Statistical properties of phonon transmission in one-dimensional disordered system with long-range correlation

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Abstract

We report statistical properties of the distribution of phonon transmission coefficient (PTC) and phonon amplitude in one-dimensional disordered systems with inverse-power-law structural correlations by numerical calculation. The distribution of PTC over an ensemble on impurity configuration is expected to have some different properties from that of standard disordered systems because of its long-range structural correlation. It is shown that the distribution of the Lyapunov exponent of PTC has a slow convergence different from that of standard disordered systems obeying a normal central-limit theorem. It is also observed that the anomalous distribution of PTC over ensemble has a non-universal form, different from the standard disordered one.

1. Introduction

Recently it has been established that a one-dimensional disordered system (1-DDS) has a pure point energy spectrum and its eigenfunctions are exponentially localized in an infinite system [1,2]. As a result, the ensemble averaged transmission coefficient of a large enough system decreases exponentially with respect to the system size [3]. This statement is established for standard 1-DDS without regard to electronic or phonon system [1].

It is also reported recently that disordered diagonal dimer model corresponding to a one-dimensional tight binding binary alloy have extended states, the number of which is proportional to $\sqrt{N}$ for a finite system size $N$ [4]. In addition to that, a set of extended modes close to a critical frequency is confirmed in a one-dimensional dimer disordered harmonic chain [5].

Furthermore, phonon transmission properties have been studied in superlattices with layer structure and with short-range correlation (SRC). The sequence of layers is generated by some kind of Markov process [6]. However, it is important to mention that most of the random sequences used up to now in these studies are of SRC. A Disordered phonon system having an inverse-power law correlation is studied in this paper. It is shown that this kind of structural long-range correlation (SLRC) causes a feature quite qualitatively different feature from that caused by SRC.

2. Models

The harmonic chain model represented by the following equation of motion is dealt:

$$m_n \frac{d^2 u_n}{dt^2} = -(u_n - u_{n-1}) + (u_{n-1} - u_n)$$

(1)
where \( u_n \) is the displacement from its equilibrium position of the \( n \)th atom and \( m_n \)'s represent sequences of masses. The sequence \( m_n \)'s are generated in this paper by a modified Bernoulli (MB) map in order to have SLRC. The MB map is one-dimensional map proposed in order to reveal the statistical properties of an intermittent chaos [7],

\[
X_{n+1} = f(X_n) = \begin{cases} 
X_n + 2^{B-1}X_n^B & \text{if } 0 < X_n < \frac{1}{2}, \\
X_n + 2^{B-1}X_n^B & \text{if } \frac{1}{2} < X_n < 1,
\end{cases}
\]

(2)

where \( B \) is a non-negative bifurcation parameter which controls the strength of correlation of the sequence \( X_n \)'s.

In this report we study only the stationary regime \( 1 \leq B < 2 \). We use the symbolized sequence made by a rule, \( m_n = m_a \) (for \( 0 < X_n < \frac{1}{2} \)), \( m_n = m_b \) (for \( \frac{1}{2} < X_n < 1 \)), as a sequence of the masses. The mass ratio \( R = m_a/m_b \) plays a role in controlling the strength of the disorder. The sequence, well approximated by a renewal process, is characterized by the residence time distribution \( P(m) \sim m^{-\beta} \), where \( \beta = B/(B - 1) \). The correlation function \( C(n) \) of this symbolic sequence decays exponentially or by power law depending on the value of \( B \), because it is a chaotic sequence [7]:

\[
C(n) = \langle m_0 m_n \rangle \sim [1 + (B - 1)n]^{B/(2B - 1)}, \quad n \gg 1.
\]

(3)

The bifurcation parameter \( B = 1 \) exhibits an exponential damping of the correlation.

Assuming the monochromatic time dependence \( u(t) = \exp(-i\omega t) \), \( u(t = 0) \), we obtain the stationary equation of motion, \(-m_\omega \omega^2 u_n = u_{n+1} - 2u_n + u_{n-1} \), characterized by a frequency \( \omega \). The solution can be written in terms of the product of the transfer matrix \( T_i \) as

\[
\begin{bmatrix} u_{n+1} \\ u_N \end{bmatrix} = M(N) \begin{bmatrix} u_1 \\ u_0 \end{bmatrix} = \prod_{i=1}^{N} T_i \begin{bmatrix} u_1 \\ u_0 \end{bmatrix}.
\]

\[
T_i = \begin{bmatrix} 2 - \omega^2 m_i & -1 \\ 1 & 0 \end{bmatrix}.
\]

(4)

We are interested in the asymptotic property of the amplitude \( u_N \) for \( N \to \infty \) or the corresponding limit theorem of the product of the matrices.

3. Numerical results and discussions

First we discuss the asymptotic behavior of the solution of Eq. (4) with respect to the system size when the set of the initial values \( u_0 \) and \( u_1 \) is given. The Lyapunov exponent (L-exponent) of phonon amplitude in the system of finite size \( N \) is defined as \( \gamma = \ln \|M(N)u_0\|/2N \), where \( u_0 = (u_0, u_0)^T = (1.0)^T \) in this case. It is worth noting that Furstenberg's theorem can be applied to the product of matrices, because the sequence is a renewal process with a finite average residence time \( \langle m \rangle \) [1]. As a result, the L-exponent in infinite system is positive definite and sample independent with probability 1 for any non-vanishing and finite initial vector [8].

Fig. 1 shows the distribution of the L-exponent of phonon amplitude over 215 samples. This calculation is performed for the system with a mass ratio of 2 for some values of squared frequency \( \omega^2 \). Contrary to the behavior of the distribution of ordinary disordered system which obeys normal central-limit theorem (CLT), the multi-peak structure is observed in the distributions in the case of \( B = 1.7 \). This kind of anomalous distribution is seen in

![Fig. 1. Histograms of the distribution of the L-exponent of phonon amplitude in the MB system for some values of squared frequency \( \omega^2 \).](image-url)
a critical regime of phase transition in statistical physics. This anomalous distribution is one of the origins of some anomalous fluctuations of the L-exponent of finite systems. We consider the fluctuation of the L-exponent distribution using the scaling form, $\sqrt{\langle (\Delta y)^2 \rangle} \propto N^{-\kappa(B)}$, by fitting numerical data. The estimated value of $\kappa(B)$ is plotted in Fig. 2. For $1 < B < \frac{1}{2}$, the value of $\kappa$ is roughly $\frac{1}{2}$, implying that the convergent property of the distribution with respect to $N$ obeys or approximately obeys CLT. However, for $\frac{1}{2} < B < 2$, the distribution converges more slowly than that obeying the CLT. The slow convergence corresponds to the anomalous large deviation property of the symbolic sequence [9].

Next we will study the statistical properties of the phonon transmission coefficient (PTC) of a finite system embedded into an infinite perfect lattice with a constant mass ($=1$) by comparing with those in the standard 1-DDS.

We study the relation between the cumulants of distribution for PTC. Some typical relations between the cumulants for some mass ratios are shown in Fig. 3 [10]. It is well observed that some data are plotted on universal curve regardless of mass ratio in the case of $B = 1.1$. This kind of universality has been strongly suggested in electronic random 1-DDS by using several methods [11].

On the other hand, some remarkable deviations are observed in the relations between cumulants for some values of the bifurcation parameter ($\frac{1}{2} < B < 2$) in Fig. 3 when compared with the universal one. We can thus say that the distribution of the PTC in MB system does depend on the bifurcation parameter $B$ controlling the structural correlation and it also depends on the mass ratio $R = m_y (m_x = 1)$.

Although the quantitative theoretical explanations for these behaviors has not been given, we can say qualitatively that the inverse-power-law correlation in the microscopic sequences survives even in the feature of the whole system.

It should be noted that the results obtained in the report are well characterized by the use of renewal process, which is a special one in the semi-Markovian class. Accordingly, it is thus not clear whether the other 1-DDS with SLRC, for example non-symbolized sequence by MB map, have similar properties which have got in this study. We have dealt with a sequence considered only two points correlation. We expect to evolve the understanding the correlated phonon system by using 1-DDS with any multi-points correlation.

Fig. 2. The exponent $\kappa(B)$ of the power for the standard deviation of the L-exponent of the phonon amplitude as a function of the bifurcation parameter.

Fig. 3. Numerical results of the second- and the third-order cumulant ($C_2$, $C_3$) of the distribution of the PTC at $\omega^2 = 2$ as a function of the first-order cumulant for MB system of the bifurcation parameter $B = 1.7$ with $m_y = 1$ and $m_x = 0.7$, 0.9. The data of $B = 1.1$ are added as a reference.
References