Heat conduction in a one-dimensional aperiodic system

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We study the energy transport properties of one-dimensional nonlinear aperiodic lattice models in this paper. It is found that, compared with their periodic and disordered counterparts, the quasiperiodic and fractal models exhibit critical macroscopic behavior in the low-temperature region, while in the high-temperature region all the models show the same property of energy transport. The relationship between the observed macroscopic behaviors and the localization theory is discussed.

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It is of fundamental importance to establish a connection between microscopic-level dynamical properties and macroscopic statistical behavior of molecular systems. In condensed matter physics, the localization theory plays a key role when aperiodic structures are involved. For one-dimensional systems, as is well known, all the eigenstates are either extended in a periodic lattice model or localized in a disordered one [1]. Between these two extremes are the quasiperiodic systems, which are believed to be dominated by critical eigenstates [2], and the fractal systems, in whose vibrational spectra exist a crossover between extended states (long-wavelength phonon) and localized states (so-called fracton) [3]. The study of quasiperiodic systems and fractal systems has attracted particular interest since they represent intermediate cases between periodic solids and disordered ones. It has been found that a lot of real-world materials have quasiperiodic order [2,4] or fractal structure [3]. Therefore, investigating the statistical properties of these systems and establishing their connection to the microscopic features mentioned above will be important for both theoretical studies and applications.

Heat conduction in a chain of coupled nonlinear oscillators is a vivid example of studying the microscopic origin of the macroscopic behaviors in terms of deterministic microscopic dynamics. It is one of the oldest but still a rather fundamental problem in nonequilibrium statistical mechanics. Intending to understand the underlying mechanism of the Fourier heat law ($J=-\kappa dT/dx$, where J is the heat flux; dT/dx is the temperature gradient; κ is the heat conductivity), the study of heat conduction has attracted increasing attention in recent years [5–11]. Normal heat transport behavior governed by the Fourier heat law implies a decay law of heat flux $J\sim N^{-1}$, where N is the system size. For one-dimensional nonlinear lattice models, it has shown that the heat conductivity is abnormal (with $J\sim N^{-0.57}$) in the case without onsite potential [5,6] and is normal (with $J\sim N^{-1}$) in the existence of an onsite potential [7–9]. The exceptions with a normal heat conduction in the absence of the onsite potential are also found in two kinds of models, one is the one-dimensional lattice with periodic potential of nearest-neighbor interaction [10], and another is the disordered FPU-β model [11].

In order to unfold the role of the localization more clearly we focus on the models without onsite potential in this paper. More specifically, we adopt a well-known molecular dynamics model, i.e., the FPU-β model described by the Hamiltonian

$$H=\sum_{i}^{N} H_i, \quad H_i=\frac{p_i^2}{2m_i}+V(x_{i+1}-x_i)$$

with $V(x)=x^2/2+\beta x^4/4$. β is fixed to 1 throughout the paper. m_i denotes the mass of the ith particle. In our study we limit m_i to the binary value A or B. When putting the particles along the chain with A and B alternately a periodic FPU model (PFPU) is obtained, and in the specific case of $A=B$ one meets the normal monatomic FPU-β model. When arranging particle masses with A or B in a random way, a disordered FPU model (DFPU) is gotten. And when managing the mass distribution of the particles following the Fibonacci sequence, one approaches a quasiperiodic FPU model (QFPU) [2]. A Fibonacci sequence $B,BA,BAB,BABBA,BABBABAB,BABBABABBABBA,\ldots$ is created according to the production rule $S_j=S_{j-1}|S_{j-2}$ for $j\geqslant 3$ with $S_1=B$ and $S_2=BA$. Meanwhile when applying an iterative rule, $A\rightarrow ABA$, $B\rightarrow BBB$ continuously one get the Cantor fractal structure model (FFPU) [12]: $A,ABA,ABABBBABA,ABABBBABABBBBBBBBBABA BBBABA,\ldots$.

We introduce the parameter $\lambda=A/B$ into controlling the ratio of mass of the two components. λ is fixed at 0.8 throughout the paper except special cases. In our numerical simulations, the Nosé-Hoover thermostats [5,13] are put on the first and the last particles, keeping them at temperatures T_+ and T_-, respectively.

It is found that the stationary state sets in after 10^5 integration time units, thereafter the time average of heat flux $\langle J_i\rangle$ $[J_i=\dot{x}_i(\partial V/\partial x_{i+1})]$ and the temperature $\langle T_i\rangle$ $(T_i=p_i^2/2m_i)$ are found to be time independent ($\langle J_i\rangle$ is also found site independent and is denoted by J). In the present paper the fixed boundary condition is adopted as is done in the usual studies of lattice heat conduction.

In previous studies the heat transport behavior of the monatomic FPU model and the disordered FPU model with the particle masses randomly distributed in an interval have been reported. In this paper, we report the numerical investigations of the diatomic periodic FPU model and diatomic disordered FPU model. The result for the diatomic periodic

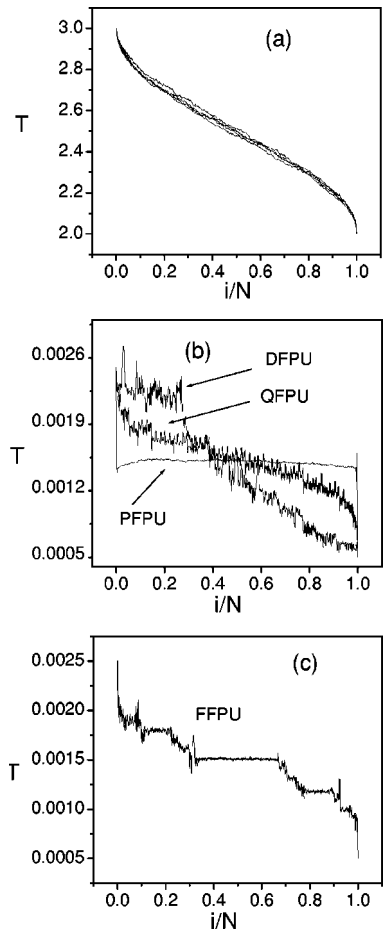

FIG. 1. Temperature profiles at (a) high-temperature region, (b) and (c) low-temperature region; *i* denotes the lattice position.

FPU model agrees qualitatively with those for the monatomic FPU model [5] and the diatomic Toda model [6]. The result for diatomic disordered FPU model also agrees with that for the disordered FPU model with the particle masses randomly distributed in an interval [11]. The results for the quasiperiodic and fractal models are presented for the first time in this paper. In our study, particular attention is paid to establish a connection between macroscopic statistical behavior and microscopic-level dynamical properties. The investigations are respectively divided into two temperature regions, high- and low-temperature cases, according to the previous knowledge on these kind of models.

Figure 1 shows spatial temperature profiles for these models. In the high-temperature case, we find an identical temperature gradient curves for all the models [Fig. 1(a)]. On the other hand, in the low-temperature region [Figs. 1(b), 1(c)], no temperature gradient is formed for PFPU model, as in the case of harmonic lattice model [14]. Temperature gradient is formed in the other cases, but difference between different models is apparent: the curve of QFPU model is located between that of DFPU and PFPU models, while the temperature profile in the FFPU case shows the fractal feature.

In Fig. 2, we present $JN(\sim\kappa)$ versus N for different models in high- and low-temperature cases, respectively. Notice that in the case of normal heat conduction JN is N independent. In the high-temperature case [Fig. 2(a)], the best fitting for all the models yields $JN\sim N^{0.43}$, which implies that the heat conductivities diverge in the same way. In the low-temperature case [Fig. 2(b)], the scene is changed completely. For the models of PFPU, QFPU, and FFPU the heat conductivities diverge, but for PFPU $JN\sim N^{1}$, for QFPU $JN\sim N^{0.83}$, and for FFPU $JN\sim N^{0.9}$. In the case of DFPU, JN becomes constant when N is sufficiently large, which indicates that the heat conduction for this model obeys the Fourier law in the low-temperature region.

It is clear that the macroscopic behaviors for all the models undergo a crossover when changing the temperature from low-temperature region to high-temperature region. In Fig. 3, we display the quantity $J(N)/J(3N)$ versus $T=(T_{+}+T_{-})/2$. $J(N)$ is the heat current for the system of size N. Notice that $J(N)/J(3N)=3$ indicates a normal heat conductivity while $J(N)/J(3N)<3$ implies a diverged one. The specific case of $J(N)/J(3N)=1$ shows that J is size independent. We find that in very low temperature region PFPU appears as a harmonic model while the DFPU model shows a normal heat conduction behavior [N is fixed to 243 for all the models, so one cannot expect that the value of $J(N)/J(3N)$ for the DFPU model is exactly equal to 3 because of the size effect. One can see from Fig. 2 that the normal heat conductivity of the DFPU model does not set up until $N>700$], while the curves for QFPU and FFPU are located between those for the two extreme models. On the other hand, the heat conductivities of all the models are abnormal in the high-temperature region and diverge in the same manner, i.e., $J(N)/J(3N)\sim 1.7$, corresponding to the diverging law of $JN\sim N^{0.43}$.

Thus, two questions arise from the above observations. First, why all the models studied here (as well as the monatomic FPU-β model [5,8,11] and the diatomic Toda model [6] studied earlier) show the same transport behavior in the high-temperature region and what the diverging law indi-

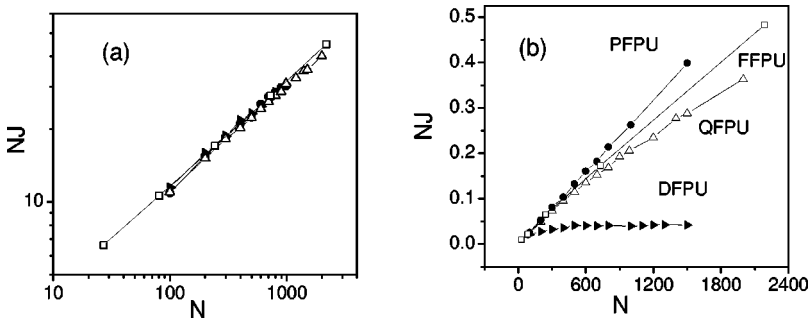

FIG. 2. Heat conductivity vs N in (a) high-temperature case and (b) low-temperature case.

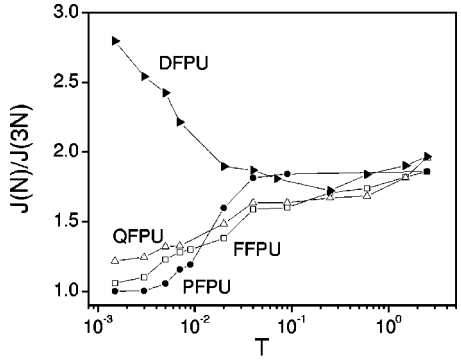

FIG. 3. Crossover from low-temperature region to high-temperature region.

cates? Second, what the different energy transport behaviors of the different models in the low-temperature region imply?

In order to fix up these two questions, we need to establish a connection between microscopic-level dynamical properties and macroscopic statistical behavior, i.e., to find out what microscopic dynamics is responsible for the observed high- and low-temperature properties. Therefore, we decompose the interaction of the thermostat into a series of kicks and observe the motion of a single kink along the chains on different initial conditions. This method has been used in Refs. [8] and [11] for similar purpose. In Fig. 4 we plot H_i versus i at $t=400$. The first column shows the results with the initial excitation $p_1=5$ and $p_i=0$ for $i\neq 1$. This excitation corresponds to high-temperature excitation. The second column is obtained on the initial excitation $p_1=0.005$ and $p_i=0$ for $i\neq 1$ and represents low-temperature case. We can see that solitary waves are excited in all the models in the first column while in the second column the excitations are linear wave packets [here we call them the linear wave packets since their shapes are similar to that of their harmonic counterparts obtained by erasing the unharmonic terms in $V(x_{i+1}-x_i)$ in their models]. In the PFPU case the solitary wave pocket shown in the first column keeps its energy when propagating along the chain, leaving behind a disconnected linear wave packet trail exactly similar with the wave packet observed in the second column. In other cases the solitary waves in the first column decrease their amplitudes slowly when propagating along the chains but keep a large fraction of initial energy. The excitations in the second column propagate essentially in the harmonic way, i.e., no clear difference can be found when comparing them with those of corresponding harmonic models (by erasing the nonlinear terms in the corresponding models).

Figure 4 indicates that the solitary waves can be excited not only in the periodic model but also in aperiodic systems with high-amplitude kinks. The solitary wave is a kind of energy localization phenomenon induced by strong nonlinearity. Andson localization theory based on normal mode analysis is not applicable in this case and cannot be used to explain the phenomena in high-temperature region. Therefore the heat conduction behaviors in high temperature case should be analyzed in the framework of solitary wave dynamics, more specifically, the scattering behaviors of the

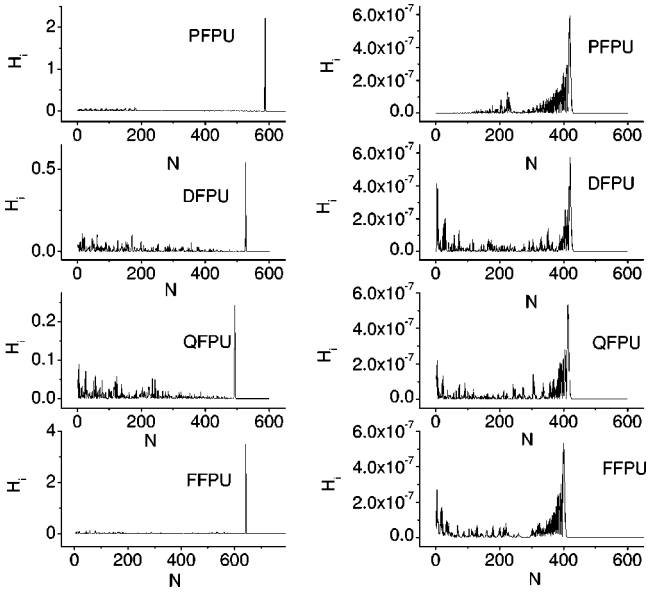

FIG. 4. The excitation in high-temperature case (first column) and low-temperature case (second column).

solitary waves. The first column of Fig. 4 indicates that a solitary wave can be scattered by the lattice structures. It also shows [8] that a solitary wave can be scattered by other solitary waves, unlike the true solitons in the integrable models such as the monatomic Toda lattice. Then which kind of scattering mechanism should be responsible for the observed devergent law of heat conductivity? Despite different structures, all models, including the monatomic FPU-β model [5,8,11] and the diatomic Toda model [6], show the same devergent law of heat conductivity. So we believe the latter is correct. As illustrated in Ref. [8], a remarkable feature of the solitary wave to solitary wave scattering is that the continuous scattering cannot destroy the correlation of an initial excitation. This makes the solitary wave scattering mechanism different from that of random-walk-like one and results in the divergent law.

Besides, the second column of Fig. 4 shows that the low-amplitude excitations behave differently in different models. One can see that the low-amplitude excitation cannot be scattered by periodic structure but can be scattered by aperiodic structures. This fact should be responsible for the different energy transport properties observed in the low-temperature region. For the periodic model, the excitations can move freely from one side of the chain to the other, which explains the fact that no temperature gradient can be formed along the periodic lattice chain and the heat flux is size independent. This result indeed agrees with Bloch's theorem, which states that the eigenstates of a system with a periodic potential are extended, having the same nominal amplitude at all positions in space. For the disordered models, the excitations are scattered by the lattice structure. The normal heat conduction behavior of this kind of model in the low-temperature region should be attributed to the fact of fully localized states together with the weak nonlinear interaction among the states. (Here we believe that the nonlinear term in the potentialshould play a role in normal heat conduction behavior

since a harmonic disordered one-dimensional lattice under the fixed boundary conditions as used in this paper has been proven to show a behavior of $\kappa \sim N^{-1/2}$ instead of a size-independent heat conductivity [15], thus disordered structure alone cannot ensure a normal heat conduction behavior.) Quasiperiodic and fractal structures also scatter energy. A one-dimensional quasiperiodic system is dominated mainly by critically localized states [2], which indicates a critical decay relationship between fully localized states and extended states. For a fractal model, the normal modes are made up of extended states, critically localized states and localized states [3]. The fact of abnormal heat conduction indicates that these features cannot ensure an energy transport behavior governed by Fourier law. The fractal model has a higher energy transport capability than the quasiperiodic structure since there exist extended states in the former.

In summary, in the high-temperature case, the main excitations in all the models studied are solitary waves, and the energy scattering is dominated by the solitary wave to solitary wave scattering mechanism. As a result, the heat conductivity diverges as $N^{0.43}$. The disordered, quasiperiodic, and fractal structures can decrease the total heat flux, but have no influence on the diverging law of heat conductivity.

On the other hand, the low-temperature scenario appears to be dominated by harmonic waves that are sensitive to the large-scale structure of the chain. As a result the transport property is different from model to model in the low-temperature region. No temperature gradient is formed along the periodic chain and the heat flux is size independent. This is because of the absence of an energy scattering mechanism for the extended eigenstates in periodic models. The disordered one-dimensional systems exhibit a normal heat conduction behavior, which can be attributed to the ''fully localized'' feature of the eigenstates. The heat conductivity in the quasiperiodic and fractal systems is abnormal. It diverges as $\kappa \sim N^{\gamma}$ with $0<\gamma<1$. The specific value of γ is determined by the specific structure of the models. Other macroscopic properties of these two systems also show critical behaviors between fully localized systems and extended ones.

The results of one-dimensional lattice models explain certain aspects of high-dimensional lattice models. Theoretical work on the classical wave problem shows that all disordered one- and two-dimensional systems must be fully localized and critically localized, respectively, and that in three dimensions there can be transitions from localized to extended states [1]. One can then expect that for two- and three-dimensional systems even the disordered structure alone cannot ensure the normal macroscopic transport behavior. So the situation for searching a lattice model with the normal heat conduction and therefore taking it as a microscopic model of studying energy transport of phonons in high-dimensional medium will be more difficult.

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