Why asymmetric interparticle interaction can result in convergent heat conductivity

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We show that the asymmetric interparticle interactions may induce rapid decay of heat current autocorrelation in one-dimensional momentum conserving lattices. When the asymmetry degree and the temperature are appropriate, the decay is sufficient rapid for resulting a convergence conductivity practically. To understand the underlying mechanism, we further studied the relaxation behavior of the hydrodynamic modes. It is shown that for lattice with symmetric potential, the heat mode relaxes in the superdiffusive manner, while in the case of asymmetric potential, the heat mode may relax in the normal manner.

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In recent decades, the heat transport properties of low-dimensional lattice models have been a particularly interesting issue. Based on intensive theoretical analysis and numerical studies (see for example [8–12] and references therein), for 1D momentum conserving fluids and lattices, at present it is generally accepted that the heat current autocorrelation should decay in power-law manner. An important consequence of the power-law decay is the divergence of the heat conductivity following the Green-Kubo formula. Recently, we found that lattice models with asymmetric inter-particle interactions may induce the rapid decay of the current-current correlation function and results in size-independent conductivity. In fact, lattice models with asymmetric interactions have been studied in the literature both analytically and numerically. In particular, the hydrodynamics analysis based on the Burgers equation suggests a divergent conductivity even for systems with asymmetric interactions, which agrees with the result based on the Zwanzig-Mori equation and the self-consistent mode coupling theory. Recently, several works appear in arXiv as in the case of the FPU-β model.

This paper present further explanation to our point of view. We explain why we can conclude that the rapid decay of the current-current correlation may result a convergent conductivity practically. To understand the mechanism and avoid the non-physical extrapolation we emphasize that one should distinguish the heat and energy. The heat mode and sound mode may behave differently between lattice models with symmetric and that with asymmetric potentials.

However, to have a solid basis to discuss or dispute, we would like to re-declare several key points of our views before present the new result.

We declared that the asymmetry interactions may result size-independent heat conductivity for one-D lattices. Not must be always. The lattice models we have studied include the FPU-αβ model, the L-J lattice models, and several other asymmetry interaction models. For these models, we have shown that with proper degree of asymmetric potential, the current-current correlation function decays in a manner faster than the power law, and the heat conductivity becomes size-independent when the system size is big enough. We emphasized the temperature should not too high and the potential parameters should be proper in the FPU-αβ model to guarantee the proper degree of the asymmetry. We agree that in the higher temperature case the heat conductivity may still divergent as in the case of the FPU-β model.

We declared that the conclusion is for lattice model, not for liquid model. We agree that for the gas model with asymmetry interaction, the conductivity diverges with the system size.

We pointed out that the so-called low-temperature region is corresponding to the room temperature. So our finding has practically importance.

We first explain why practically the rapid decay of the current correlation function can induce a size-independent conductivity. Here we take only the Fermi-Pasta-Ulam-α-β (FPU-α-β) model to be an example, though we have also studied a lot of asymmetry-potential lattice models such as the Lennard-Jones (L-J) model. The model is defined by the Hamiltonian

\[ H = \sum_i \frac{p_i^2}{2} + V(x_i - x_{i-1} - 1), \]

where \( p_i \) and \( x_i \) are the momentum and position of the \( i \)th particle, respectively, and \( V \) is the potential between two neighboring particles. The component particles are assumed to be identical and have unit mass, and the lattice constant is set to be unity so that the system length \( L \) equals the particle number \( N \). The inter-particle interactions in the FPU-α-β model are given by

\[ V(x) = \frac{1}{2} x^2 - \frac{\alpha}{3} x^3 + \frac{1}{4} x^4, \]

where the parameter \( \alpha \) controls the degree of asymmetry as illustrated in Fig. 1(a). For \( \alpha = 0 \) the system
reduces to the Fermi-Pasta-Ulam-β (FPU-β) model with symmetric potential only. To well reveal the effects of the asymmetry in this model, in our simulations the average energy per particle, denoted by \( \varepsilon \), is fixed to be \( \varepsilon = 0.1 \) such that the averaged potential energy per particle is about 0.05.

The energy current \( J_q \) is defined as \( J_q \equiv \sum_i \dot{q}_i \frac{\partial V}{\partial x_i} \). For a lattice the energy current is equal to the heat current because there is no residual global velocity \( \left[ \right] \). To numerically measure the current in equilibrium state, the system is first evolved from an appropriately assigned random initial condition for a long enough time (\( > 10^6 \)) to ensure that it has relaxed to equilibrium state; then the current at ensuing times is measured. The periodic boundary condition is applied in the calculations, and the total momentum is set to be zero.

In Fig. 1 we show the autocorrelation function of the energy current \( C(t) \equiv \frac{\langle J(t)\rangle - \langle J(t) \rangle_0}{\langle J(0)J(0) \rangle_0} \) for high and low temperatures respectively. The results are presented in log-log scale. In generating Fig. 1, the system size is fixed to be \( N = 2048 \). It can be seen that in the high-temperature cases the correlation function decays in power-law \( C_{qq}(t) \sim t^{-\gamma} \), which agrees qualitatively with previous studies and theoretical predictions \( 2, 6, 23, 24 \). Therefore in high-temperature case the long-time-tail prediction applies. However, at low-temperature case, we can see that the decay becomes faster than the power-law manner (see also Fig. 2), which can be roughly regarded to be exponential.

Some researchers argue that it could not conclude that the correlation function may still become as power-law decay when the evolution time is long enough. Yes, with numerical simulations we can not exclude such a possibility. But, what can be concluded is that such a long-period of rapid decay as shown in the figure can already insure a size-independ conductivity practically. To explain this, it is better to divide the Green-Kubo formula into two parts,

\[
\kappa = \lim_{\tau \to \infty} \lim_{L \to \infty} \frac{1}{2kBT} \int_0^\tau C(t) dt - \frac{1}{2kBT} \left[ \int_0^{\tau_e} C(t) dt + \int_{\tau_e}^{\tau_{tail}} C(t) dt \right]
\]

where \( \tau_e \) represents the exponential-decay time period and \( (\tau_e, \tau_{tail}) \) represents the tail. In the case of \( T = 0.1 \), it has \( \tau_e = 2000 \). Therefore, it has \( \int_0^{\tau_e} C(t) dt \sim 123 \) by direct integral. The second part, even assume it decays as the power-law of \( t^{-0.67} \), it contribute a sum of \( \int_{\tau_e}^{\tau_{tail}} C(t) dt \sim 10^{-2} = 0.01 \). In this case, with even \( \tau_{tail} \sim 10^{12} \) it has \( \int_{\tau_e}^{\tau_{tail}} C(t) dt \sim 1 \). To correlate the result of the Green-Kubo formula to that of the direct nonequilibrium simulation, it is usually suggested \( 23 \) that the integral time should be truncated at \( \tau_{tail} = L/v \), where \( v \) is the sound speed of the system. Therefore, even the

![Figure 1](image1.png)  
**Figure 1:** (Color online) Temperature dependence of the decay behavior of current correlation function for the FPU-α-β lattice model with \( \alpha = 2, \beta = 1 \).
tail is power-law, the conductivity may turn to power-law divergence till at least $L > 10^{12}$, which is about 100 meter length and thus physically meaningless.

The fundamental mechanism should be understood by studying the relax behavior of hydrodynamic modes [26–28]. According to the hydrodynamical theory, fluctuations of a physical quantity will relax as a superposition of the hydrodynamical modes of heat and sound. To calculate the modes, one can apply the method described in [27, 28]. In such a way, we obtain the scaling exponent $\gamma$ of the Prähofer-spohn scaling function for several one-dimension systems.

In Fig. 3 (a)-(b), we show the relax behavior of the heat mode in the case of the FPU-\(\alpha-\beta\) model as an example. These plots indicate that the heat mode relax in the normal manner with $\gamma = 0.5$.

This is the fundamental reason why the heat current in the FPU-\(\alpha-\beta\) model may still obey the Fouré law at low-temperature region. Our studies remind us to distinguish the heat part and the sound part to be transported. In the lattice models with proper degree and asymmetry, the heat part relax in the normal manner, while the sound may still be transported to infinite. The energy current carried by the sound mode thus may decay in the power-law manner. In this case, the heat in a heat bath is transported following the Fouré heat conduction law. In real material, one would find a normal heat conduct behavior. Meanwhile, there are a small part of sound energy in the heat bath, no matter how small it is, it will contribute a power-law decay energy current. When applying the Green-Kubo formula, it will result the divergence of the integral. This is a non-physical effect and should be avoided, instead to declare a abnormal heat conduct behavior for this kind of systems.

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