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Heat conduction and long-range spatial correlation in 1D models

Xin Zhou[1,2] **and Mitsumasa Iwamoto**[1]

[1] Department of Physical Electronics, Tokyo Institute of Technology, O-okayama 2-12-1, Meguro-ku, Tokyo 152-8552, Japan
[2] Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

E-mail: zhou@mpip-mainz.mpg.de and iwamoto@pe.titech.ac.jp

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Abstract

Heat conduction in one-dimensional (1D) scattering models is studied based on numerical simulations and an analytical S-matrix method which is developed in the mesoscopic electronic transport theory. In the models, it is found that the heat conduction is closely related to a spatial correlation of particle motions: if the correlation exists, the heat conduction is abnormal; otherwise (i.e. if the correlation vanishes), the heat conduction is normal. The randomization of scatterers in the models is found to determine the existence of correlation. Our simulations are in agreement with the theoretical expectations. We generalize the result and study the property of heat conduction by directly analysing the correlation in general 1D dynamical systems.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The study of heat conduction in one-dimensional (1D) systems is an interesting subject in the context of nonequilibrium statistical physics, which has been attracting much attention in recent years [1]. Most works aim at understanding the dynamical properties of heat transport in 1D systems [2–10]. Many modelling systems have been carefully studied and their thermal conductivities and temperature profiles have been calculated; however, the key dynamical properties of normal conduction are still unknown. Generally, normal heat conduction is specified by a diffuse-type motion, hence the investigation of random behaviour of systems is necessary. It is well known that chaos can generate the required random behaviour in some systems. For example, thermal conductivity is characterized normal in the ding-a-ling model [2] and the Lorentz gas channels [6], due to their dynamical instability. However, heat conduction is still considered abnormal in other systems, such as Fermi–Pasta–Ulam (FPU) model [3] in spite of their dynamical instability. Recently, Li *et al* [9] studied three models with the same zero-Lyapunov exponents (i.e. these models are dynamically stable) and found that heat conduction can be either normal or abnormal depending on details of the models. Consequently, they draw such a surprising conclusion that there is no direct connection between the dynamical instability and normal heat conduction.

Among all researches of heat conduction in 1D systems, most works are short-time numerical simulations of small systems. It is very difficult to get definite conclusions on the macroscopic transport properties of these nonlinear systems. A general conclusion that the momentum conservation systems with non-zero pressure have anomalous conductivity had been proved by Prosen and Campbell [11]. Unfortunately, the proof is criticized to be wrong by Narayan and Ramaswamy [12]. Until now, many current numerical results are still very confusing. For example, in the diatomic gas models, the heat conduction was first thought as normal by Jackson *et al* [13] and was in agreement with a recent work of Garrido *et al* [14], but it was against the numerical results by Hatano [5], Dhar [8], Savin *et al* [15] and Grassberger *et al* [10]. It is necessary to study generally the required dynamical characteristics that guarantee normal heat conduction.

In this paper, we try to relate the normal heat conduction of 1D systems to a spatial correlation along the systems. By considering a 1D system with N scatterers and non-interacting classic particles, we find that the classic model can be theoretically treated using S-matrix theory [16] developed in the mesoscopic electronic transport theory (METT). In METT, if the scattering is random, electronic transport will be incoherent, electronic phase correlation at the two ends of a 1D chain will be absent and eventually Ohm's law will be observed. Similarly, in our model, defining a 'phase' correlation, we find that normal heat conduction is characterized by the breaking of the phase correlation which is ascribed to the randomization of the scatterers. We generalize the finding to other 1D systems: the absence of a spatial correlation along a 1D system implies a normal heat conduction. The supposition is supported by some physical considerations and some previous theoretical and numerical researches. From the view of breaking the spatial correlation, in 1D systems, it is easy to know that other kinds of randomness characteristics are of equal value with dynamical instabilities. Therefore, we conclude that dynamical instability is not necessary to get normal heat transport only while other kinds of randomness effects exist. The result is helpful in explaining the surprising finding of Li *et al* [9] about the relation between the normal heat conduction and the dynamical instabilities. Some related discussions are given in section 4. In section 3, the results of numerical simulations are presented. We begin, in section 2, with a description of our models and some theoretical treatment.

2. Theory

2.1. Model and scattering theory

Consider a 1D classical chain with N scatterers $s_k, (k = 1, \ldots, N)$ and non-interacting particles, which are elastically transmitted or reflected at these scatterers, we place this chain between two heat baths. Without loss of generality, the length of chain (L) is set as N. If the transmission coefficient (t_k) of each scatterer is a number between 0 and 1, it is a typical random walk process, hence heat conduction is normal and independent of the kind of heat baths. However, here we suppose that scatterers periodically turn on or off on time, so particles will completely transmit through a scatterer in some time segments, but reflect at the scatterer in the other time segments. So the transmission coefficients, $t_k(\phi)$, are function of time ϕ. Here, we set $t_k(\phi)$ as a period function with the period 1 and the average transmit coefficient 1/2. If there are different initial time shifts δ_k for different scatterers, we have $t_k(\phi) = t(\phi - \delta_k)$, and

$$t(\phi) = \begin{cases} 1, & 0 \leqslant \phi < 1/2 \\ 0, & 1/2 \leqslant \phi < 1. \end{cases} \tag{1}$$

The term ϕ and δ_k are thought as 'phases'. Another parameter of the kth scatterer is its positions x_k. $\{\delta_k\}$ and $\{x_k\}$ will determine the properties of the model. Actually, the model is very similar to the Lorentz channel model [6] or the Ehrenfest gas channel model [9].

We define the average of the particle current density $J(x, v, t)$ at position x and velocity v as

$$j(x, v, \phi; n) = \frac{1}{M} \sum_{m=0}^{M-1} J(x, v, \phi + m + n), \tag{2}$$

where n, m are integer numbers M is a large integer number and $0 \leqslant \phi < 1$. In steady state, $j(x, v, \phi; n)$ is independent of n, and is noted as $j(x, v, \phi)$. Due to the particle current conservation, as x is between two nearest-neighbour scatterers, x_k and x_{k+1}, $j(x, v, \phi)$ can be written as function of $\phi - x/v$, thus we have,

$$j(x, v, \phi) = \sum_m j_m^{(k)}(v) \exp\{2m\pi \mathrm{i}(x/v - \phi)\}, \qquad \text{if} \quad x_k < x < x_{k+1}. \tag{3}$$

The heat current density $J_u(x)$ and temperature profile $\mathcal{T}(x)$ can be written as

$$J_u(x) = \frac{1}{2} \int_0^\infty \mathrm{d}v\, v^2 \big[j_0^{(k)}(v) - j_0^{(k)}(-v) \big], \tag{4}$$

and

$$\mathcal{T}(x) = \frac{\int_0^\infty \mathrm{d}v\, v \big[j_0^{(k)}(v) + j_0^{(k)}(-v) \big]}{\int_0^\infty \mathrm{d}v\, v^{-1} \big[j_0^{(k)}(v) + j_0^{(k)}(-v) \big]}, \tag{5}$$

respectively, while $x_k < x < x_{k+1}$.

On the basis of the properties of scatterers, we easily obtain the following scattering formula:

$$\begin{pmatrix} \hat{j}^{(k)}(v) \\ \hat{j}^{(k-1)}(-v) \end{pmatrix} = \begin{pmatrix} \hat{t}^{(k)}(v) & \hat{r}'^{(k)}(v) \\ \hat{r}^{(k)}(v) & \hat{t}'^{(k)}(v) \end{pmatrix} \begin{pmatrix} \hat{j}^{(k-1)}(v) \\ \hat{j}^{(k)}(-v) \end{pmatrix} \tag{6}$$

where $\hat{j}^{(k)}(v)$ is a vector with infinite components ($j_m^{(k)}$, m is any integer number). $\hat{t}, \hat{r}, \hat{t}'^{(k)}$ and $\hat{r}'^{(k)}$ are nothing but S-matrix elements, and each S-matrix element is an infinite-dimensional matrix. For example, the element $t_{mn}^{(k)}$ of matrix $\hat{t}^{(k)}$ is a coefficient which the mode m at the left transmits the scatterer k to mode n at the right,

$$t_{mn}^{(k)}(v) = t^{(m-n)} \exp\{-2\pi \mathrm{i}(m - n)(x_k/v - \delta_k)\}, \tag{7}$$

where $t^{(p)} = \int_0^1 \mathrm{d}\phi\, t(\phi)\, \mathrm{e}^{2p\pi \mathrm{i}\phi}$, is the pth Fourier's expanded coefficient of transmission function $t(\phi)$. Similarly, other matrices can be written as

$$\begin{aligned} r_{mn}^{(k)}(v) &= r_k^{(m-n)} \exp[-2\pi \mathrm{i}(m + n)x_k/v], \\ t_{mn}'^{(k)}(v) &= t^{(m-n)} \exp[-2\pi \mathrm{i}(m - n)(x_k/(-v) - \delta_k)], \\ r_{mn}'^{(k)}(v) &= r_k^{(m-n)} \exp[-2\pi \mathrm{i}(m + n)x_k/(-v)], \end{aligned} \tag{8}$$

where $r_k^{(p)} = (\delta_{p,0} - t^{(p)}) \exp(2p\pi \mathrm{i}\delta_k)$.

For whole N scatterers, we have

$$\begin{pmatrix} \hat{j}^{(N)}(v) \\ \hat{j}^{(0)}(-v) \end{pmatrix} = \begin{pmatrix} \hat{T}(v) & \hat{R}'(v) \\ \hat{R}(v) & \hat{T}'(v) \end{pmatrix} \begin{pmatrix} \hat{j}^{(0)}(v) \\ \hat{j}^{(N)}(-v) \end{pmatrix} \tag{9}$$

where $\hat{T}$, $\hat{R}$, $\hat{T}'$ and $\hat{R}'$ are whole transmitting and reflecting matrix of all scatterers from left to right and from right to left, respectively. $\hat{j}^{(0)}$ and $\hat{j}^{(N)}$ correspond to the current densities at the left and right ends, respectively.

Since the parameters of the system (x_k and δ_k) determine the S-matrix, we study heat conduction of models with different parameters. Without loss of generality, we set

$$\delta_k = c * R, \tag{10}$$

$$x_k = k - 0.5 + d * (R - 0.5), \tag{11}$$

where R is a random number uniformly distributed between 0 and 1, c and d are the magnitude of disorder in scattering phases and positions, respectively. If both c and d are equal to zero, it is a periodic scattering system, otherwise, it is a disordered system. For the latter, we can consider two kinds of different disordered systems: (1) the dynamical random system (DRS), where x_k or δ_k are random in time, (2) the static random system (SRS), where random x_k or δ_k are fixed rather than depending on time in each realizations of system. We are interested in the average properties of many realizations. DRS and SRS correspond to the phonon scattering and impurity scattering in electronic transport, respectively. Obviously, the disorder of x_k or δ_k will induce some random phases in the S-matrix, it may affect the transport property of the system.

The combined S-matrices of N scatterers can be easily written according to the well-known rules generated in METT: it is written as a summation of many terms, where each term is depicted by a 'Feynman path' [16]. For example, the combining transmitting matrix of any two parts of scattering $s^{(1)}$ and $s^{(2)}$ is

$$\begin{aligned} \hat{t}(12) &= \hat{t}^{(2)}[I - \hat{r}'^{(1)}\hat{r}^{(2)}]^{-1}\hat{t}^{(1)}, \\ &= \hat{t}^{(2)}[I + \hat{r}'^{(1)}\hat{r}^{(2)} + \cdots]\hat{t}^{(1)}. \end{aligned} \tag{12}$$

Generally, we have $T_{mn}(N) = \sum_P A_P$, where each A_P is a complex number contributed from path P which starts from mode n at the left end, to mode m at the right end. If $t_k(\phi)$ of each scatterer is independent of time ϕ, then there is only one mode, $T = \sum_{P_0} A_{P_0}$, where P_0 are all the 'Feynman' paths with mode 0 for all scatterers. We easily obtain

$$T(N) = \left(\sum \frac{1 - t_i}{t_i} + 1\right)^{-1} \sim \frac{t}{N(1-t) + t}. \tag{13}$$

While $N \to \infty$, we have $T(N) \to \frac{t}{N(1-t)}$, satisfying the Fourier law, which is the expectation of the random walk process.

2.2. Heat baths

Before going on to the study of the transport properties of the model, we analyse the effects of heat baths. Here, the temperatures of the left and right heat baths are noted as T_1 and T_2, respectively. Many kinds of heat baths can be selected. For example, we can choose complete-reflecting heat baths: as a particle hits a heat bath, it will be reflected with a velocity distribution $P_T(v)$, where T is the temperature of the heat bath. $P_T(v)$ can be of the Maxwellian distribution, $P_T(v) = v/T \exp(-v^2/2T)$, or of a single velocity distribution,

$P_T(v) = \delta(v - \sqrt{T})$, or other forms. In this case, we have complete-reflecting conditions at the boundaries:

$$j_m^l(v) = J_m^l P_{T_1}(v) \tag{14}$$

$$j_m^r(-v) = J_m^r P_{T_2}(v), \tag{15}$$

where v is larger than 0, $j_m^l(v)$ or $j_m^r(-v)$ corresponds to the currents entering into the 1D system from the left or right heat bath ($x = 0/L$), which has a different phase from $j_m^0(v)\big/j_m^N(-v)$ which are used in equation (9). $J_m^l = \int_0^\infty \mathrm{d}v\, j_m^l(-v)$ and $J_m^r = \int_0^\infty \mathrm{d}v\, j_m^r(v)$. Actually, J_m^l and J_m^r are the Fourier expanded coefficients of the current densities $J^l(\phi)$ (at the left end, $x = 0$) and $J^r(\phi)$ (at the right end, $x = L$) of 1D chain, respectively. From equation (9), we easily obtain,

$$\begin{pmatrix} \hat{j}_m^r(v) \\ \hat{j}_m^l(-v) \end{pmatrix} = \begin{pmatrix} \tilde{T}_{mn}(v) & \tilde{R}'_{mn}(v) \\ R_{mn}(v) & \tilde{T}'_{mn}(v) \end{pmatrix} \begin{pmatrix} \hat{j}_n^l(v) \\ \hat{j}_n^r(-v) \end{pmatrix} \tag{16}$$

where there are some phase differences between the matrix elements and the original S-matrix elements in equation (9),

$$\begin{aligned} \tilde{T}_{mn}(v) &= \exp(2m\pi \mathrm{i} L/v) T_{mn}(v) \\ \tilde{T}'_{mn}(v) &= T'_{mn} \exp(2n\pi \mathrm{i} L/v) \\ \tilde{R}'_{mn}(v) &= \exp(2m\pi \mathrm{i} L/v) R'_{mn} \exp(2n\pi \mathrm{i} L/v). \end{aligned} \tag{17}$$

Then, we know J_m^l and J_m^r are not arbitrary, but satisfy the following equation:

$$\begin{pmatrix} \langle R_{mn}\rangle_1 - \delta_{mn} & \langle \tilde{T}'_{mn}\rangle_2 \\ \langle \tilde{T}_{mn}\rangle_1 & \langle \tilde{R}'_{mn}\rangle_2 - \delta_{mn} \end{pmatrix} \begin{pmatrix} J_n^l \\ J_n^r \end{pmatrix} = 0 \tag{18}$$

where $\langle f_{mn}\rangle_i$, ($i = 1$, or 2), means the average value of $f_{mn}(v)$ under the velocity distribution function $P_{T_i}(v)$. The physical meaning of equation (18) will be easily understood. In fact, we can treat the right boundary as $(N + 1)$th scatterer (complete reflecting), J_m^l must satisfy the linear equation, $(R^{Nr} - I)J^l = 0$, where R^{Nr} is the total reflecting matrix of all N scatterers as well as the right heat bath. From equation (18), we have

$$R^{Nr} = \langle R\rangle_1 + \langle \tilde{T}'\rangle_2 [I - \langle \tilde{R}'\rangle_2]^{-1} \langle \tilde{T}\rangle_1. \tag{19}$$

Since

$$[I - R]^{-1} = I + R + RR + \cdots, \tag{20}$$

we find that the result is nothing but the summation of 'Feynman path'. Similarly, we also have the formula of R^{lN} and equation $(R^{lN} - I)J^r = 0$. If there is only one linear-independent solution of the equation, we will get a unique steady state (a free constant J_0^l is decided by the particle density and average temperature of system).

However, the asymptotic N dependence of the heat current is only determined by the N dependence of transmission coefficient $|\hat{T}|$, which is independent of the details of heat baths. In this paper, we only consider a simpler case, replacing with the complete-reflecting heat baths: particles uniformly enter into the system from two heat baths at time (ϕ) with the single velocity distribution $\delta(v - \sqrt{T})$, therefore the heat current is simply proportional to the transmission coefficient T_{00}. When calculating $\mathcal{T}(x)$, we choose another uniform incoming current from the right heat bath at the same time, making the total particle current zero.

2.3. Phase correlation

It is well established that, if the scattering is random, the contributions from different Feynman paths are incoherent in electronic transport, therefore, we can find Ohm's law and normal electric conductivity. But if there are some long range correlations between scatterers, the electronic phase-relaxation length may be larger than the length of the system, the transport will be coherent and we can find anomalous electric conductivity. So the existence of the phase correlation between electrons at the two ends can be used to judge whether the transport is coherent or not, hence whether the conductivity is abnormal or normal. Comparing the results, we expect a similar relationship between heat conduction and a long range correlation of particles in 1D systems. We also expect the random characteristic of scatterers to be responsible for the correlations.

For any incoming particle current from the left heat bath, $J_+^l(\phi)$, we have the transmit current density at the right boundary $J_+^r(\psi) = \int T(\psi,\phi) J_+^l(\phi)\,\mathrm{d}\phi$, where $T(\psi,\phi)$ is the transmit function,

$$T(\psi,\phi) = \sum_{mn} \exp(-2m\pi\mathrm{i}\psi) T_{mn} \exp(2n\pi\mathrm{i}\phi). \qquad (21)$$

Similarly, the reflecting function is $R(\psi,\phi)$. Since for any ϕ, $\int [T(\psi,\phi) + R(\psi,\phi)]\,\mathrm{d}\psi = 1$, so $R_{0n} = \delta_{0n} - T_{0n}$.

The probability that we observe a current with phase ψ at the right end and a current with ϕ at the left end is $W_2(\psi, L; \phi, 0) = T(\psi,\phi) J_+^l(\phi)$. We define a normalized two-point current distribution function as $f_2(\psi,\phi) = W_2(\psi, N; \phi, 0)/A$, where A is a normalized constant,

$$A = \int W_2(\psi, L; \phi, 0)\,\mathrm{d}\phi\,\mathrm{d}\psi = \int J_+^r(\psi)\,\mathrm{d}\psi. \qquad (22)$$

The left and right normalized distributions are

$$f_l(\phi) = \int f_2(\psi,\phi)\,\mathrm{d}\psi, \qquad (23)$$

and

$$f_r(\psi) = \int f_2(\psi,\phi)\,\mathrm{d}\phi, \qquad (24)$$

respectively.

On the basis of these distributions, we define a motion correlation of particles at two ends of the 1D chain as

$$D = \frac{\langle \phi\psi \rangle_2 - \langle \phi \rangle_l \langle \psi \rangle_r}{\sigma_l \sigma_r}, \qquad (25)$$

where $\langle \cdots \rangle_i$ ($i = 2, l$ or r) means the average value under the distribution functions $f_2(\psi,\phi)$, $f_r(\psi)$ and $f_l(\phi)$, respectively. $\sigma_{l/r} = \sqrt{\left(\langle \phi^2 \rangle_{l/r} - \langle \phi \rangle_{l/r}^2\right)}$ is the width of the current distribution at the left/right end. Hence, $D = 0$ implies the breaking of the correlation and $T(\psi,\phi) = F(\psi)G(\phi)$ (or $T_{mn} = F_m G_n$). Here, D corresponds to the electronic phase correlation at both ends of 1D electronic transport system, and the particle velocity plays the role of wavevector of the electron.

2.4. Theoretical results

Based on the rules of the 'Feynman' paths on scattering theory, the transmission matrix T_{mn} can be written as

$$T_{mn} = \sum_{pq} t_{mp}^{(N)} t_{qn}^{(1)} B_{pq}(N), \qquad (26)$$

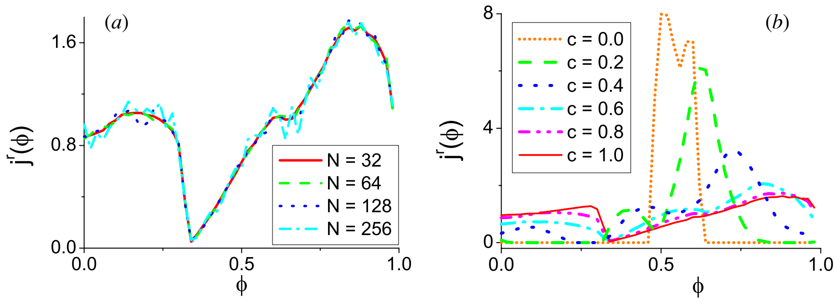

Figure 1. The particle current distribution $J^r(\phi)$ at the right end in DRS with random phases. (a) $J^r(\phi)$ of systems with different N are identical to each other, where $c = 0.8$. (b) The distribution $J^r(\phi)$ of DRS with different c. $c = 0$ means a periodic system.

where $t^{(N)}$ and $t^{(1)}$ are the transmission matrix of the scatterer N and the scatterer 1, respectively. $B_{pq}(N)$ is the sum of all 'Feynman' paths which start from mode q of the scatterer 1, end to mode p of the scatterer N. Expanding $B_{pq}(N)$ in large N, the lead term is noted as α_{pq}/N^{γ}, therefore we have the first result that the asymptotic N dependence of T_{mn} is independent of m and n,

$$T_{mn} = T(N)h_{mn}, \tag{27}$$

where $T(N) \sim 1/N^{\gamma}$, is a simple notation of T_{00} and h_{mn} is independent of N. If the correlation is absent, T_{mn} can be written as $T(N)f_m g_n$.

For DRS, due to the random time-dependent positions/phase of the scatterers, the contributions from different Feynman paths are not coherent with each other, so they can be first averaged in time, then be summed up. This indicates that only zero-mode contribute to the total transmission coefficient, so the heat conduction shall be normal. We also easily know that the correlation is absent in DRS due to the incoherent Feynman contribution.

3. Numerical simulation

In this section, by using a uniform input current with single velocity $v_1 = \sqrt{T_1}$ from the left end, we numerically simulate the transmit coefficient $T(N)$, the distribution function $f_r(\psi)$, $f_l(\phi)$ and the temperature profile $\mathcal{T}(x)$ in different systems. First, we find that both $f_r(\psi)$ and $f_l(\psi)$ are independent of N for all models including the periodic scattering system, DRS and SRS with the same disordered magnitude (c and d). The results verify very well our theoretical expectations in equation (27) and indicate that h_{mn} is only dependent on the disordered magnitude. As c (or d) increases, $f_r(\psi)$ and $f_l(\phi)$ become flatter, but they are not uniform even though the disordered magnitudes arrive at their maximum value, 1. For example, the results in DRS are shown in figure 1, where $J^r(\phi)$ is the un-normalized current distribution function at the right end. Then, we show the temperature profiles $\mathcal{T}(X/N)$ of DRS in figure 2(a), which are found to be independent of N but dependent on the disorder magnitude c (or d). It indicates that $\mathrm{d}\mathcal{T}/\mathrm{d}X$ is proportional to $1/N$. The heat current $J_u \sim 1/N^{\gamma}$ is shown in figure 2(b), and fitted $\gamma \approx 0.9989 \pm 0.0045$. Therefore, the heat conduction is normal in DRS with disordered scattering phases, which verifies our theoretical expectation. In this case, our obtained spatial correlation D is very small but with the same-order statistic error. To obtain a better correlation estimation, we used the non-uniform input currents $J_+^l(\phi)$ with different distributions and found the right-end distribution functions $f^r(\psi)$ independent of the selection of $J_+^l(\phi)$ (not shown). This indicates that the transmission function $T(\psi, \phi)$

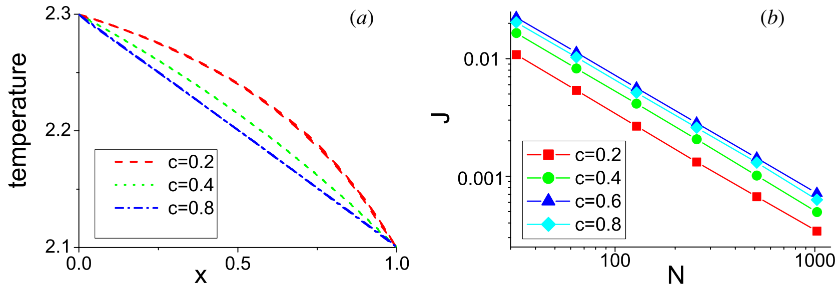

Figure 2. The results of DRSs with random phase. (*a*) Temperature profile, where $x = X/N$. For every c, we show four temperature profiles, the corresponding chain lengths are 32, 64, 128 and 256, respectively. They are almost identical to each other. (*b*) Heat current J versus N.

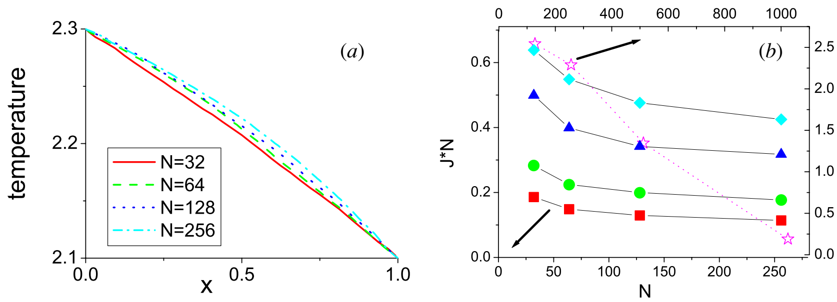

Figure 3. The results of SRSs with random phase and periodic systems. (*a*) Temperature profile of four chains, where $c = 0.8$. (*b*) NJ_u versus N of SRS and periodic system. The results of SRS with $c = 0.2$ (squares), $c = 0.4$ (circles), $c = 0.6$ (triangles) and $c = 0.8$ (diamonds) of the left and bottom axes. The results of periodic systems (stars) of the right and top axes.

can be written as $F(\psi)G(\phi)$, hence $D = 0$. For DRS with disordered scattering positions, the obtained results are similar to that of DRS with disordered phases.

We also numerically simulate the heat conduction of SRS. Since the position disordered system is similar to the phase disordered system, we only show the results of the latter. In our calculations, the temperature and heat flux are averaged over 1000 disordered realizations. There are not obvious differences using more realizations to calculate these average values. The obtained temperature profile $\mathcal{T}(x)$ and the N dependence of J_u in SRS are similar as that in DRS, but the fitted $\gamma \approx 1.19$ from four SRS systems with $N = 32, 64, 128$ and 256, respectively. It is slightly far from the normal thermal conduction. However, the deviations are due to the limiting chain length N in our simulation. In figure 3(*b*), we show the N dependence of NJ_u. It is easily seen that NJ_u will arrive at a constant as N increases. Obviously, the obtained larger fitted value of γ is ascribed to the adopted smaller N in our simulation. From figure 5(*a*), we know the deviation originates from some very minor high-J_u disordered realizations in small-N systems. In large-N systems, the realization distribution of NJ_u is a Gaussian curve with N-independent centre value. Therefore, we conclude that the heat conduction of SRS is normal. We calculated four systems with different disordered magnitudes $c = 0.2, 0.4, 0.6$ and 0.8, respectively. The heat conduction of all systems are found to be normal. Approximately, we numerically have $J_u \approx c/2N$. For very small c, it is difficult to numerically detect whether heat conduction is normal, since very large systems need to be simulated. In our simulations, it is found that the fluctuation of D similarly decreases

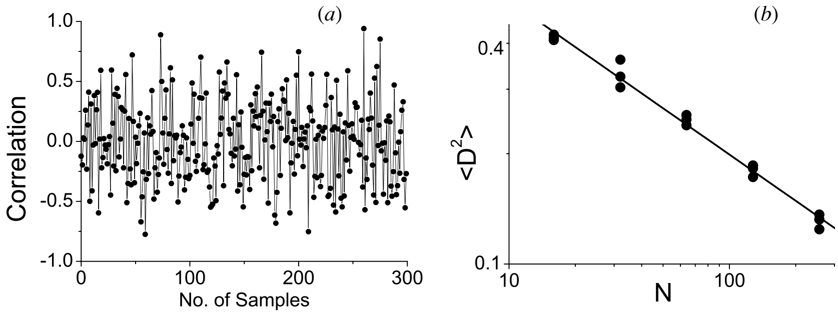

Figure 4. The correlation of SRSs with random phase. (a) The correlation distribution of different samples, where $N = 32$ and $c = 0.2$. (b) The fluctuation of correlation $\langle D^2 \rangle$ versus N. We show the results of three SRSs with different c ($c = 0.2$, 0.5 and 0.8), they are almost indistinguishable. The solid line is the best fit one.

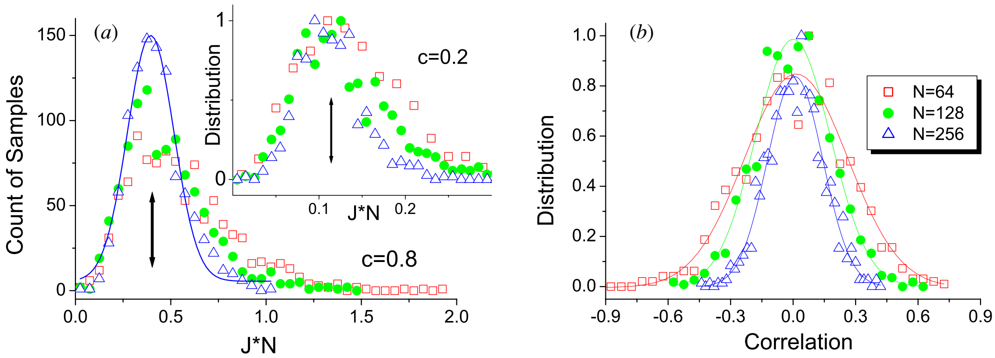

Figure 5. The distribution of heat flux J_u and correlation D of 1000 different disordered realizations. The data of three SRSs with $N = 64$ (squares), $N = 128$ (circles) and $N = 256$ (triangles) are shown, respectively. (a) The distribution of NJ_u with $c = 0.8$. The data of three systems with different N show a Gaussian profile with same centre value, but for small-N systems, there is very low tail in the high-J_u range, which cause a small deviation from normal heat conduction in small-N systems (see text). The solid line is a Gaussian curve fitted from the data of $N = 256$. In the inset of (a), similar results of SRSs with $c = 0.2$ in centre zone are shown. (b) The distribution of correlation D with $c = 0.8$. Solid lines are the fitted Gaussian curves. It is clearly found that the width of correlation distribution decreases as N increases. Here, the distributions in inset of (a) and (b) have been normalized.

as N increases for very different c. For comparison, in figure 3(b), we also show J_u of periodic scattering systems with $N = 128$, 256, 512 and 1024, respectively. The found NJ_u obviously decreases as N increases, so the heat conduction of periodic systems is abnormal. To detect the relation between heat conduction and phase spatial correlation D, we calculate the correlation of SRS. Thousand disordered realizations are used to get the distribution of the correlation. In figure 4(a), we show the correlation D of 300 disordered samples of SRS with $N = 32$ and $c = 0.2$. D is found to fluctuate largely around zero point. However, the fluctuation decreases as N increases, $\langle D^2 \rangle = N^{-0.42}$ is shown in figure 4(b). From figure 5(b), we find the D is a wonderful Gaussian curve with a decreasing width as N increases. It indicates that $D \to 0$ even in single disordered realization of SRS while $N \to \infty$. On the other hand, as our expectation, the numerical results show the correlation of periodic system is non-zero. These results strongly support the conclusion that the normal heat conduction is characterized by the breaking of the spatial correlation.

4. Summary

Defining a spatial correlation in 1D scattering systems, we have connected the property of the heat transport with a spatial correlation. In randomness scattering systems, the correlation is broken, as is our expectation, where the heat conduction is found to be normal. In contrast, in periodic scattering systems, the correlation exists even in the thermodynamic limit and the heat conduction is abnormal. Our classic scattering systems can be compared with quantum systems studied in electronic transport. The S-matrix theory developed in the latter can be used very well in the former. By drawing an analogy between the two kinds of systems, we suggest that the normal heat conduction be characterized by the breaking of the spatial correlation. On the basis of the S-matrix theory, we directly prove the relation between the correlation and heat conduction in DRS. For SRS and periodic systems, the numerical results support our conclusion. Considering to exist a distribution of the particle's spent time to transport through the chain in our studied 1D system, the spatial correlation might be related to the current–current time correlation function. Thus, our results may be related to the Kubo formula of heat conduction.

A noted fact is that our model is very similar to the Ehrenfest gas channel [9]. In the latter, the channel is quasi-1D systems with a small transverse coordinate (the height of the channel). Actually, the height corresponds to the 'phase' in our models, a similar scattering theory can be derived. In the Ehrenfest channel, the surprising declaration of Li *et al* [9], where there is no direct connection between chaos and normal thermal conduction, can be easily understood from our results. Actually, their found normal heat conduction should be ascribed to their adopted randomization of the scatterers. In their model, the randomness scattering plays the role of chaos in other models (such as the Lorentz gas channels) to guarantee the normal heat conduction. Therefore, the relation between chaos and normal thermal conduction is only while other kinds of randomness effects exist, dynamical instability is not necessary to get normal heat transport.

The obtained relation between heat conduction and the spatial correlation may be universal in general 1D systems by comparing it with quantum transport. It is possible to study properties of heat conduction by detecting the spatial correlation. The correlation might be known by analysing dynamical characteristics of systems. For example, we consider a variant of ding-a-dong model, where its even-numbered particles are oscillatedly coupled to each other, rather than coupled with its individual lattice site in the initial model [2]. Since there exist some long-wave modes in the model, the motion correlation is present even in the thermodynamic limit, then we can directly expect that its thermal conductivity is abnormal. For general 1D systems, an important question is how to define a suitable correlation and judge directly its existence from the characteristic of systems. We wish to study these problems in the future.

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References

[1] Bonetto F, Lebowitz J L and Rey-Bellet L 2000 *Preprint* math-ph/0002052
[2] Casati G *et al* 1984 *Phys. Rev. Lett.* **52** 1861
[3] Lepri S, Livi R and Politi A 1997 *Phys. Rev. Lett.* **78** 1896

[4] Hu B, Li B and Zhao H 1998 *Phys. Rev.* E **57** 2992
[5] Hatano T 1999 *Phys. Rev.* E **59** R1
[6] Alonso D, Artuso R, Casati G and Cuarneri I 1999 *Phys. Rev. Lett.* **82** 1859
[7] Gendelman O V and Savin A V 2000 *Phys. Rev. Lett.* **84** 2381
[8] Dhar A 2001 *Phys. Rev. Lett.* **86** 3554
[9] Li B, Wang L and Hu B 2002 *Phys. Rev. Lett.* **88** 223901
[10] Grassberger P, Nadler W and Yang L 2002 *Phys. Rev. Lett.* **89** 180601
[11] Prosen T and Campbell D K 2000 *Phys. Rev. Lett.* **84** 2857
[12] Narayan O and Ramaswamy S 2002 *Phys. Rev. Lett.* **89** 200601
[13] Jackson E A and Mistriotis A D 1989 *J. Phys.: Condens. Matter* **1** 1223
[14] Garrido P L, Hurtado P I and Nadrowski B 2001 *Phys. Rev. Lett.* **86** 5486
[15] Savin A V, Tsironis G P and Zolotaryuk A V 2002 *Phys. Rev. Lett.* **88** 154301
[16] Datta S 1995 *Electronic Transport in Mesoscopic Systems* (Cambridge: Cambridge University Press)