

Wave transmission, phonon localization, and heat conduction of a one-dimensional Frenkel-Kontorova chain

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We study the transmission coefficient of a plane wave through a one-dimensional finite quasiperiodic system—the Frenkel-Kontorova (FK) model—embedding in an infinite uniform harmonic chain. By varying the mass of atoms in the infinite uniform chain, we obtain the transmission coefficients for *all* eigenfrequencies. The phonon localization of the incommensurate FK chain is also studied in terms of the transmission coefficients and the Thouless exponents. Moreover, the heat conduction of the Rubin-Greer-like model for the FK chain at low temperature is calculated. It is found that the stationary heat flux $J(N) \sim N^\alpha$, and α depends on the strength of the external potential. [S0163-1829(99)12713-9]

I. INTRODUCTION

In recent years, there has been growing interest in studying incommensurate structures and commensurate-incommensurate phase transitions in condensed-matter physics and dynamical systems.^{1–15} On the one hand, incommensurate structures appear in many physical systems such as quasicrystals, two-dimensional electron systems, magnetic superlattices, charge-density waves, organic conductors, and various atomic monolayers adsorbed on crystalline substrates. One of the simplest prototypes for incommensurate structures is the Frenkel-Kontorova (FK) model¹ which describes a one-dimensional (1D) chain of atoms with an elastic nearest-neighbor interaction, and subjected to an external periodic potential. If the mean distance between consecutive atoms is not in rational ratio to the period of the external potential, the corresponding state is incommensurate. It has been shown by Aubry^{3–5} in his pioneering work that there exists two different configurations for an incommensurate state by changing the strength of the external potential. These two configurations are called the sliding phase and pinned phase, and the transformation between these two phases has been called the *transition by breaking of analyticity*. On the other hand, the ground-state equation of the 1D FK model is nothing but the standard map which is widely studied in the field of nonlinear dynamics.^{12–14} The two incommensurate configurations correspond to the invariance circle and the Cantorus, respectively.

In the past two decades, most of the works about 1D FK model have been focused on the study of the ground state. Little attention has been paid to the linear excitation or phonon modes. As is well known, the excitation of phonons is very important; it determines the fundamental properties,

such as the wave transmission, heat conduction, and other low-temperature thermodynamics properties of the underlying material. In turn, the study of the transmission coefficients and energy transport gives us insights of the excitation. In this paper we shall study systematically these related properties, namely, the wave transmission, the heat conduction, and the phonon localization in 1D FK model. Through this study we shall have a clear picture about how the macroscopic phenomena such as the transmission coefficients and heat conduction are related to the localization properties of the phonon excitation. Moreover, our study suggests a possible way for experimental observation of the phonon gap which characterizes the *phase transition by breaking analyticity*.

Recently, Burkov *et al.*¹⁵ have studied the localization properties of the phonon eigenstates. They solved the equation of phonon numerically for a FK chain of finite length. It is found that the phonon eigenstates are extended and quasiperiodic functions for $V < V_c$, whereas for $V > V_c$ the eigenstates at band edges of phonon spectrum are more localized than that one in the middle of the spectrum, but no exponential localization states have been found.¹⁵ In their numerical study, the localization property is inferred by computing the participation ratio. Ketoja and Satija¹⁶ have studied the eigenfunctions corresponding to the minimum frequency ω_{min} of the phonon spectra in Cantorus regime by using an exact decimation scheme. The phonon eigenstates of the minimum frequency are found to be critical for $V > V_c$.

The method used by Burkov *et al.* is limited to the small system size. In our calculation we shall study the wave transmission by making use of the transfer-matrix method due to the following reason. As is known that there is a nice correspondence between the phonon and electron properties. The

transmission coefficient has been found to be a very useful quantity for the study of localization of electron eigenstates.¹⁷ The transfer-matrix method is a powerful method to study the systems with much larger size. In this paper, we shall study systematically the properties of the phonon eigenstates by computing the transmission coefficients of a plane wave through a 1D FK chain. By using the transmission coefficient, we are not restricted to only one frequency, instead we can study the localization properties for *all* frequencies. To quantify the localization, we shall also calculate the Thouless exponents in addition to the conventional participation ratio and transmission coefficients.

Another interesting and fundamental property that is related to the phonon excitation is the thermal conductivity. Recently, there has been a renaissance interest in heat conduction in a variety of 1D systems,^{19–25} since this problem is essential for our understanding of the microscopic origin of the macroscopic irreversibility.²⁶ At low temperature, the linear excitations of the underlying system are most important for heat conduction. Rubin and Greer^{27,28} have established the relation between the stationary energy flux and the transmission coefficients of the phonons. They found that the stationary energy flux approach to a finite positive value as the number of atoms goes to infinity for uniform periodic harmonic chains, and the thermal conductivity is proportional to N . However, for random mass binary harmonic chains, the stationary energy flux is found to be proportional to $N^{-1/2}$ as the number of atoms N tends to infinity, and the thermal conductivity is thus proportional to $N^{1/2}$. Therefore how the stationary energy flux and the thermal conductivity depends on the particle number N for an incommensurate system is of great interest. This will be also investigated in the present paper.

The paper is organized as follows. In Sec. II, we shall describe the model and numerical method for calculating the wave transmission coefficient. The phonon localization and heat conduction problems shall be discussed in Sec. III and Sec. IV, respectively. A brief discussion and conclusion is given in Sec. V.

II. THE MODEL AND NUMERICAL METHOD

The 1D FK model can be described by

$$H = \sum_n \left[\frac{p_n^2}{2m} + \frac{1}{2} (x_{n+1} - x_n - a)^2 - V \cos(x_n) \right], \quad (1)$$

where p_n and x_n are the momentum and position of the n th atom, respectively. V is the strength of the external potential. a is the distance between consecutive atoms without external potential. Aubry and Le Daëron⁵ showed that the minimum-energy configurations are periodic when $a/2\pi$ is rational (commensurate model) and quasiperiodic when $a/2\pi$ is irrational (incommensurate model). For an incommensurate FK model, there are qualitatively different ground-state configurations separated by *the transition by breaking analyticity* predicted by Aubry. For each irrational a there exists a critical value V_c of the external potential. The

$$V_c = 0.971\ 635\ 4 \dots$$

(Refs. 13 and 14) corresponds to the most irrational number, golden mean value $a/2\pi = (\sqrt{5} - 1)/2$. Without loss of generality, we restrict ourselves to this particular value of a in the numerical calculations throughout the paper.

The phonon equation describing the physical stability of the atoms in the FK model at ground state is

$$\psi_{n+1} + \psi_{n-1} - [2 + V \cos(x_n^0)] \psi_n = -\omega^2 \psi_n, \quad (2)$$

where x_n^0 is the equilibrium position of the n th atom in ground state, ψ_n is displacement of the n th atom from its equilibrium position, and ω is the eigenfrequency.

This equation can be written in the form of transfer matrix

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = T_n \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix} \quad (3)$$

with

$$T_n = \begin{pmatrix} -\omega^2 + 2 + V \cos(x_n^0) & -1 \\ 1 & 0 \end{pmatrix}. \quad (4)$$

Thus

$$\begin{pmatrix} \psi_{N+1} \\ \psi_N \end{pmatrix} = P_N \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} \quad \text{with } P_N = T_N T_{N-1} \dots T_1. \quad (5)$$

In order to study the transmission of a plane wave through the 1D FK system, we first consider a uniform harmonic atom chain with atom mass m_0 , and the external potential V is equal to zero. The eigenstates and eigenfrequencies of this chain are simply

$$\psi_n = A_+ e^{iqna} + A_- e^{-iqna} \quad \text{and} \quad \omega^2 = \frac{4}{m_0} \sin^2 \left(\frac{1}{2} qa \right), \quad (6)$$

respectively.

Then we replace the segment between $n = 1$ and $n = N$ by a finite incommensurate FK chain. The atom in the FK chain has mass m . Now we consider an incoming plane wave from $n = -\infty$ with frequency $\omega = \sqrt{4/m_0} \sin(\frac{1}{2} qa)$. Thus in the range of $n \geq N + 1$ there is only outgoing wave. That is

$$\psi_n = A e^{iqna} + A_R e^{-iqna} \quad \text{for } n \leq 0,$$

$$\psi_n = B e^{iqna} \quad \text{for } n \geq N + 1. \quad (7)$$

From Eqs. (5) and (7), after long calculation, we obtain the transmission coefficient

$$t = \frac{|B|}{|A|} = \frac{4 \sin^2(qa)}{|-(P_N)_{11} e^{-iqna} + (P_N)_{21} - (P_N)_{12} + (P_N)_{22} e^{iqna}|^2}, \quad (8)$$

where $(P_N)_{ij}$, $i, j = 1, 2$ are the elements of matrix P_N in Eq. (5).

If we let the atom mass of the uniform harmonic chain be equal to the atom mass in the FK chain, i.e., $m_0 = m$, as done

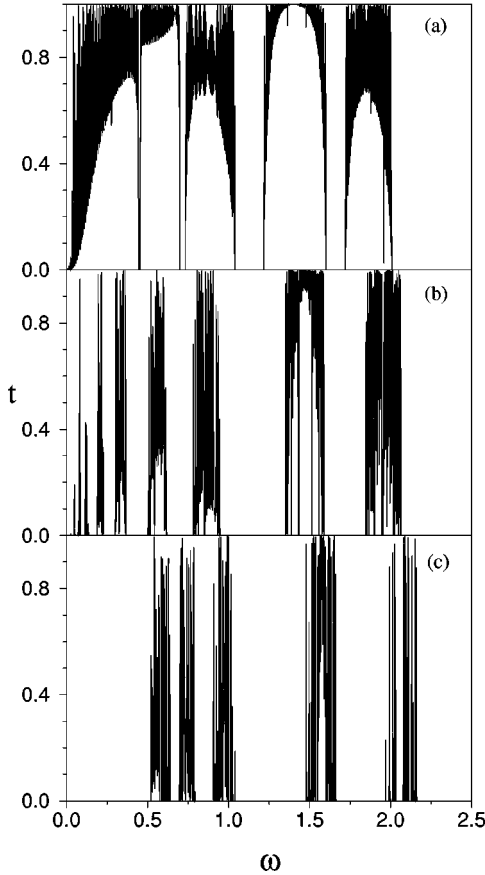


FIG. 1. The transmission coefficients as functions of frequency ω for different values of V . (a) $V=0.4$, (b) $V=1$, and (c) $V=1.6$. The parameters in the calculations are $N=1597$, $m_0=0.8$, and $a/2\pi=(\sqrt{5}-1)/2$. The critical value $V_c=0.971\ 654\ 3\dots$

in the usual study of electron systems,¹⁷ then we could not obtain the transmission coefficients of the phonons with frequency larger than $2/\sqrt{m}$. However, for $V \neq 0$, there do exist phonons whose frequencies are larger than $2/\sqrt{m}$. Therefore, in order to study the transmission coefficients of *all* eigenfrequencies, we should let the mass m_0 of the uniform harmonic chain differ from the mass of the FK chain. In Figs. 1(a)–(c) we show the transmission coefficients of the finite FK chains as the functions of frequency for different V . The parameter $a/(2\pi)=(\sqrt{5}-1)/2$ is approximated by a converging series of truncated fraction: F_n/F_{n+1} ($n=1,2,\dots$), where $\{F_n\}$ is the Fibonacci sequence. The results of Figs. 1(a)–(c) are obtained for $N=F_{16}=1597$, $m_0=0.8$, and $m=1$. In our calculations, we first obtained the N atomic positions of the equilibrium ground state of the FK chain with free boundary condition, i.e., $x_0=0$ and $x_N=2\pi Na$, by the gradient method.^{3–5} Evidently, for the plane wave with frequency in the gaps of the phonon spectra, the transmission coefficients are zero. From Fig. 1 we see that for small V there exists a wider frequency range with nonzero transmission coefficients than that for large V . This can be understood by the following facts. For $V=0$, there exists only one frequency band from $\omega=0$ to $2/\sqrt{m}$. When $V \neq 0$, the ground-state positions of atoms deviate from that in the FK chain without external potential. For small V ($<V_c$), the ground-state positions of atoms are periodic or quasiperiodic. Therefore, one band splits into several subbands and the bandgaps

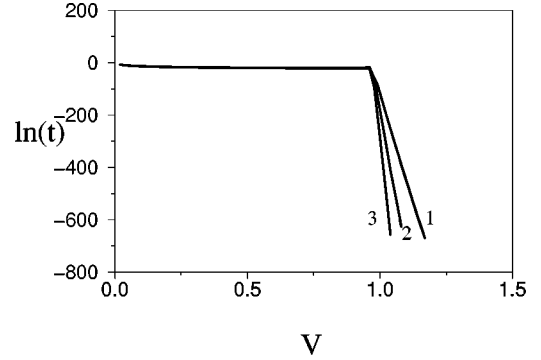


FIG. 2. The transmission coefficient of low-frequency ($\omega = 10^{-6}$) wave through the FK chain as a function of V . For all three curves $m_0=1$ and $a/2\pi=(\sqrt{5}-1)/2$. The curves 1, 2, and 3 are for $N=1597, 2548, \text{ and } 4181$, respectively.

show up. As V increases, more and more subbands and gaps show up. Also, we found that the range of the eigenfrequency becomes smaller as V is increased beyond V_c . This implies that the eigenfrequencies are attracted somehow for $V > V_c$ [see Fig. 1(c)], which is similar to the band gaps of the Harper model at the critical point.¹⁸ Because the eigenstates of the Harper model at critical point are critical, this result is one of the signature showing that the eigenstates of an incommensurate FK chain in Cantorus regime are critical.

It is well known³ that the phase transition by breaking of analyticity is manifested by the phonon gap for $V > V_c$. In fact, from Fig. 1, we have seen that as V increased to 1.6 there is a wide range of frequencies around $\omega=0$, in which the transmission coefficient is zero. This is the direct consequence of the appearance of the phonon gap. In order to see this transition of an incommensurate FK model, we calculate the transmission coefficient of a low-frequency wave at different values of V , which are shown in Fig. 2. In this figure we plot the transmission coefficients of the plane wave with frequency $\omega = 10^{-6}$ as a function of V for the FK segments having different lengths. It is obviously seen that there is a sharp decrease after $V > V_c$ and the decrease becomes sharper for larger N . The corresponding particle numbers are 1597, 2584, and 4181 for curves 1, 2, and 3, respectively. This clearly demonstrates the existence of the phonon gap for $V > V_c$. In turn, our results illustrated here suggest that the transmission coefficient might be a very good quantity for probing the existence of phonon gap in the underlying system. Therefore measuring the transmission coefficient would enable us to detect the *phase transition by breaking analyticity* experimentally.

III. PHONON LOCALIZATION

The above-discussed wave transmission is a macroscopic phenomenon. To some extent, it reflects the microscopic origin, namely, the phonon excitation in the underlying systems. In this section, we would like to study the phonon localization from different approaches.

Participation ratio. Burkov *et al.*¹⁵ studied this quantity for the finite FK chain by numerically solving Eq. (2) and computing the participation ratio (PR):

$$\text{PR} = \frac{1}{N} \frac{\left(\sum_n \psi_n^2 \right)^2}{\sum_n \psi_n^4}. \quad (9)$$

Here N is number of atoms. If the eigenfunction is extended, PR tends to be a finite limit as $N \rightarrow \infty$. If an eigenfunction is exponentially localized, $N \times \text{PR}$ will be a finite number as the length N goes to infinity. Burkov *et al.* found that for $V < V_c$, all eigenfunctions are extended for N up to 987 and for $V > V_c$ the PR of states near the band edges decrease with increasing N , but the true exponential localization was not observed. Their method has been limited by computer memory (RAM). Therefore, in addition to study the participation ratio, we shall also study other quantities such as the transmission coefficients and the Thouless exponent. Our results given in this section can be regarded as an extension and supplement to the previous study by others.^{15,16}

Transmission coefficient. The transmission coefficient is also a very good quantity reflecting the localization property of eigenstates of electron, and has been used widely to study the eigenstates of electron moving in random and quasiperiodic fields.¹⁷ If the transmission coefficient associated with the eigenstate tends to be a finite limit as $N \rightarrow \infty$, the eigenstate is extended. If the eigenstate is exponentially localized, the transmission coefficient will decrease exponentially as N increasing. This method has the advantage that it can compute transmission coefficients for much larger systems.

Thouless exponent. Another important quantity that describes the localization of eigenstates is the Thouless exponent. The Thouless exponent for an eigenfunction corresponding to the eigenfrequency ω_i of Eq. (2) is

$$\gamma(\omega_i) = \frac{1}{N-1} \sum_{j \neq i}^N \ln |\omega_j^2 - \omega_i^2|. \quad (10)$$

If $\gamma(\omega_i)$ goes to zero as $N \rightarrow \infty$, then the eigenfunction corresponding to ω_i is localized exponentially.

In Figs. 3–5, we show the transmission coefficients, the Thouless exponents, and PR's for the eigenstates of a finite FK chain with $N=987$ for $V=0.4, 1.0$, and 1.6 , respectively. From the numerical results, we find that the transmission coefficients of the phonon eigenstates at the band edges (actually, these are quasiband edges because the phonon spectra are the Cantor-like sets, the quasibands consist of many subbands if we consider a larger FK chain) are smaller than that in the center of the bands. Because the transmission coefficient depends on m_0 , its absolute value is not meaningful for the study of localization of phonon eigenstates. In order to see if these eigenstates at band edges are exponentially localized. We calculate the transmission coefficients for several FK chains having different lengths. Figure 6 shows numerical results for some eigenstates at band edges. We can see that these eigenstates are not exponentially localized. This is nicely demonstrated by the Thouless exponents shown in Figs. 3(b), 4(b), and 5(b). There the Thouless exponents are about $0.005 \sim 0.02$, thus the decay length $\xi = 1/\gamma \sim 10^2$, which is about the order of the size of the FK chains. We also calculated these quantities for larger systems (up to 4181, in fact the transfer-matrix method allows us to

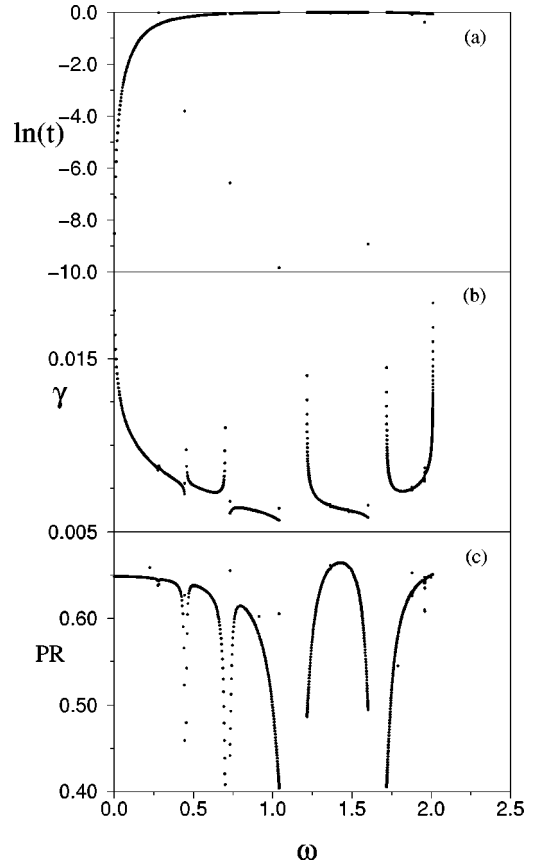
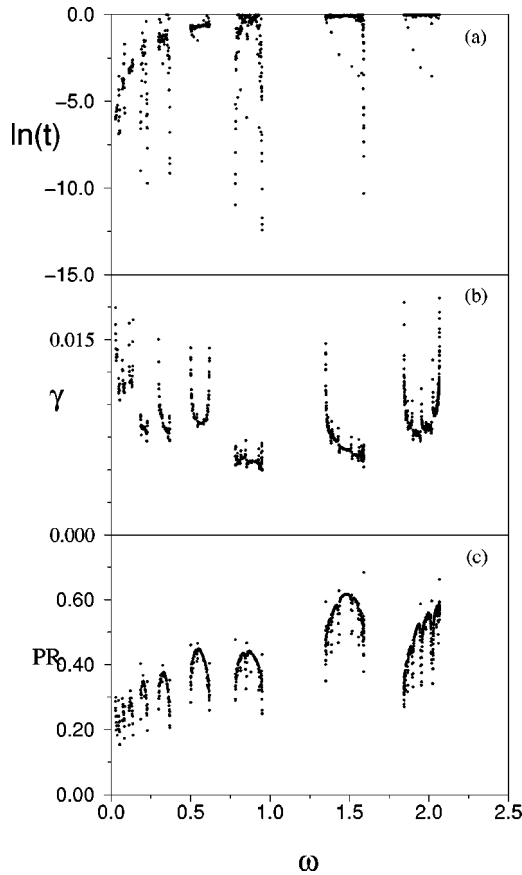


FIG. 3. The transmission coefficients (a), the Thouless exponents γ (b), and the participation ratio (c) for eigenfunctions of the FK chain at $V=0.4$. The particle number of the FK chain is $N=987$, the mass of the atom is $m_0=0.8$, and the winding number is $a/2\pi=(\sqrt{5}-1)/2$.

go to even larger size, e.g., more than 10 946), but no significant difference has been found.

Recently, by using the renormalization-group transformation, Ketoja and Satija¹⁶ have studied the eigenfunctions of the minimum frequency for $V > V_c$. They found that phonon eigenstates defy localization and remain critical. Furthermore, there exists an infinite sequence of parameter values in the regime of $V > V_c$ where the renormalization limit cycle degenerates into a trivial fixed point.¹⁶

Here we would like to get a further picture about the localization for other different scenarios. We shall study not only the transmission coefficients of the degenerated point, but also those cases corresponding to the nondegenerated and pseudodegenerated situation at the regime of $V > V_c$. The results are shown in Fig. 7. There the transmission coefficients as functions of N are drawn for $V=1.756\ 562\ 083\ 826\ 74\dots$, 2.33 , and $3.894\ 742\ 854\ 929\ 86\dots$, respectively. These three values correspond to degenerated, nondegenerated, and pseudodegenerated cases, respectively. We find that there are not qualitative differences of transmission coefficients for the degenerated parameter values and other values of $V > V_c$. The only minor difference is that the curves for degenerated and pseudodegenerated points are more regular than that for nondegenerated. Another thing worthy to be mentioned is that for N fixed, the transmission coefficients decrease as n^{-2} for $n < N/2$ and increase as n^2 for $n > N/2$ [see the insets of Figs.

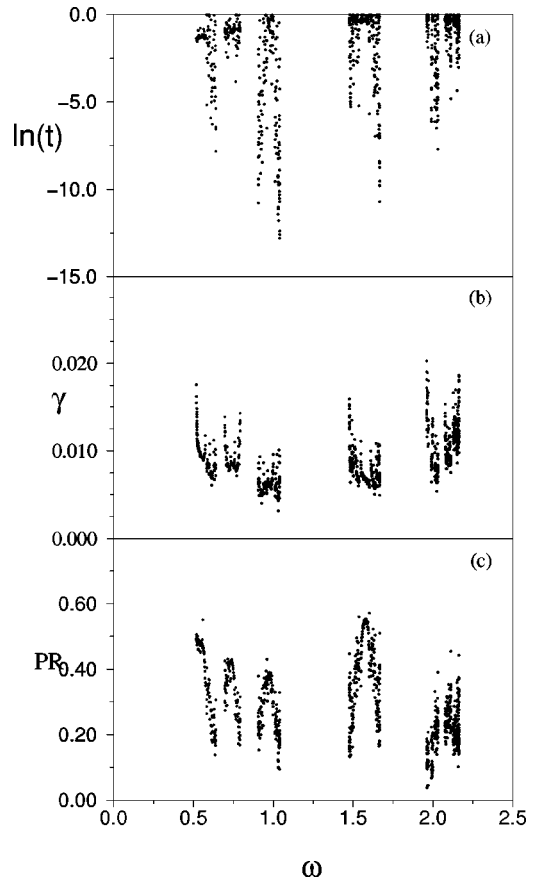
FIG. 4. Same as Fig. 3, but $V=1.0$.

7(a)–7(c)]. This can be understood by realizing that for a small part of the finite FK chain the positions of atoms look irrelative, but not real random, and the plane wave seems to propagate through a pseudorandom medium. But for a large part of finite FK chain, there exists a certain correlation between the positions of atoms, and the correlation increases as $n \rightarrow N$. The plane wave transports through a correlated media, and the transmission coefficients increase as N increased.

IV. HEAT CONDUCTION

The properties of the phonon excitations will be also manifested in another macroscopic quantity—the heat conduction. It is time now to discuss the transport of energy flux or the heat conduction in the finite FK chains. This is a quite interesting problem that attracted much attention in recent years.^{19–25} In this section, we consider a different model of heat conduction, which was discussed by Rubin and Greer²⁷ originally. In this model, the chain of N particles (which constitute the system) is connected at both ends to semi-infinite chains of identical particles. The left and right ends are put in thermal equilibrium at temperatures T_L and T_R , respectively. The original Rubin-Greer model was for periodic and random mass chains with harmonic nearest-neighbor interaction. They found that the stationary heat flux as a function of N can be expressed in terms of the transmission coefficient:

$$J(N) = \frac{T_L - T_R}{4\pi} \int_0^2 t_N^2(\omega) d\omega. \quad (11)$$

FIG. 5. Same as Fig. 3, but $V=1.6$.

It is shown that $J(N) \sim N$ for the uniform and periodic chains and $J(N) \sim N^{1/2}$ for random mass chains. For the FK chains both T_L and T_R must be very low so that the formula (11) can be applied. Figure 8 shows some typical results of $j = J(N)/(T_L - T_R)$ for different V . In the calculation of transmission coefficients, we let the mass of atoms in the left- and right-hand semi-infinite uniform harmonic chains be equal to the mass of atoms in the FK chain. We found that the

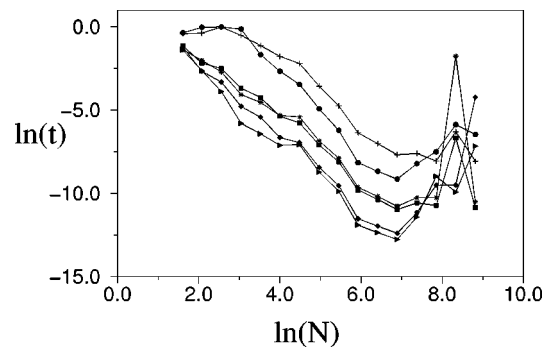


FIG. 6. The transmission coefficients of plane waves with frequencies near the band edges of phonon spectra as functions of N . The solid circles, squares, and diamonds correspond to $\omega = 0.369\ 915\ 599\ 017\ 013\ 597$, $0.782\ 580\ 479\ 119\ 728\ 611$, and $0.950\ 165\ 600\ 964\ 576\ 584$ for $V=1.0$, respectively. The solid stars, triangles, and crosses correspond to $\omega = 0.907\ 882\ 097\ 032\ 394\ 975$, $1.040\ 462\ 163\ 089\ 725\ 28$, and $2.033\ 317\ 415\ 572\ 499\ 79$ for $V=1.6$, respectively. In all cases $m_0 = 0.8$. The lines are drawn for guiding the eye.

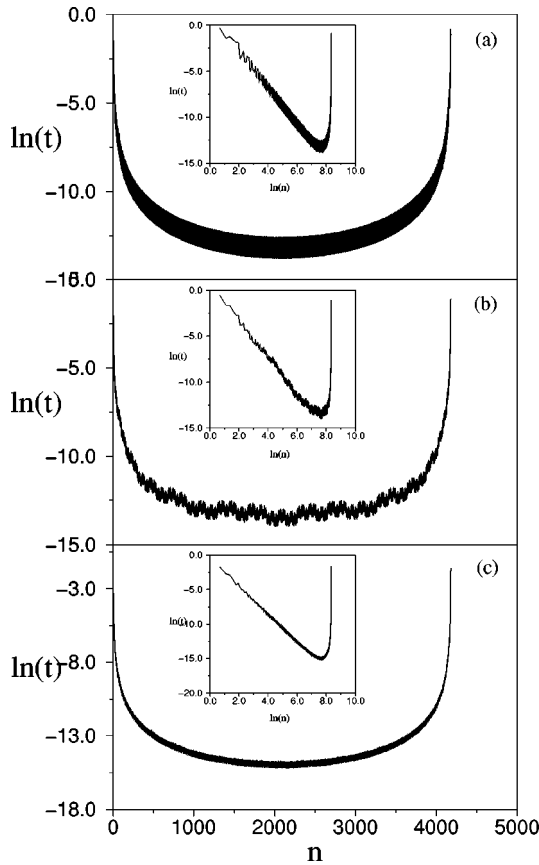


FIG. 7. The transmission coefficient at the minimum frequency ω_{min} versus N for different V . (a) $V=1.756208382674\dots$, (b) $V=2.33$, and (c) $V=3.89474285492986\dots$. Insets are $\ln(t)$ versus $\ln(N)$.

$J(N) \sim N$ for $V < V_c$ and $J(N) \sim N^\alpha$ for $V > V_c$. For $V > V_c$, the α depends on the V . But its range is approximately from 0.83 to 0.87, which is larger than 0.5 for random systems. This also implies that the phonon eigenstates of the FK chain are extended for $V < V_c$ and critical for $V > V_c$.

It should be pointed out that to express the heat flux in terms of the transmission coefficients is valid only at very low temperature, namely the particles oscillate nearby their equilibrium positions. In fact, this is a linearization result of the FK model. In real case, the FK model is nonlinear, thus for the general simulation of heat conduction, one should take the approach of molecular dynamics simulation.^{22,23}

V. DISCUSSION AND CONCLUSIONS

In this paper, we have studied the transmission coefficient of a plane wave through the FK chain by making use of the

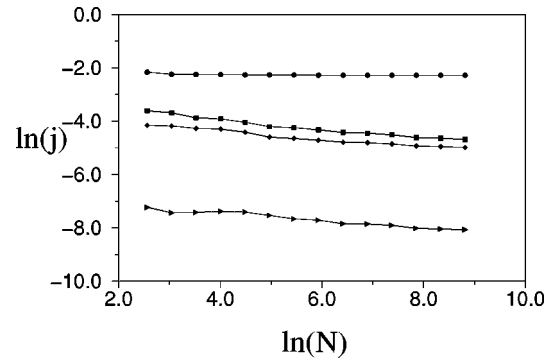


FIG. 8. The ratio $[j=J(N)/(T_R-T_L)]$ of the stationary energy flux to temperature difference for the FK chain as a function of N for different values of V . The solid circles, squares, diamonds, and triangles are for different values of $V=0.4, 1.6, 3.0,$ and $5.0,$ respectively. The lines are drawn for guiding the eye.

transfer-matrix method. We have been able to calculate the transmission coefficients of *all* phonon frequencies. The localization properties of the phonons based on the transmission coefficient and the Thouless exponents agree with that by the participation ratio. We also studied the Rubin-Greer-like model for the FK chain and find that the FK chain likes a periodic chain for $V < V_c$, whereas it looks like a chain somewhat between random and periodic for $V > V_c$. Our numerical results confirm that all eigenstates are critical in Cantorus regime. This result can be understood as the following. For $V < V_c = 0.9716354\dots$, the ground-state configuration of atoms is quasiperiodic. The $V \cos(x_n^0)$ in Eq. (2) is also quasiperiodic and continuous. It corresponds to the phonon problem of the Harper equation in the extended regime ($V < 2$). Therefore all phonon eigenstates are extended. For $V > V_c$, the ground-state configuration of atoms is a Cantorus-like set. The $V \cos(x_n^0)$ takes only some finite values. Consequently, the exponentially localized state does not exist, and all eigenstates are critical.²⁹

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