these different temperature ranges, there exists a simple nontrivial scaling relation for the temperature profile as aforementioned, i.e. $T_l = T(l/N)$ (see figure 1 in LLP's paper and figures 2 and 3 in [6]), which means that the temperature gradient $dT/dx \sim 1/N$. The heat flux J is found to be N^α, $\alpha \approx \frac{1}{2}$. Thus, the thermal conductivity

$$\kappa = \frac{J}{dT/dx} \tag{1}$$

diverges as $N^{1/2}$ approximately.

Compared with that case of the ding-a-ling model [11], where the heat transport obeys the Fourier heat law, i.e. the thermal conductivity is independent of the particle number N, LLP concluded that the chaotic behaviour is not sufficient to ensure the Fourier heat law. However, a sound explanation for this puzzling result has until now been lacking.

Although it is commonly believed that the anharmonicity or the nonlinear interaction leads to the scattering of phonons, the mechanism leading to the divergence of the thermal conductivity in the FPU model and other similar nonlinear oscillator chains is not clear. In fact, it is a very general problem in the field of statistical physics to understand the origin of the irreversibility and its compatibility with the time-reversible deterministic microscopic dynamics.

In this paper, we shall restudy the FPU model and make further analysis. We shall try to give an answer, at least qualitatively and phenomenologically, to the puzzle. To this end, we should concentrate on the long-time evolution of the system. As we shall see later, there exists a long-wavelength mode propagating along the chain which assists the energy transport. We believe that it is due to this long-wavelength mode that the thermal conductivity is divergent.

2. The model and numerical simulation

The Hamiltonian of the 1D FPU β model is:

$$H = \sum_{i=0}^{N+1} \frac{p_i^2}{2m_i} + V(x_{i-1}, x_i) \qquad V(x_{i_1}, x_i) = \frac{1}{2}(x_i - x_{i-1})^2 - \frac{\beta}{4}(x_i - x_{i-1})^4 \tag{2}$$

where p_i is the momentum of the ith particle, x_i the displacement from the equilibrium position, and β is a nonlinear parameter. In our calculation, m_i is taken to be unity.

As in LLP, the ends of the chain are kept fixed, namely, $x_0 = 0$ and $x_{N+1} = 0$. The equation of motion for the central particles is,

$$\ddot{x}_i = f_i - f_{i+1} \qquad i = 2, \ldots, N-1 \tag{3}$$

where $f_i = -V'(x_{i-1} - x_i)$ is the force acting on the particle.

The first and last particles are kept at the 'thermostats' having temperatures T_+ and T_-, respectively. Thus, the equations of motion of the two particles being kept at the

'thermostats' are determined by (in our calculation, the Boltzman constant $k = 1$)

$$\ddot{x}_1 = -\zeta_+ \dot{x}_1 + f_1 - f_2$$
$$\ddot{x}_N = -\zeta_- \dot{x}_N + f_N - f_{N+1} \tag{4}$$

where ζ_+ and ζ_- are thermodynamic friction coefficients. They describe microscopically the action of the heat reservoirs. The time evolution is determined by the Nosé–Hoover dynamical equations [8, 9]

$$\dot{\zeta} = (\dot{x}^2 - T)\frac{1}{Q} \tag{5}$$

where Q is a parameter of dimension energy $\times$ (time)^2. It can be written as $Q = T\tau^2$, where T is the temperature of the reservoir and τ is the response time of the reservoir and are chosen as $\tau = 1$ throughout this paper. The notation means that the kinetic energy of the boundary particles fluctuates around the imposed average value, which in principal should simulate a 'canonical' dynamics. It is obvious that the dynamical equations are invariant under time reversal combined with the change $p_i \to -p_i$.

The above-mentioned Nosé–Hoover 'thermostats' were proposed as the extension of molecular dynamics methods to treat the problem of whether the statistical mechanics can be derived from the underlying dynamics [2, 8].

It has been shown that the canonical distribution with a given temperature can be generated with smooth, deterministic and time-reversible trajectories. However, simple numerical examples given in [9] illustrate that a single oscillator which is usually used for the boundary 'thermostat' in equations (4) cannot be sufficiently chaotic to yield the canonical distribution from a single initial condition. Indeed, for the parameter we chose, $T_+ = 152$, $T_- = 24$ (as in LLP), and $\beta = 0.5$, the time evolution of the two 'thermostats' are not sufficiently random. There are some periodic-like structures in the phase space (see figures 1(*a*) and (*b*)). Therefore, these two 'thermostats' are not really thermostats, instead they are attractors covering only part of the phase space. This means that, we are dealing with a long but finite system which consists of two attractors connected by a 1D FPU β chain.

Since the dissipation is absent in this system, we expect that some excitations once generated, may not disappear during the process of thermalization. In figures 1(*c*) and (*d*), we plot the time evolution of the displacement at the initial time period (10^2 time units) as well as after a long time (the same time interval, but after 10^4 time units), respectively. These two approaches indeed give strong evidence that some kind of nonlinear excitations are propagating inside the system. They do not vanish even after a very long time. Interestingly, this structure is not reflected in the 'temperature' profile, (the temperature is defined as twice the kinetic energy), namely, the temperature profile is smooth and has exactly the same scaling $T_l = T(l/N)$ as observed by LLP. Since the parameters we chose are the same as that used by LLP, the resulting temperature profile and thermal conductivity are basically the same as that obtained by LLP. We shall not repeat all of these results here, instead we shall concentrate on investigating the reasons why the thermal conductivity is divergent.

We would like to point out that there are at least two different kinds of regular motion present in the system even after a very long time. They are: (a) localized nonlinear excitation performing nondiffusive energy transport between two boundary attractors; (b) stationary long-wavelength eigenmode. We shall discuss these two regular motions in detail in the following.

The first one is a nonlinear excitation which moves back and forth, and is scattered by the boundaries. Its presence is the main reason for the apparent singularity of the
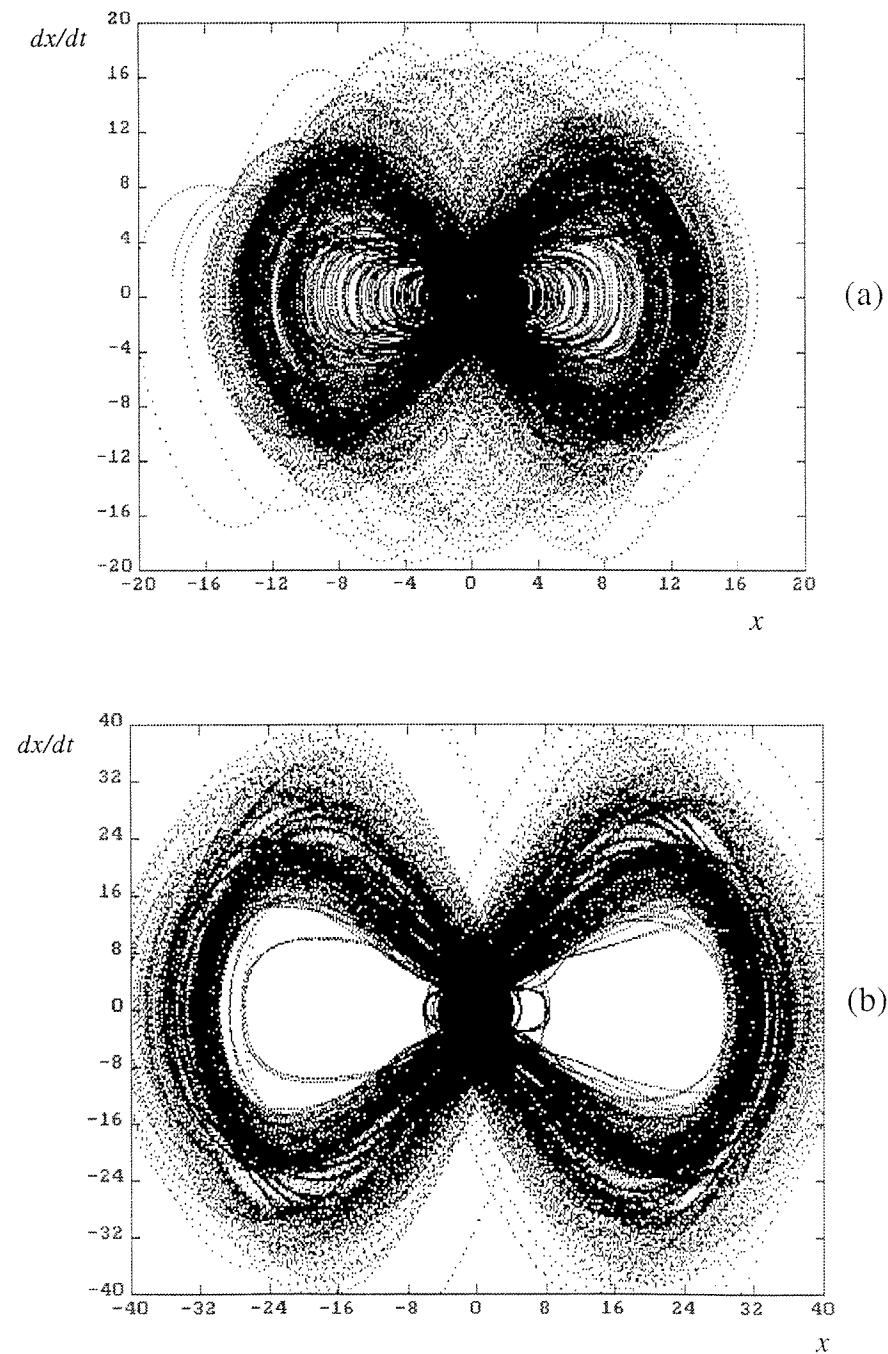
Figure 1. The phase space of the two 'thermostats' at (*a*) the left end and (*b*) the right end with temperatures $T_+ = 152$ and $T_- = 24$, respectively. The time evolution of the particles' displacements for the time interval of 100 steps at (*c*) the initial period and (*d*) the intermediate period (after 10^4 steps).
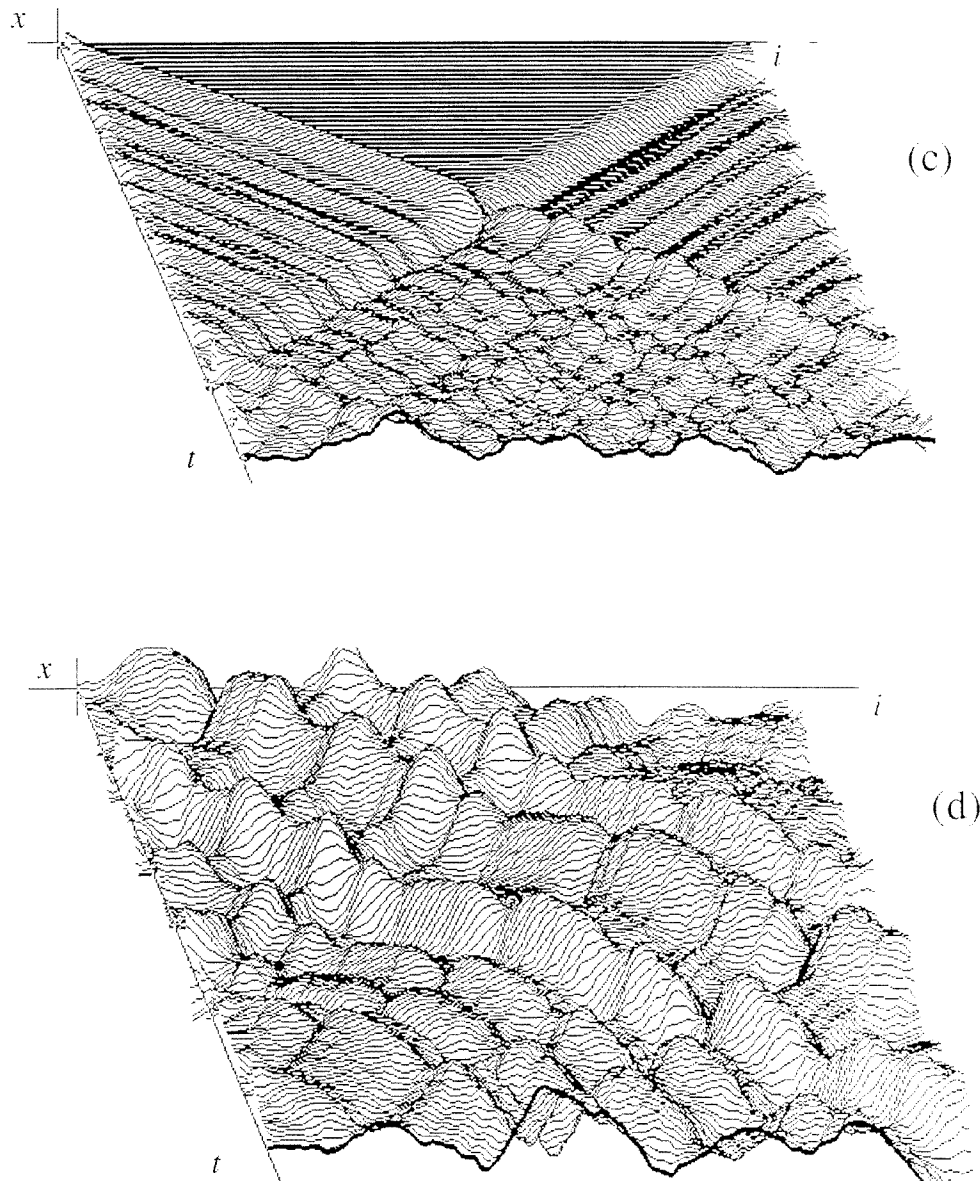
Figure 1. (Continued)

temperature profile near the boundary (see, e.g. figures 2 and 3 of [6] and figure 1 of LLP). To demonstrate this effect, we initialized the particles' displacement of the chain by a localized excitation, and let it propagate along the chain. The time evolution of this localized excitation is shown in figure 2(*a*). After a very long time the 'temperature' profile caused by the propagation of this excitation can be calculated, which is plotted in figure 2(*b*). This figure clearly displays the specific singular structure near the boundaries as originally observed in this model by Kaburaki and Machida [6] and then confirmed by LLP in the temperature profile. As we argued before, these kinds of nonlinear localized excitations are
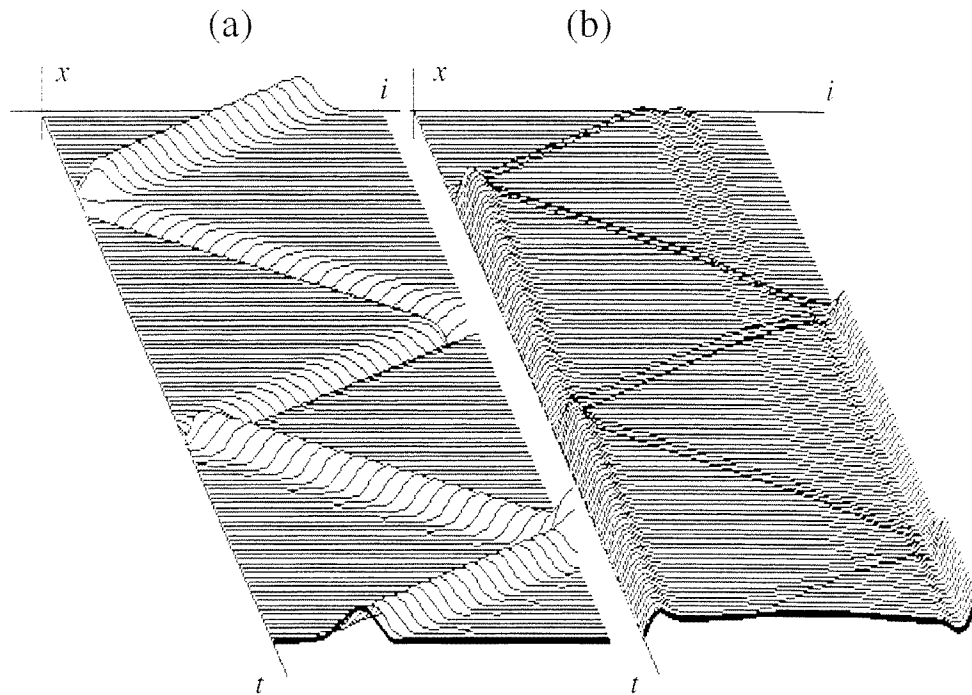
Figure 2. (*a*) The time evolution of a localized excitation and (*b*) the temperature profile caused by this excitation.

due to the absence of the dissipation and/or scattering mechanism of the phonons. If either of these two mechanisms are introduced, this singular behaviour in the temperature profile will disappear [10].

The second kind of motion can be compared to that of an effective harmonic oscillator with rescaled frequencies and modulated amplitudes existing at different timescales. If we allow enough time for the simulation, then the very-long period oscillations are observable. Besides, the time taken to reach the same level of thermalization essentially grows with the chain length N. Strictly speaking, this makes the simulation of the thermodynamic limit impossible. Nevertheless, the thermalization-like process is realized in the nonequilibrium stationary state. Figure 3 shows the probability distribution function of the velocity of the particles near the boundary and inside the chain far from the boundaries. They are really good Gaussian functions, with their widths proportional to the averaged temperatures at the points.

Let us now turn to the long-time evolution of particles' displacement. In figure 4, we plot this for a system having 64 particles. We have performed an extensive simulation by changing the particle numbers from 32 to 1024, and qualitatively the same pictures have been obtained. Therefore, at least in this particle number range, the conclusions given below are length independent. The equations of motion have been integrated through a standard fifth-order Runge–Kutta routine by using double precision with a maximal step size of 10^{-3}. The time in figure 4(*a*) begins after a transient time of 10^8 steps and changes from 0 to 163.84 time units. The grey-scale changes from white to black correspond to the amplitude of the displacements change from minimum to maximum. It has also been checked for the structures obtained after very long transient times as well as much longer time intervals of observation (up to 1638.4 units).
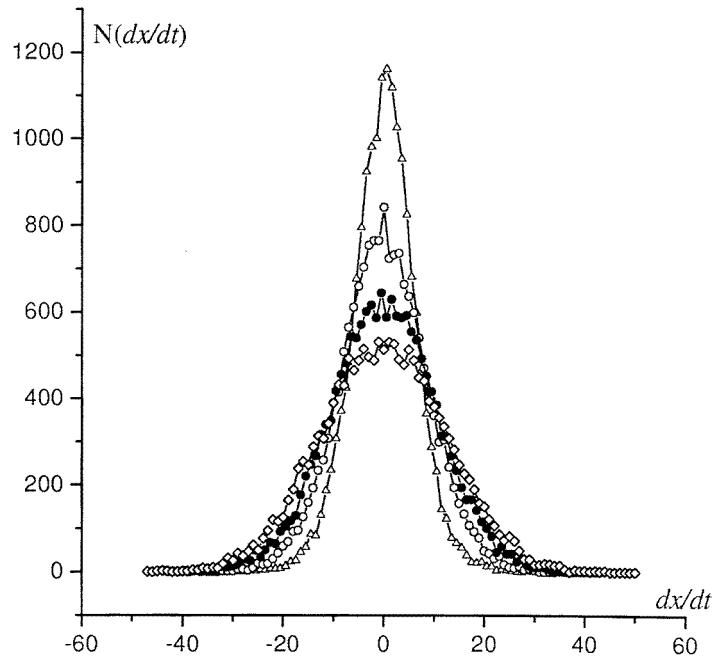
Figure 3. The probability distribution function of the velocity for the particles. $\Diamond$ for $i = 2$, $\bullet$ for $i = 16$, $\bigcirc$ for $i = 43$, and $\triangle$ for $i = 62$.

This picture gives us clear evidence of the periodic structure. It corresponds to the longest oscillation visible during the demonstration time†. However, it shades other waves in the system. The presence of excitations with different scales makes it impossible to separate them by using ordinary Fourier transforms. However, it can be done with the help of a more sophisticated tool, i.e. wavelet transform [12]. The wavelet transform allows us to separate the excitations into different scales. To filtrate the modes, standard Daubechies wavelets of 20th-order DAUB20 have been used [13]. The wavelet transform over time has been performed for every particle and a truncation is made over the first 0.39% wavelet coefficients.

After filtration we have a clear picture of the long-wavelength motion as is shown in figure 4(*b*). The fine (or mesoscopic) structures can be seen by subtracting figure 4(*b*) from figure 4(*a*), which is shown in figure 4(*c*). It is not difficult to distinguish many short-wave excitations moving left and right without energy loss from this picture. We found that these excitations might be responsible for instant local heat flux $J_i(t)$ in the system. Here, the heat flux is interpreted as the flow of potential energy from the ith particle to its neighbours and can be written in the form

$$J_i(t) = \dot{x}_i f_{i+1}. \tag{6}$$

The time–space distribution for the $J_i(t)$ value is displayed (without a wavelet transform) in figure 4(*d*) and should be compared with the mesoscopic structure in figure 4(*c*).

Finally, as further evidence to demonstrate the existence of the long-wavelength mode, we would like to carry out an analysis of the correlation function. We argue that the regular

† Note that the period of this structure is found to be proportional to N, whereas that of the soliton in the FPU model is proportional to $N^{5/2}$.
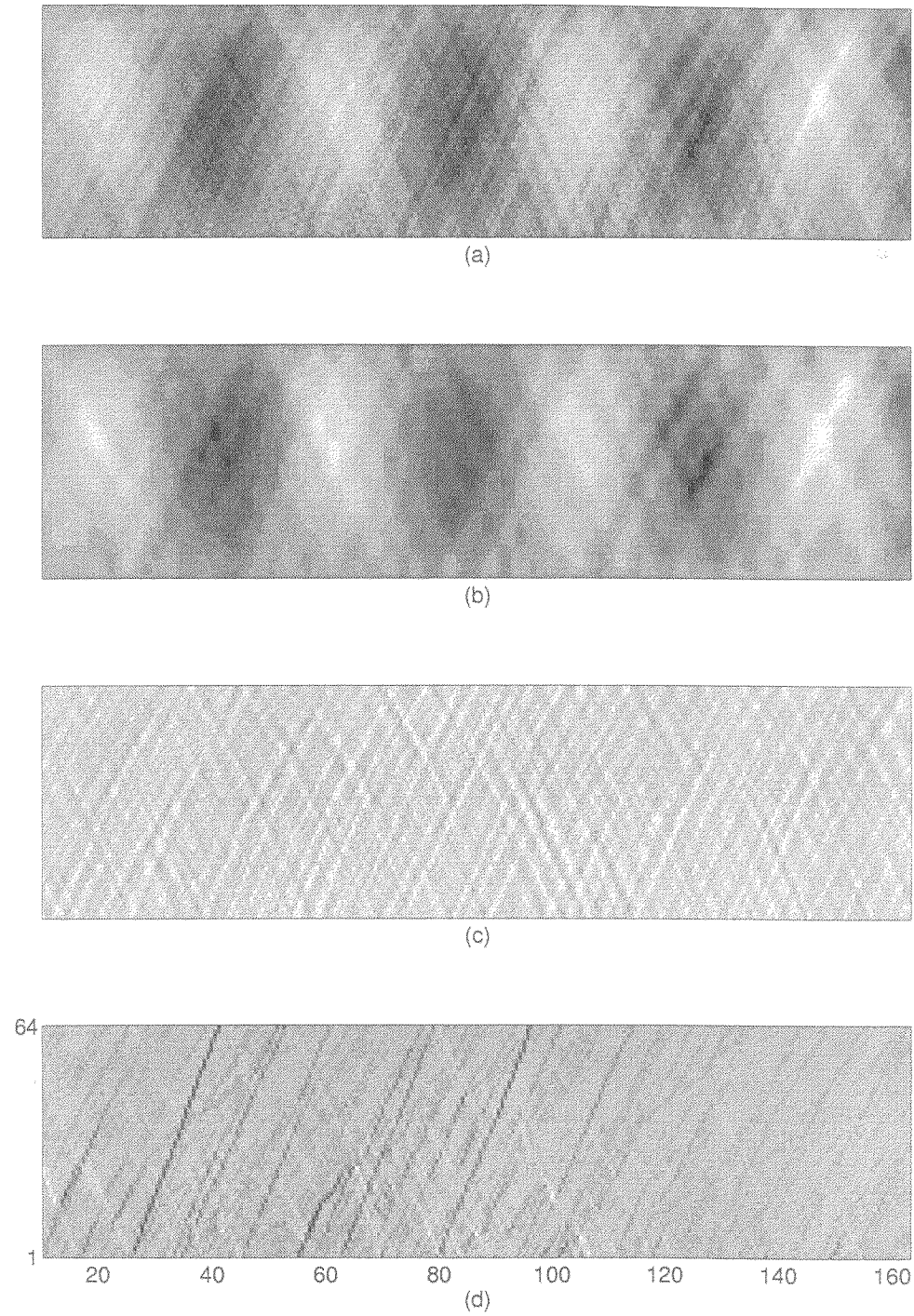
Figure 4. (*a*) Time evolution of the displacement of a chain with 64 particles. (*b*) The picture after wavelet transform. (*c*) The subtraction of (*b*) from (*a*). (*d*) The time evolution of local heat flux. The grey-scale changes from white to black correspond to the change of (*a*)–(*c*) the amplitude of displacement and (*d*) heat flux from minimum to maximum.
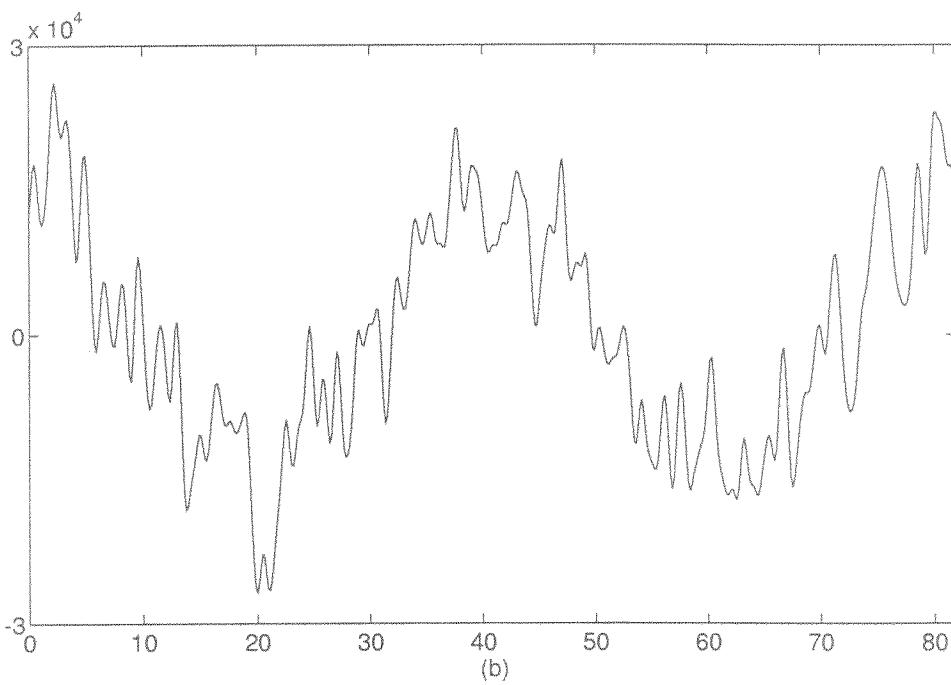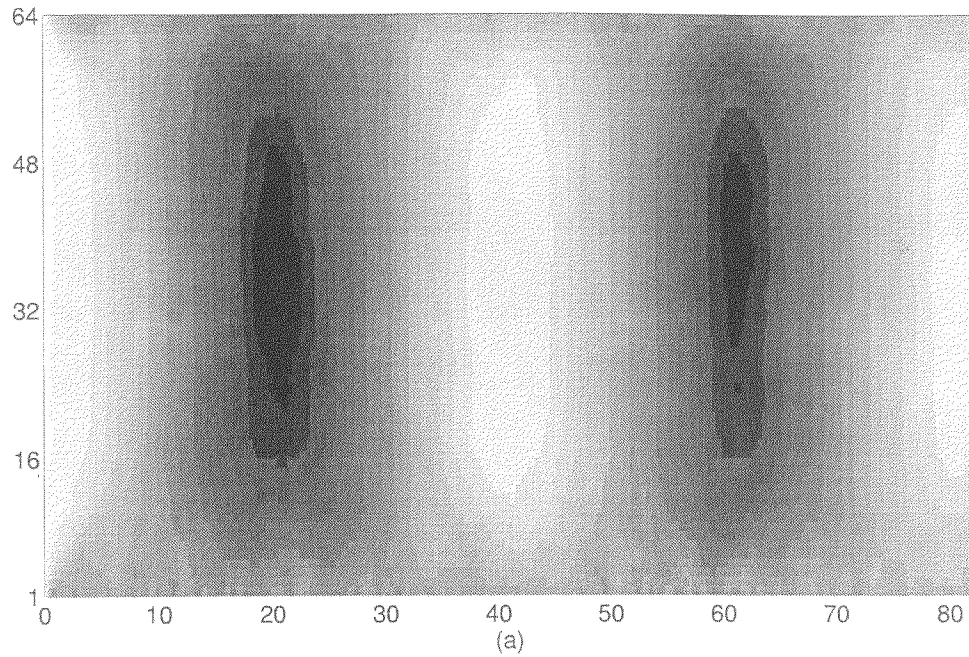
Figure 5. (*a*) Time evolution of the autocorrelation function for the chain with 64 particles. (*b*) The cross-correlation function between the first particle (at the high-temperature 'thermostat') and the last particle (at the low-temperature 'thermostat').

energy transport along the chain leads to a long-time correlation between particles in the system. This can be quantified by the following function

$$C_{ij}(t') = \langle x_i(t)x_j(t + t')\rangle. \tag{7}$$

We plot the autocorrelation function C_{ii} (each of which is normalized by its maximum) in figure 5(a). It is clearly seen from this picture that C_{11} and C_{NN} have a form qualitatively close to that of independent attractors. In addition, the quasiperiodic correlations inside the chain are also visible. Surprisingly, even the particles kept at the two reservoirs are found to be correlated. This is depicted by C_{1N} shown in figure 5(b).

3. Conclusions

In this paper, we have numerically demonstrated that the singular behaviour in the temperature profile near the boundary of the 1D FPU chain is caused by a kind of localized nonlinear excitation. Moreover, by studying the long-time evolution of the system, we have observed a long-wavelength eigenmode propagating in the chain. This is also supported by the analysis of the correlation function between particles. This long-wavelength mode is responsible for assisting the energy transport. We believe that the existence of this long-wavelength eigenmode makes the heat conduction energy in the FPU model *impossible* to obey the Fourier heat law. Our results suggest that in order to have the thermal conductivity obey the Fourier heat law, one needs to add some elements such as an external periodic potential [10], which is analogous to the lattice, or dissipation and/or disorder (e.g. taking different masses for different particles) to inhibit such kinds of long-wavelength propagating modes. Indeed, we have observed that if we replace the FPU chain by the Frenkel–Kontorova chain (which has external potential), this kind of long-wavelength mode disappears, and consequently the Fourier heat law is justified [10].

Acknowledgments

References

 [1] Fermi E, Pasta J, Ulam S and Tsingou M *Los Alamos Report* LA-1940
     Fermi E, Pasta J, Ulam S and Tsingou M 1993 *The Many-body Problem: An Encyclopedia of Exactly Solved Models in One Dimension* ed D C Mattis (Singapore: World Scientific)
 [2] Ford J 1992 *Phys. Rep.* **213** 271 and references therein
 [3] Lichtenberg A J and Lieberman M A 1992 *Regular and Chaotic Dynamics* (New York: Springer)
 [4] Kantz H 1989 *Physica* **39D** 322
 [5] Pettini M and Cerruti-Sola M 1991 *Phys. Rev.* A **44** 975
 [6] Kaburaki H and Machida M 1993 *Phys. Lett.* A **181** 85
 [7] Lepri S, Livi R and Politi A 1997 *Phys. Rev. Lett.* **78** 1896
 [8] Nosé S 1984 *J. Chem. Phys.* **81** 511
 [9] Hoover W G 1985 *Phys. Rev.* A **31** 1695
[10] Hu B, Li B and Zhao H 1998 *Phys. Rev.* E **57** 2992
[11] Casati G, Ford J, Vivaldi F and Visscher W M 1984 *Phys. Rev. Lett.* **52** 1861
[12] Poularikas A D (ed) 1996 *The Transforms and Applications Handbook* (Boca Raton, FL: Chemical Rubber Company)
[13] Press W H, Teukolsky S A and Flannery B P (ed) 1995 *Numerical Recipes* (Cambridge: Cambridge University Press)