Heat flux distribution and rectification of complex networks

Zonghua Liu\textsuperscript{1,2,5}, Xiang Wu\textsuperscript{2}, Huijie Yang\textsuperscript{2}, Neelima Gupte\textsuperscript{3} and Baowen Li\textsuperscript{2,4,5}

\textsuperscript{1} Institute of Theoretical Physics and Department of Physics, East China Normal University, Shanghai 200062, People's Republic of China
\textsuperscript{2} Department of Physics and Centre for Computational Science and Engineering, National University of Singapore, 117546 Singapore, Singapore
\textsuperscript{3} Department of Physics, Indian Institute of Technology, Madras, Chennai 600036, India
\textsuperscript{4} NUS Graduate School for Integrative Science and Engineering, Singapore 117597, Singapore
E-mail: zhliu@phy.ecnu.edu.cn and phylibw@nus.edu.sg

\textit{New Journal of Physics} 12 (2010) 023016 (16pp)
Received 31 August 2009
Published 12 February 2010
Online at http://www.njp.org/
doi:10.1088/1367-2630/12/2/023016

\textbf{Abstract.} It was recently found that the heterogeneity of complex networks can enhance transport properties such as epidemic spreading, electric energy transfer, etc. A trivial deduction would be that the presence of hubs in complex networks can also accelerate the heat transfer although no concrete research has been done so far. In the present study, we have studied this problem and have found a surprising answer: the heterogeneity does not favor but prevents the heat transfer. We present a model to study heat conduction in complex networks and find that the network topology greatly affects the heat flux. The heat conduction decreases with the increase of heterogeneity of the network caused by both degree distribution and the clustering coefficient. Its underlying mechanism can be understood by using random matrix theory. Moreover, we also study the rectification effect and find that it is related to the degree difference of the network, and the distance between the source and the sink. These findings may have potential applications in real networks, such as nanotube/nanowire networks and biological networks.

\textsuperscript{5} Authors to whom any correspondence should be addressed.
1. Introduction

It is well known that heat transfer in a solid obeys Fourier’s law:

\[ J = -\kappa \nabla T, \]

(1)

where the heat flux \( J \) is the amount of heat energy transported through the unit surface per unit time and \( T(x, t) \) is the local temperature. It is not a trivial task to find a microscopic foundation of Fourier’s law, namely find the necessary and/or sufficient condition for the heat conduction to obey the Fourier law. To this end, great effort has been made and some significant results have been achieved in the past decade [1]–[3].

The last decade’s studies have revealed many striking features of heat conduction in low-dimensional systems; in particular, it is found that normal heat conduction (heat conduction following Fourier’s law) only works for limited and specific models. In the general case, abnormal heat conduction has been observed; namely, heat conductivity depends on the system size \( L \), \( \kappa \propto L^\beta \) [4]–[13].

On the other hand, heat conduction is, in fact, a kind of energy diffusion. A lot of attention has been paid to anomalous diffusion. Depending on the exponent \( \alpha \) in \( \langle \Delta x^2 \rangle = 2Dt^\alpha \), the diffusion can be classified into ballistic motion (\( \alpha = 2 \)), superdiffusion (\( 1 < \alpha < 2 \)), normal diffusion (\( \alpha = 1 \)) and subdiffusion (\( \alpha < 1 \)). Normal diffusion has been observed only in the Frenkel–Kontorova (FK) model [14], the disordered FPU model [15], the Lorentz gas channel [16] and billiard models [17, 18], respectively. Recently, it has been pointed out that there exists a corresponding relationship between anomalous heat conduction and anomalous diffusion in the form \( \beta = \alpha - 1 \) [19] or \( \beta = 2 - 2/\alpha \) [2, 20].

However, real systems such as biological systems [21] and artificial networks such as nanotube/nanowire networks in thin-film transistors and nanosensors [22, 23] are not simple one-dimensional (1D) or 2D lattices but complex networks. Owing to the fast development of nanotechnology, it is now very easy to fabricate or grow nanotube/nanowire networks in the laboratory [24]–[27]. Thus the heat conduction in complex networks has now become a realistic problem and we have to face it. To the best of our knowledge, there is no research work on heat conduction in complex networks so far. Thus the purpose of this paper is to provide a first model to study the heat conduction in complex networks.
In contrast with the case of heat conduction, other dynamics in complex networks have been well studied recently, such as epidemic spreading [28]–[32], traffic communication [33]–[37], synchronization [38], electricity transport [24], [39]–[49], etc., owing to the rapid progress in the field of complex networks [50]–[52]. Among them, electric conduction is the one closest to heat conduction. It is found that electric transport changes linearly with the number of added bonds [24, 43], and the heterogeneity of complex networks enables fast mutual access of all nodes and thus improves electric transport [45, 46]. The dependence of electrical current and flow on multiple sources and sinks is also discussed [44]. The whole electric resistance of the network can be figured out by the Kirchhoff second law for the complicated parallel and serial electric circuits [45, 47]. A trivial deduction would be that the presence of hubs in complex networks can also accelerate the heat transfer. According to the best of our knowledge, there is no concrete work to justify this argument so far.

Can we apply the effective approach of the electric network to the case of the heat conduction network? Toward this direction, some primary efforts have been made, such as in small size networks [53, 54] and in coupled chains [55]. For the former, it is found that a small size network can exhibit ‘strange’ transport phenomena. In particular, circulation of heat flux may appear in the steady state of a network of three oscillators only [54]. For the latter, we have found that the coupling between two chains will form an interface and thus introduces an interface thermal resistance. The value of interface thermal resistance depends sensitively on the position and strength of the coupling [55]. These features imply that there are essential differences between the electric network transferred by electrons and the heat conduction network transferred by lattice vibrations. That is, the Kirchhoff second law is applicable to heat conduction network only after considering the induced interface resistance, which is different from the situation of the electric network (circuit) where no interface resistance is considered and the Kirchhoff second law can be directly applied [24], [39]–[43]. These ‘strange’ properties revealed in the small size networks and coupled chains will definitely exist in the case of a complex network, which consists of a lot of chains or small size networks. In complex networks, a diversity of couplings among the chains exist, resulting in a lot of inter-resistances, thus making it difficult to calculate the effective heat resistance of the network. Thus, it is a challenge to study heat conduction in a complex network. To understand heat conduction in complex networks, we need to consider a completely new model, i.e. a model based on the topological structure of a complex network. Therefore the purpose of this paper is to understand how a heat current can be regulated or manipulated by the structures of complex networks.

In this paper, instead of using the effective circuit approach, we will investigate heat conduction in complex networks by using numerical simulations. We demonstrate that the heat flux will decrease with the increase of heterogeneity of the network caused by degree distribution or the clustering coefficient. The effect of rectification will become significant when the degrees of the source and sink nodes have a large difference. This result may shed light on the heat manipulation and regulation in biological systems where the network structure and the dynamical processes may interact with each other and reach an optimal relationship.

The paper is organized as follows. In section 2, we briefly introduce the FPU model of heat conduction in the 1D lattice. In section 3, we present our heat conduction model in complex networks and discuss how heat conduction depends on the network topology. We illustrate the influence of network topology by using random matrix theory. We also discuss the rectification of heat flow caused by the heterogeneity of the network. In section 4, we give our conclusions and discussions.
2. The FPU model

The heat conduction in 1D systems is usually studied by a chain of \( N \) coupled atoms with the two ends contacting a thermal bath of higher or lower temperature, respectively \([1, 2]\). The Hamiltonian of the chain has the form

\[
H = \sum_{i=1}^{N} \left( \frac{p_i^2}{2m_i} + U(x_i) + V(x_{i+1} - x_i) \right),
\]

where \( m_i \) and \( x_i \) represent the mass and the position of the \( i \)th particle, respectively, \( U(x) \) denotes the on-site potential on a substrate and \( V(x) \) is the nearest-neighbor interaction. For convenience, let \( m_i = 1 \) and let \( x_i \) be the displacement from the equilibrium position. As the two ending atoms have special positions, they will have different dynamical equations with the medium atoms. The medium atoms satisfy the canonical equations

\[
\dot{x}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial x_i}, \quad i = 2, 3, \ldots, N - 1.
\]

(3)

Let the first and last atoms be kept at the Nose–Hoover thermostat \([56]\) with temperature, \( T_h \) and \( T_\ell \), respectively. Thus, they satisfy

\[
\dot{x}_1 = \frac{\partial H}{\partial p_1}, \quad \dot{p}_1 = -\frac{\partial H}{\partial x_1} - \xi_{h} p_1,
\]

\[
\dot{x}_N = \frac{\partial H}{\partial p_N}, \quad \dot{p}_N = -\frac{\partial H}{\partial x_N} - \xi_{l} p_N,
\]

(4)

where \( \xi_{h} \) and \( \xi_{l} \) are thermodynamic friction coefficients and satisfy

\[
\dot{\xi}_{h} = \frac{\dot{x}_1^2}{T_h} - 1, \quad \dot{\xi}_{l} = \frac{\dot{x}_N^2}{T_\ell} - 1.
\]

(5)

The thermostat equations (4) and (5) will produce canonical distributions of \( \dot{x}_1 \) and \( \dot{x}_N \) with the given temperatures \( T_h \) and \( T_\ell \), respectively \([56]\). Thus, the medium atoms will be influenced by these two ending atoms and gradually reach their equilibrium state.

The system (2) is momentum conserved when \( U(x) = 0 \) and not conserved when \( U(x) \neq 0 \). Equation (2) will give different models when the potentials \( U \) and \( V \) have different forms. The most general model used in heat conduction is the FPU model where an abnormal process of heat transfer was detected for the first time \([57]\). The potential of the FPU model is defined as \( U(x) = 0 \) and

\[
V(x) = \frac{g_2}{2} x^2 + \frac{g_3}{3} x^3 + \frac{g_4}{4} x^4,
\]

(6)

which can be regarded as resulting from an expansion of \( V \) around its equilibrium position \( x = 0 \). It is called the FPU-\( \alpha \) model when \( g_4 = 0 \) and the FPU-\( \beta \) model when \( g_3 = 0 \) \([1]–[3]\).

After the transient process, the chain will reach a stationary state. A local temperature at each atom can be defined as \([1]–[3]\)

\[
T(i) = \langle p_i^2 \rangle.
\]

(7)
When two neighboring atoms have different local temperatures, there will be a heat flux, $J_i$, from the higher temperature to the lower temperature, which can be calculated by using \([1, 14, 58, 59]\)

$$J_i = \langle \dot{x}_i \frac{\partial V}{\partial x_{i+1}} \rangle,$$  \hspace{1cm} (8)

where $\langle \cdots \rangle$ is the time average. Because of the fluctuation of $\dot{x}_i$, the time for taking the average in equation (8) should be long enough to stabilize $J_i$, such as $10^6$ in this paper. For a single chain, $J_i$ will be site independent.

Except for the FPU model, there are several other models such as the FK model, the $\phi^4$ model, disordered harmonic chains, the ding-a-ling model, Toda lattice, Klein–Gorden lattice, etc, which are also used very often in heat conduction \([1, 2]\). The generalization of these models to two dimensions is rather straightforward; see examples in \([60]–[62]\).

3. Heat conduction in complex networks

As we have pointed out in the introduction, the heat conduction in complex networks is fundamentally different from the regular 1D and 2D chains. To understand the mechanism of heat conduction in complex networks, we present a network model of heat conduction in this section, which is based on the topological structure of complex networks.

3.1. Adjusting the structure of complex networks

The complex network has been well studied in recent years, and a lot of models have been proposed \([50]–[52]\. Two typical models are the random network and the Barabasi–Albert (BA) scale-free network \([50]\. The distinct difference between them is the degree distribution, where the random network has a Gaussian-type distribution $P(k) \sim e^{-k}$, the BA model has a power-law degree distribution $P(k) \sim k^{-3}$, with $k$ being the links of a node.

Based on the BA model, a general network model has been presented, which can produce any network structures in between the random and SF networks by adjusting a parameter $p$ \([63]\. The general network can be constructed as follows: we first take $m$ nodes as the initial nodes and then add one node with $m$ links at each time step. The $m$ links from the added node go to $m$ existing nodes with probability $\Pi_i \sim (1 - p)k_i + p$, where $k_i$ is the degree of node $i$ at that time and $0 \leq p \leq 1$ is a parameter. The resulting network has an average degree $\langle k \rangle = 2m$ for large $N$. Obviously, $(1 - p)k_i$ in $\Pi_i$ represents the preferential attachment and $p$ in $\Pi_i$ represents the random attachment. The resulting connectivity distribution is shown to be \([63]\)

$$P(k) \sim [k + p/(1 - p)]^{-\gamma},$$

where the scaling exponent $\gamma$ is $\gamma = 3 + p/[m(1 - p)]$. We see that the power-law scaling for SF networks is recovered for $p = 0$ and the distribution becomes exponential $P(k) \sim e^{-k/m}$ as $p \to 1$. That is, it is a random network for $p = 1$, the BA model for $p = 0$ and other complex networks in between the random and SF for $0 \leq p \leq 1$.

For a fixed degree distribution $P(k)$, its topology can be changed by adjusting its clustering coefficient $C$, which represents the possibility that two neighbors of a given node will also be neighbors \([50]\. The clustering coefficient can be changed in several ways \([64]–[66]\. We here choose the rewiring approach \([66]$, which has the advantage that the degree of each node will remain unchanged when we change its clustering coefficient. The algorithm of the rewiring approach can be stated as follows \([66]$: randomly choose two links, one connecting nodes $A$
and $B$, and the other $C$ and $D$. Each node changes its partner and the original links $A–B$ and $C–D$ are altered to $A–D$ and $B–C$. The link exchange trial is accepted only when the new network configuration has a higher clustering coefficient.

In this paper, we will use the general network model to discuss the influence of degree distribution on the heat conduction, and then use the rewiring approach to change the clustering coefficient of the general network model and discuss how the clustering coefficient influences the heat conduction.

3.2. The complex network model of heat conduction

Our model can be described as follows: a complex network of heat conduction consists of a lot of atom chains with different lengths and the chains are entangled/intersected at many places. Let each intersection of the atom chains be a node; thus the nodes are connected by short chains, i.e. part of the atom chain. A short chain between two connected nodes can be considered as a 1D chain and its length may be different for different short chains. For simplicity, we replace the short chains by springs, i.e. the nodes are connected/coupled by springs. Thus, these springs form the links of the network. Considering the fact that heat conductivity $\kappa$ is size dependent [1]–[3], we represent the different lengths of short chains between two connected nodes by different spring coefficients or coupling strengths, i.e. the links have different weights, which can be implemented by a given distribution. Therefore, we obtain a weighted network with different weights/couplings on the links. The distribution of weights will be determined later.

We consider the situation in which each node oscillates around its equilibrium position; thus for simplicity, each node $i$ can be considered as a 1D FPU-$\beta$ model with the Hamiltonian $H = \sum_{i} E_i^k + E_i^\gamma$, where $E_i^k = \frac{1}{2}p_i^2$, $E_i^\gamma = \frac{1}{2} \sum_j \gamma_{ij} \left[ \frac{1}{2} (x_j - x_i)^2 + \frac{1}{4} (x_j - x_i)^4 \right]$, $x_i$ represents the displacement from the equilibrium position of node $i$, $\gamma_{ij}$ the coupling/spring strength between nodes $i$ and $j$, and the sum is for all the neighbors $j$ of node $i$. We randomly choose two nodes $i_0$ and $j_0$ to contact two heat baths with temperature $T_h$ and $T_c$ ($T_h > T_c$), respectively. The heat baths are the Nose–Hoover thermostat [1]. Different from the case of 1D chains where the heat can be transported only through one path, here the heat may go from node $i_0$ to node $j_0$ through a number of paths. That is, the heat flux will be transmitted to other nodes through all the links of $i_0$. Near $j_0$, all the fluxes will gradually merge and finally go to $j_0$ through the links of $j_0$. Therefore, the heat flux from $i_0$ to $j_0$ depends on the structure of networks, such as the degree distribution, the clustering coefficient, etc. We are interested in how heat flux from $i_0$ to $j_0$ depends on the network structure.

In short, the heat conduction in complex networks depends on both the induced interface resistance and the network topology. To illustrate how heat flux depends on the network topology, we put the influence of interface resistance aside for a while and consider the specific situation of $\gamma_{ij} = 1$. In this situation, we can write the network in the form of matrix $A = (a_{ij})$ with $a_{ij} = 1$ if $i$ and $j$ are connected and 0 otherwise. Let $a_{ii} = 0$ for avoiding self-connection. Denote $M$ as the temperature vector of $N$ components. For convenience, we reorganize the network and let the source with $T_h$ be node 1 and the sink with $T_c$ be node 2. Thus, the temperature vector $M$ can be expressed as $M = (T_h, T_c, T_3, \ldots, T_N)^T$ and can be divided into block-1 with $M_1 = (T_h, T_c)^T$ and block-2 with $M_2 = (T_3, \ldots, T_N)^T$. The discrete Laplace operator on the network, an analogue of $\nabla^2$, is $L = D - A$, where $D$ is the diagonal degree matrix. Correspondingly, the matrix $L$ can be divided into four submatrices $L_{11}, L_{12}, L_{21}$
and $L_{22}$. In the steady state we have $LM = J$, where $J$ is the external flux. Note that this is the discrete analogue of $-\kappa \nabla^2 T(r) = \nabla \cdot j(r)$ with $M$ playing the role of $\kappa T(r)$ and $J$ playing the role of $-\nabla \cdot j(r)$ [67], where $j(r)$ is the flux vector field. Except for the source and sink nodes, the equilibrium condition demands that no net heat flux should occur, i.e. $J = 0$ for the nodes $i = 3, \ldots, N$. Thus, we have

$$L_{11}M_1 + L_{12}M_2 = J,$$

$$L_{21}M_1 + L_{22}M_2 = 0,$$

where $J = (J_0, -J_0)^T$ with $J_0$ being the outgoing flux at the source $T_h$.

Rewrite the second equation of equation (9) as $L_{22}M_2 = -L_{21}M_1$. As $M_1$ and the submatrices $L_{11}$, $L_{12}$, $L_{21}$ and $L_{22}$ are all known for a network with chosen $i_0$ and $j_0$, so $-L_{21}M_1$ is a $(N - 2) \times 1$ matrix or a $(N - 2)$-dimensional vector. Therefore, the equation $L_{22}M_2 = -L_{21}M_1$ has a unique nonzero solution $M_2$. Then substituting $M_2$ into the first equation of equation (9), we can obtain $J$. That is, $J$ can be analytically solved. $(J)$ is just the ensemble average of $J$ for different pairs of $i_0$ and $j_0$. From the fact that the number of $a_{ij} \neq 0$ in a row of A is the degree of node $i$, we see that the random network has a relatively ‘uniform’ distribution of elements $a_{ij} \neq 0$ in the rows of $A$, while the SF network has a non-uniform $a_{ij} \neq 0$ in the rows of $A$. Another factor to cause heterogeneity of $A$ is the clustering coefficient $C$. For larger $C$, the links form groups and make the elements $a_{ij} \neq 0$ in $A$ become local clusters. The heterogeneity will seriously influence the flux $(J)$ through equation (9).

Go back to our model. Both the interface resistance and the network heterogeneity will influence the flux $(J)$. It is difficult to analytically solve this problem. Thus, in the following, we will use numerical simulations to study the heat conduction in complex networks and the components of $M$ will be calculated by equation (7).

### 3.3. Heat conduction in complex networks

In numerical simulations, we take the network size $N = 100$ and the average links $\langle k \rangle = 6$ and assign each link a coupling strength $\gamma_{i,j}$ from the uniform distribution in $[0.5, 1.5]$. Considering that heat conduction can be considered as a diffusion process of continuous energy pulses from the source to the sink, we need to first understand how an energy pulse is spread out. For this purpose, we first thermalize the network to temperature $T = 0.6$. That is, we randomly choose a few nodes and let them contact a heat bath of temperature $T = 0.6$. The heat bath will continuously provide energy to the nodes and the energy will be gradually transferred to other nodes through the links/couplings. After the transient process, the network will reach a stationary state. Then we remove the heat baths and add an energy pulse $\delta E_i = 9E^i_0$ at a randomly chosen node $i$ at time $t = 0$ by increasing its velocity. We observe that this energy pulse will be gradually transported to its neighbors and then to its neighbors’ neighbors and so on. An interesting finding is that both the variations of $\delta E_i$ at the source node $i$ and the $\delta E_j$ at the neighbors of $i$ and other nodes are not monotonically decreasing or increasing but oscillatory, in contrast to the smooth decay of electric energy.

This oscillatory spreading can be understood as follows. The energy spreading is through the variation of potential between two neighboring nodes. As the vibrations of nodes make the potentials change periodically, the losses or gains of energy at node $i$ depend on its instantaneous
Figure 1. Heat fluxes $J_{i_0 \rightarrow j_0}$ for different pairs $(i_0, j_0)$ at the stationary state with $T_h = 0.7$ and $T_\ell = 0.5$ where the $x$- and $y$-axes denote the node indexes $i_0$ and $j_0$. They are (degree) ordered descendingly, respectively; (a) and (b) denote the cases of $p = 1$ and 0, respectively, and (c) and (d) denote the results of $C = 0.6$ for the cases of $p = 1$ and 0, respectively.

Heat conduction can be considered as a diffusion of continuous energy pulses from the source to the sink. To investigate the influence of network structure, we randomly choose two nodes $i_0$ and $j_0$ and put them in contact with heat baths maintained at temperatures $T_h = 0.7$ and $T_\ell = 0.5$, respectively. The heat bath $T_h$ will continuously provide energy pulses to the node $i_0$; then the energy will be transferred to other nodes through the links/couplings and be finally absorbed at $j_0$ by the heat bath $T_\ell$. After the transient process, the network will reach a stationary state. The heat flux sent out from $i_0$ is the sum of all the paths from $i_0$ to its neighbors and the part on each individual path can be calculated by equation (8), i.e. $\langle p_{i_0}(\partial E^V_{i_0})/(\partial x_{i_0+1}) \rangle$, where $x_{i_0+1}$ denotes one neighbor of node $i_0$ and $\langle . \rangle$ is the time average. In the same way, we can calculate the total heat flux absorbed at $j_0$. After the transient process, the heat flux sent out from $i_0$ will equal that absorbed at $j_0$. We denote it as the heat flux from $i_0$ to $j_0$, $J_{i_0 \rightarrow j_0}$. By changing the node pair $(i_0, j_0)$, we can calculate another $J_{i_0 \rightarrow j_0}$. In this way, we obtain $J_{i_0 \rightarrow j_0}$ for all the possible pairs $(i_0, j_0)$. Figures 1(a) and (b) show the distribution of $J_{i_0 \rightarrow j_0}$ for the cases of $p = 1$ and 0, respectively, where the $x$-axis denotes the node index $i_0$ and the $y$-axis the index $j_0$ and they are degree ordered descendingly. Obviously, the flux $J_{i_0 \rightarrow j_0}$ is different from pair to pair and the fluxes in (a) are much larger than those in (b), indicating that the flux $J_{i_0 \rightarrow j_0}$ depends on the chosen pair $(i_0, j_0)$ and the random network is in favor of energy diffusion. The reason is that the random network is relatively ‘uniform’, most of the nodes have the degree around the average value and thus they spread out the energy fast, while the SF network is heterogeneous with hub nodes, which results in a bottleneck problem and thus suppresses the energy spreading.
We use the rewiring approach [66] to increase the clustering coefficient of the network and then perform the heat conduction simulations. Without rewiring, the clustering coefficient is $C = 0.08$ in figure 1(a) and $C = 0.14$ in figure 1(b). With rewiring, we can increase $C$ to over 0.6. Figures 1(c) and (d) show the results of $C = 0.6$ for the cases of $p = 1$ and 0, respectively. Compared with figures 1(a) and (b), it is easy to see that the fluxes in figures 1(c) and (d) are heavily suppressed, indicating that the fluxes decrease with further increase of heterogeneity.

A common feature of figures 1(a)–(d) is that the fluxes are not continuously varied but interweaved by higher and lower values. This can be understood as follows. For a chosen pair $(i_0, j_0)$, the energy pulse first spreads to the neighbors of $i_0$ and then to the neighbors of the neighbors of $i_0$ and so on. After that, the energy pulses will be gradually merged into the neighbors of $j_0$ and finally absorbed at $j_0$. Thus, the energy is transferred by a lot of paths and each path consists of several intermediate stops. The total flux $J_{i_0 \rightarrow j_0}$ is a sum over all paths. For a different chosen pair $(i_0, j_0)$, the sum $J$ will be different. All the $J$ will satisfy a distribution $P(J)$. For a homogeneous network, each path of heat transmission can be approximately considered as equivalent to others. The sum of heat fluxes on different paths can be approximately treated as the sum of random variables, thus resulting in normal distribution of $P(J)$. For a heterogeneous network, the paths are not equivalent because of the existence of hubs or local loops, i.e. some paths will go through hubs or local loops but others may not. That is, the paths are ‘weighted’ with different weights. The sum of these weighted random variables will deviate from the Gaussian distribution.

Figures 2(a) and (b) show the results for the case without rewiring and the case with rewiring to $C = 0.6$, respectively, where ‘triangles’ denotes the case of $p = 1$, ‘circles’ the case of $p = 0$ and dashed lines are the fit by Gaussian distribution. It is easy to see that the case of the random network with $p = 1$ is fitted very well, but the other three cases are not fitted so well. To make a better fitting, figures 2(c) and (d) show the results in a log–log plot, where the dashed lines are fitted by log-normal distribution. Obviously, the log-normal fit does not work for the case of the random network with $p = 1$ where there is a significant difference between the fitting (red dashed line) and the numerical simulations (triangles) for $J < 0.1$, but works very well for the other three cases. Thus, we conclude that $P(J)$ satisfies Gaussian distribution for the homogeneous network and log-normal distribution for the heterogeneous network.

From figure 2 we see that the peaks of the distribution for the four cases are located at different places, indicating they will have different average flux $\langle J \rangle = \int J P(J) dJ$. To understand how the network structure influences $\langle J \rangle$, we now adjust the degree distribution by the parameter $p$ and change the clustering coefficient $C$ by the rewiring approach. We find that $\langle J \rangle$ increases monotonically with $p$, as shown in figure 3(a), and decreases with the increase of $C$ for fixed degree distribution $P(k)$, as shown in figure 3(b) where ‘squares’ and ‘circles’ represent the cases of $p = 1$ and 0, respectively. As the degree of heterogeneity decreases with the increase of $p$ but increases with $C$, $\langle J \rangle$ decreases with the increase of the degree of heterogeneity.

The underlying mechanism of the influence of network topology on heat conduction can be understood from the structure-induced localizations of collective waves. This topic has been studied in typical complex networks such as small world, random and SF networks [68]–[70], in analogy to the Anderson transition or metal–insulator transition where an injected wave will spread all over the system in a metallic phase but will be localized in the vicinity of the injection point in the insulating phase. An interesting question here is whether a wave injected into one of the nodes will produce a signal at all other nodes or only at a finite set of other nodes. By
studying the spectral statistics, Sade et al [68] found that the connectivity influences the degree of localization. In the case of heat conduction, the energy propagates through the links and redistributes at the nodes into the outgoing links. To show the influence of network on the heat conduction, we consider an electron walking on the network. A simple computation shows that the tight-binding Hamiltonian of the system is the same as the adjacency matrix of the network, \( A \). The elements of \( A \) are given by the coupling strength \( \gamma_{ij} \), i.e. \( a_{ij} = \gamma_{ij} \) if nodes \( i \) and \( j \) are connected; \( a_{ij} = 0 \) otherwise. The nearest-neighbor-level-spacing distribution of the spectrum of \( A \), denoted by \( P(s) \), is given by the Brody distribution

\[
P(s) = (1 + \beta) B \left( \frac{s}{D} \right)^{\beta} \exp \left( -B \left( \frac{s}{D} \right)^{1+\beta} \right),
\]

where \( D \) is the average of \( s \) and \( B = \left[ \Gamma(2+\beta/1+\beta) \right]^{1/\beta} \) [71, 72]. For the cases of \( \beta = 0 \) and 1, \( P(s) \) reduces to the Poisson and Wigner distributions, which correspond to localized and extended states, respectively. Generally, \( \beta \) values are in between 0 and 1 and represent the behavior in between localized and extended states. The structure-induced localization can be quantitatively measured by \( \beta \) [71]–[74].

**Figure 2.** Distributions of heat fluxes: ‘triangles’ denotes the case of \( p = 1 \), ‘circles’ denotes the case of \( p = 0 \) and the dashed lines represent the fit. (a, b) The linear–linear plot with Gaussian fit; (c, d) the log–log plot with log-normal fit.
Figure 3. (a) The ensemble average $\langle J \rangle$ versus $p$; (b) the ensemble average $\langle J \rangle$ versus $C$ for $p = 1$ (‘squares’) and 0 (‘squares’); (c, d) The nearest-neighbor spacing distribution $P(s)$ versus the actual spacing in units of the mean level spacing $s/D$ for the cases without rewiring and with rewiring with $C = 0.5$, respectively, where the zigzag lines denote the experimental results and the smooth curves the Brody distribution fit and the insets are the Brody exponent.

For each fixed parameter $p$ and $C$, we construct 200 network realizations and calculate their eigenvalues and then obtain the normalized $s/D$ by the unfolding approach [73, 74]. Then we construct its histogram by choosing bin = 0.1. The zigzag curves in figures 3(c) and (d) show typical histograms of $p = 0, 1$ for the case without rewiring and the case with rewiring for $C = 0.5$, respectively. The smooth curves in figures 3(c) and (d) are their Brody distribution fits. In this way, we find that the $\beta$ value increases with $p$ for the case without rewiring, see the inset in figure 3(c). For the fixed degree distribution, we find that the $\beta$ value decreases with the increase of $C$ for the case with rewiring; see the inset in figure 3(d). Obviously, the change in the tendency of $\beta$ curves in figures 3(c) and (d) is consistent with the change in the tendency of $\langle J \rangle$ in figures 3(a) and (b), implying that the $\beta$ value is closely related to the heterogeneity of the network. Therefore, the heterogeneity suppressing heat conduction is due to the localization of vibration modes or phonons.

3.4. Rectification in complex networks

Among many ways of manipulating heat flow, rectification is the most fundamental [75]–[78]. Experiment on nanotubes has verified the rectification [25]. Can this phenomenon be observed in the heat conduction of complex networks?
Figure 4. Rectification $R_{ij}$ where figures 4(a)–(d) correspond to figures 1(a)–(d), respectively.

Another feature shown in figures 1(a)–(d) is the asymmetric fluxes, i.e. the heat flux from $i_0$ to $j_0$ is not equal to the inverse. This rectification may be useful in manipulating heat flow, by using the network topology. We here introduce a quantity

$$R_{ij} = \frac{|J_{i\rightarrow j} - J_{j\rightarrow i}|}{\max(J_{i\rightarrow j}, J_{j\rightarrow i})}$$

as the rectification coefficient. Larger $R_{ij}$ corresponds to larger relative difference between $J_{i\rightarrow j}$ and $J_{j\rightarrow i}$, i.e. larger rectification effect. Let $i$ and $j$ be ordered degree descendingly; then the matrix $R_{ij}$ must be symmetric on the diagonal line $i = j$. That is, $R_{ij}$ represents the value of asymmetric transport but ignores the direction of the net flux, i.e. the direction of difference $J_{ij} - J_{ji}$. Figure 4 shows the rectification matrix where figures 4(a)–(d) correspond to figures 1(a)–(d), respectively. From figure 4(a) it is very easy to see that the node index $i = 1$ (or $j = 1$) has higher $R_{ij}$ with all the nodes of $j \geq 5$ (or $i \geq 5$) and the node indexes $i \leq 20$ have higher $R_{ij}$ with most of the other nodes of $j \geq 25$, see the ‘flames’ there, and there are lower $R_{ij}$ among the pairs with both $i \geq 25$ and $j \geq 25$. By checking their degrees we find that the node with $i < 25$ has degree $k_i > k_{max}/2$ and the node with $i \geq 25$ has degree $k_i < k_{max}/2$, indicating statistically that the larger degree difference between $i$ and $j$ makes a larger $R_{ij}$. Considering that the number of those nodes with degree $k_i > k_{max}/2$ is very small and thus can be approximately considered as hubs, we conclude that the $R_{ij}$ between the hubs and the general nodes are significant.

Apart from the degree difference, the distance between $i$ and $j$ and the paths will also influence the rectification; thus we also observe lower $R_{ij}$ between two ‘flames’ in figure 4(a). We observe a similar phenomenon in figure 4(b) except for the first three indexes, i.e. $i \leq 3$. We know that the SF network has hubs. By checking their degrees we find that the node with $i \leq 3$ has degree $k_i > k_{max}/2$ and the node with $i > 4$ has degree $k_i < k_{max}/2$. That is, the degrees of
the first three nodes are much larger than the others. This characteristic feature means that the hubs are directly connected with most of the other nodes without intermediate stops, indicating that their heat transfer is approximately symmetric, thus resulting in lower $R_{ij}$. This point can be seen more clearly as follows. Take a hub and a node connected to it as an example. As the hub has much larger degree than the connected node, the number of paths for sending out heat flux from the hub is much larger than that from the connected node. An intuitive deduction is that the heat flux from the hub to the connected node should be much larger than that from the connected node to the hub. Is this correct? Notice that the shortest path in all the paths from the hub to the connected node has the smallest thermal resistance and thus the maximal heat flux. Especially, this maximal heat flux will be the majority of the total flux from the hub to the connected node when they are directly connected. We have the same conclusion for the inverse process, i.e. heat flux from the connected node to the hub. As the maximal heat flux in the shortest path is the same for both directions because of the same thermal resistance, so their heat transfer is of some difference but the difference is not significant, indicating that their heat transfer is approximately symmetric. Moreover, we find that the $k_{\text{max}}$ of the SF network is two times the $k_{\text{max}}$ of the random network, implying the nodes with $i > 4$ in the SF network are equivalent to all the nodes in the random network and thus they have similar behavior. Figures 4(c) and (d) can be explained in the same way.

To see the influence of degree difference better, we calculate the rectification on degree difference $\Delta k$ and let $R(\Delta k)$ be the average of $R_{ij}$ on those pairs of nodes with $|k_i - k_j| = \Delta k$. Figure 5 shows the results. From both figures 5(a) and (b) we can see that the rectification $R(\Delta k)$ increases with the degree difference of node pairs for all four cases.

4. Conclusions and discussions

The dynamics of complex networks can be classified into two classes. The first class is that the node’s behavior does not change with time, such as epidemic spreading and electric...
current transfer. In epidemic spreading, nodes provide the locations for agents to infect each other; and in electric flow transmission, the resistance at each node is fixed. For this kind of dynamics, because of the existence of hubs, the SF network usually accelerates its transport and results in significant effects such as the absence of epidemic threshold [29] and the improved electric transmission [45]. The second class is that the node’s behavior changes with time, such as the synchronization of oscillators and heat conduction. It is now very clear that the synchronization in complex networks depends on both the network topology and the dynamics of the oscillators [38]. Combining with results obtained in this paper, we would conclude that the SF network may not accelerate the transport for the second dynamics.

In conclusion, we have studied heat conduction in a complex network model. It is found that as an energy flow, heat flow in complex networks is quite different from the electric flow. We have demonstrated that the network structure greatly influences the heat current, and hence it is possible to regulate the heat current via the structure of the complex network. We also demonstrate that the rectification is closely related to the network topology. This result may shed light on the heat manipulation and regulation in biological systems where the network structure and the dynamical processes may interact with each other and reach an optimal relationship.

Acknowledgments

ZL is supported in part by the NNSF of China under grant numbers 10775052 and 10635040 and by National Basic Research Program of China (973 Program) under grant number 2007CB814800.

References

[1] Lepri S, Livi R and Politi A 2003 Phys. Rep. 377 1
[2] Li B, Wang J, Wang L and Zhang G 2005 Chaos 15 015121
[3] Dhar A 2008 Adv. Phys. 57 457
[4] Lepri S 1998 Phys. Rev. E 58 7165
[5] Pereverzev A 2003 Phys. Rev. E 68 056124
[6] Narayan O and Ramaswamy S 2002 Phys. Rev. Lett. 89 200601
[7] Payton D N III and Visscher W M 1967 Phys. Rev. 156 1032
[8] Li B, Casati G and Wang J 2003 Phys. Rev. E 67 021204
[9] Kaburaki H and Machida M 1993 Phys. Lett. A 181 85
[10] Dhar A 2001 Phys. Rev. Lett. 86 3554
[11] Rieder Z, Lebowitz J L and Lieb E 1967 J. Math. Phys. 8 1073
[12] Savin A V and Gendelman O V 2003 Phys. Rev. E 67 041205
[13] Liu Z and Li B 2008 J. Phys. Soc. Japan 77 074003
[14] Hu B, Li B and Zhao H 1998 Phys. Rev. E 57 2992
[15] Li B, Zhao H and Hu B 2001 Phys. Rev. Lett. 86 63
[16] Alonso D, Artuso R, Casati G and Guarneri I 1999 Phys. Rev. Lett. 82 1589
[17] Zaslavsky G M 2002 Phys. Rep. 371 461
[18] Metzler R and Klafter J 2000 Phys. Rep. 339 1
[19] Denisov S, Klafter J and Urbakh M 2003 Phys. Rev. Lett. 91 194301
[20] Li B and Wang J 2003 Phys. Rev. Lett. 91 044301
[21] Diller K R (ed) 1998 Biotransport: Heat and Mass Transfer in Living Systems (New York: Academy of Sciences)
[22] Hu L, Hecht D S and Grüner G 2004 *Nano Lett.* **4** 2513
[23] Hecht D S, Hu L and Grüner G 2006 *Appl. Phys. Lett.* **89** 133112
[24] Kumar S, Murthy J Y and Alam M A 2005 *Phys. Rev. Lett.* **95** 066802
[25] Chang C W, Okawa D, Majumdar A and Zettl A 2006 *Science* **314** 1121
[26] Chang C W, Okawa D, Garcia H, Majumdar A and Zettl A 2008 *Phys. Rev. Lett.* **101** 075903
[27] Pop E, Mann D, Cao J, Wang Q, Goodson K and Dai H 2005 *Phys. Rev. Lett.* **95** 155505
[28] Liljeros F, Edling C R, Amaral L A, Stanley H E and Aberg Y 2001 *Nature* **411** 907
[29] Pastor-Satorras R and Vespignani A 2001 *Phys. Rev. Lett.* **86** 3200
[30] Liu Z and Hu B 2005 *Europhys. Lett.* **72** 315
[31] Zhou J, Liu Z and Li B 2007 *Phys. Lett. A* **368** 458
[32] Colizza V, Pastor-Satorras R and Vespignani A 2007 *Nat. Phys.* **3** 276
[33] Dorogovtsev S N and Mendes J F F 2003 *Evolution of Networks: From Biological Nets to the Internet and WWW* (Oxford: Oxford University Press)
[34] Echenique P, Gomez-Gardenes J and Moreno Y 2004 *Phys. Rev. E* **70** 056105
[35] Echenique P, Gomez-Gardenes J and Moreno Y 2005 *Europhys. Lett.* **71** 325
[36] Liu Z, Ma W, Zhang H, Sun Y and Hui P M 2006 *Physica A* **370** 843
[37] Zhang H, Liu Z, Tang M and Hui P M 2007 *Phys. Lett. A* **364** 177
[38] Arenas A, Diaz-Guilera A, Kurths J, Moreno Y and Zhou C 2008 *Phys. Rep.* **469** 93
[39] Noh J D and Rieger H 2004 *Phys. Rev. Lett.* **92** 118701
[40] Gallos L K 2004 *Phys. Rev. E* **70** 046116
[41] Sood V, Redner S and Ben-Avraham D 2005 *J. Phys. A: Math. Gen.* **38** 109
[42] Wu Z, Lopez E, Buldyrev S V, Braunstein L A, Havlin S and Stanley H E 2005 *Phys. Rev. E* **71** 045101
[43] Chubynsky M V and Thorpe M F 2005 *Phys. Rev. E* **71** 056105
[44] Carmi S, Wu Z, Havlin S and Stanley H E 2008 *Europhys. Lett.* **84** 28005
[45] Lopez E, Buldyrev S V, Havlin S and Stanley H E 2005 *Phys. Rev. Lett.* **94** 248701
[46] Lee D-S and Rieger H 2006 *Europhys. Lett.* **73** 471
[47] Wu Z, Braunstein L A, Havlin S and Stanley H E 2006 *Phys. Rev. Lett.* **96** 148702
[48] Strelniker Y M, Berkovits R, Frydman A and Havlin S 2004 *Phys. Rev. E* **69** 065105
[49] Li G, Braunstein L A, Buldyrev S V, Havlin S and Stanley H E 2007 *Phys. Rev. E* **75** 045103
[50] Albert R and Barabási A-L 2002 *Rev. Mod. Phys.* **74** 47
[51] Boccaletti S, Latora V, Moreno Y, Chavez M and Hawang D-U 2006 *Phys. Rep.* **424** 175
[52] Dorogovtsev S N, Goltsev A V and Mendes J F F 2008 *Rev. Mod. Phys.* **80** 1275
[53] Maes C, Netocny K and Verschueren M 2003 *J. Stat. Phys.* **111** 1219
[54] Eckmann J-P and Zabey E 2004 *J. Stat. Phys.* **114** 515
[55] Liu Z and Li B 2007 *Phys. Rev. E* **76** 051118
[56] Nose S 1984 *J. Chem. Phys.* **81** 511
[57] Hoover W G 1985 *Phys. Rev. A* **31** 1695
[58] Fermi E, Pasta J and Ulam S 1995 *Los Alamos Report No.* LA-1940 (unpublished)
[59] Hu B, Li B and Zhao H 2000 *Phys. Rev. E* **61** 3828
[60] Li B, Wang L and Casati G 2004 *Phys. Rev. Lett.* **93** 184301
[61] Yang L 2002 *Phys. Rev. Lett.* **88** 094301
[62] Shimada T, Murakami T, Yukawa S, Saito K and Ito N 2000 *J. Phys. Soc. Japan* **69** 3150
[63] Lee L W and Dhar A 2005 *Phys. Rev. Lett.* **95** 094302
[64] Liu Z, Lai Y, Ye N and Dasgupta P 2002 *Phys. Lett. A* **303** 337
[65] Holme P and Kim B J 2002 *Phys. Rev. E* **65** 026107
[66] Wu X and Liu Z 2008 *Physica A* **387** 623
[67] Kim B J 2004 *Phys. Rev. E* **69** 045101
[68] Zhang Y, Blattner M and Yu Y 2007 *Phys. Rev. Lett.* **99** 154301
[69] Sade M, Kalisky T, Havlin S and Berkovits R 2005 *Phys. Rev. E* **72** 066123

New Journal of Physics 12 (2010) 023016 (http://www.njp.org/)
[69] Zhu C P and Xiong S-J 2000 Phys. Rev. B 62 14780
[70] Sade M and Berkovits R 2003 Phys. Rev. B 68 193102
[71] Brody T A, Flores J, French J B, Mello P A, Pandey A and Wong S S M 1981 Rev. Mod. Phys. 53 385
[72] Papenbrock T and Weidenmuller H A 2007 Rev. Mod. Phys. 79 997
[73] Yang H, Zhao F and Wang B 2006 Chaos 16 043112
[74] Zhu G, Yang H, Yin C and Li B 2008 Phys. Rev. E 77 066113
[75] Li B, Wang L and Casati G 2004 Phys. Rev. Lett. 93 184301
[76] Li B, Lan J and Wang L 2005 Phys. Rev. Lett. 95 104302
[77] Hu B, Yang L and Zhang Y 2006 Phys. Rev. Lett. 97 124302
[78] Lan J and Li B 2006 Phys. Rev. B 74 214305