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Heat Transport in Low-dimensional Systems with Asymmetric Inter-particle Interaction (Transport and Relaxation in one-dimensional Models)

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Transport and relaxation in one-dimensional models

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Abstract

Studying the transport and relaxation properties of low-dimensional systems is a long-term project of our group (Complex Systems Group, Xiamen University, China). Recently, we have found that: (a) The asymmetric inter-particle interactions may break the power-law decay of current-current correlation functions in one-dimensional, momentum conserving lattices and result in a finite thermal conductivity in the thermodynamical limit; (b) In the thermodynamic limit, a universal divergent behavior(s) of the thermal conductivity may be absent for systems with only symmetric inter-particle interactions; (c) In a given system, diffusion of a physical quantity can be very different from those of others; In particular, diffusion of heat can be completely distinct from that of energy, and thus a universal connection between heat conduction and energy diffusion can not exist; (d) To numerically calculate the current-current correlation functions, the time scale over which the results are free from the finite-size effect can be much shorter than that assumed in the literature. In my talk these results will be briefed with examples.

[1] S. Chen, Y. Zhang, J. Wang and H. Zhao, arXiv:1106.2896.

[2] S. Chen, Y. Zhang, J. Wang and H. Zhao, arXiv:1204.5933.

[3] S. Chen, Y. Zhang, J. Wang and H. Zhao, arXiv:1208.0888.

[4] D. Xiong, J. Wang, Y. Zhang, and H. Zhao, Phys. Rev. E 85, 020102(R) (2012).

[5] Y. Zhong, Y. Zhang, J. Wang, and H. Zhao, Phys. Rev. E 85, 060102(R) (2012).

[6] H. Zhao, Phys. Rev. Lett. 96, 140602 (2006).

[7] H. Zhao, Z. Wen, Y. Zhang, and D. Zheng, Phys. Rev. Lett. 94, 025507 (2005).

Part I: Breakdown of the power-law decay of current-current correlation in one-dimensional, momentum conserving lattices

We find that the asymmetric inter-particle interactions can induce rapid decay of the autocorrelation function of the energy current in one-dimensional (1D), momentum conserving lattices. In particular, with certain degree of asymmetry, it may decay exponentially. This fact suggests that the hydrodynamic prediction of the power-law decay may be invalid and the Fourier law may hold in lattices with asymmetric inter-particle interactions. The mechanism is probably due to that the energy current has to drive to form a mass current additionally. [1,2]

Models：Lattices with asymmetry inter-particle interactions

$$H=\sum_i\left[\frac{p_i^2}{2m}+V(q_i-q_{i-1}-a)\right] \quad \text{with}$$

(a) $V(x)=(x+r)^2+e^{-rx}$

(b) $V(x)=\frac{1}{2}x^2-\frac{\alpha}{3}x^3+\frac{1}{4}x^4 \quad FPU-\alpha\beta$ model

(c) $V(x)=[(\frac{x_c}{x+x_c})^m-2(\frac{x_c}{x+x_c})^n+1] \quad L-J$ model

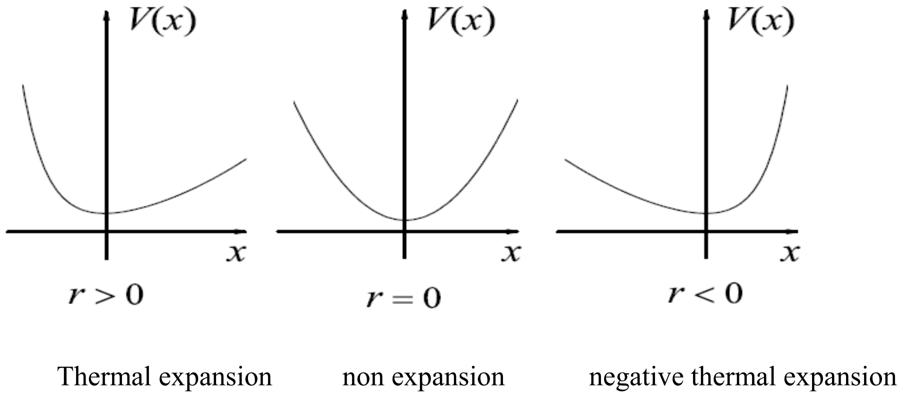


Fig.1 Illustration of the asymmetry potential

Results: The current-current autocorrelation decay faster than the power-law manner

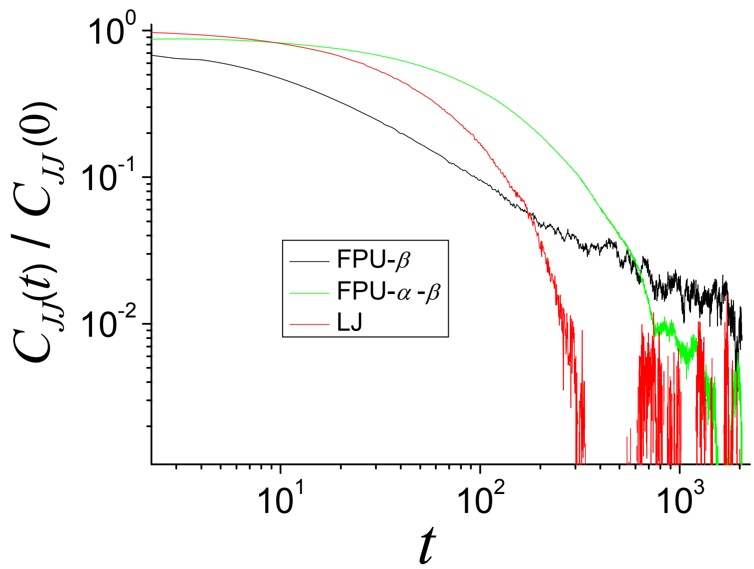


Fig.2 The decay of the autocorrelation functions with log-log scale. The L-J model is for (m, n)=(12,6);The FPU-αβ model is with α=2.

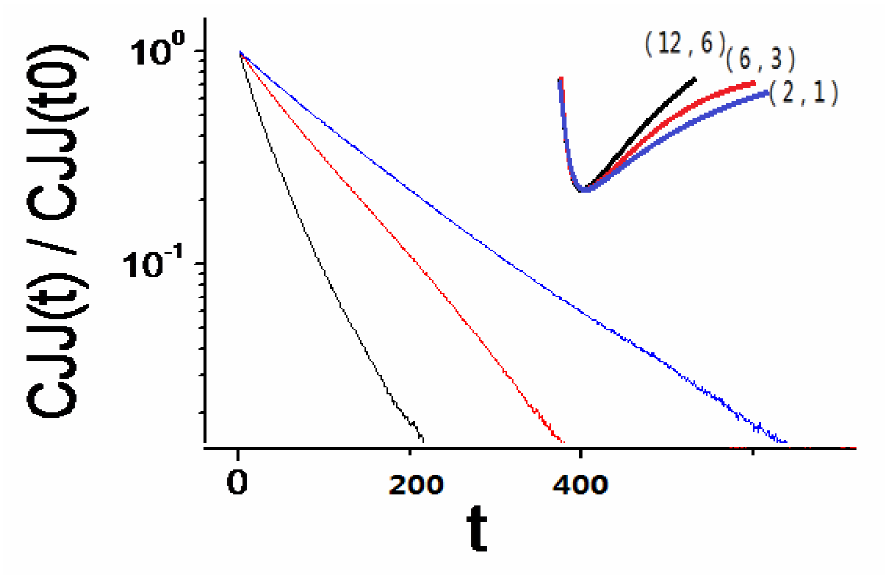


Fig.3 The decay of the autocorrelation functions approaches the perfect exponential decay with the increase of the degree of the asymmetry in the case of L-J model.

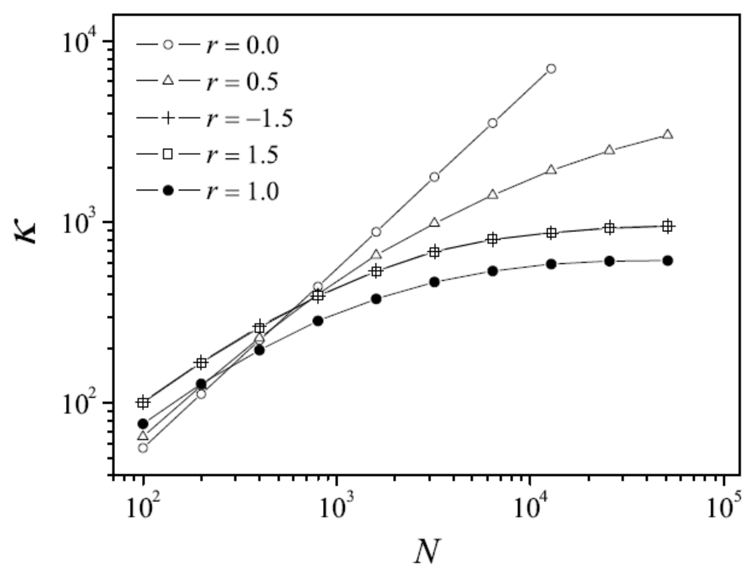


Fig.4 Convergence of the thermal conductivity when the asymmetry is introduced [5].

Part II: Non-universal heat conduction of 1D momentum conserving lattices

For 1D nonlinear lattices with momentum conserving interparticle interactions, intensive studies have suggested that the heat conductivity κ diverges with the system size L as $\kappa \sim \mathrm{L}^{\alpha}$ and the value of α is universal. But in the Fermi-Pasta-Ulam-β lattices with nearest-neighbor (NN) and next-nearest-neighbor (NNN) coupling, we find that α strongly depends on γ, the ratio of the NNN coupling to the NN coupling. Our analysis shows clear evidence of the correlation between the γ-dependent heat conduction behavior and the in-band discrete breathers. [4,6,7]

Model:

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + V(x_i - x_{i-1}) + \gamma V(x_i - x_{i-2})$$

$$with \quad V(x) = \frac{1}{2}x^2 + \frac{1}{4}x^4$$

Results: The index α is a function of γ

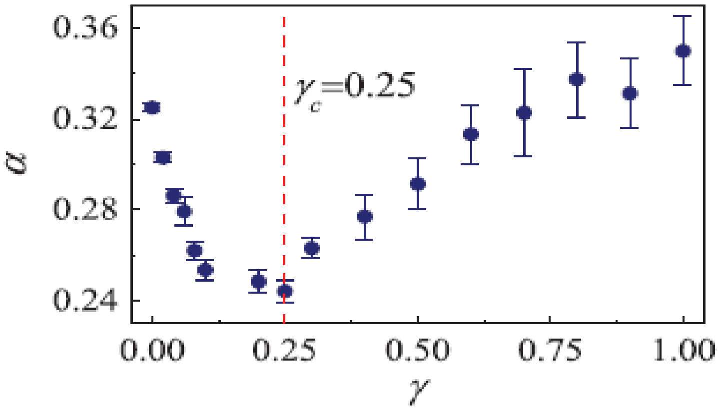
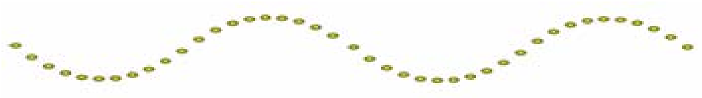


Fig. 5 The dependence of α on the parameter γ [4].

Mechanism: Phonon physics, Soliton physics, breather physics may result different α

Phonon physics



Soliton physics [6,7]

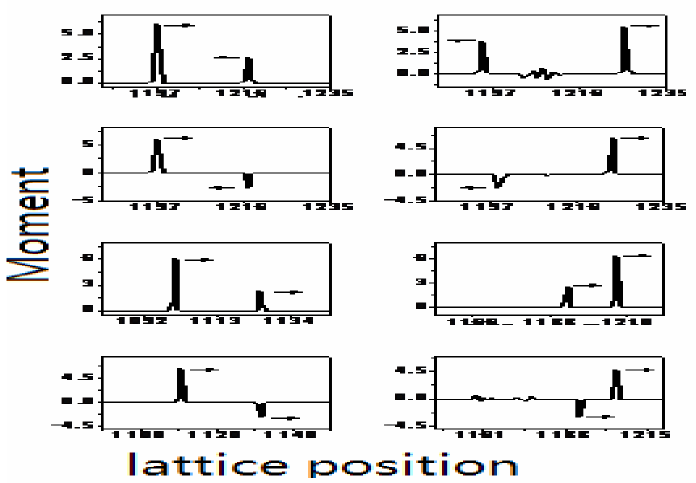


Fig. 6 Four types of soliton collisions in the FPU-β model. The formation of the solitons are same. Z. Wen and H. Zhao, Chin. Phys. Lett. 22, 1341 (2005).

Breather physics

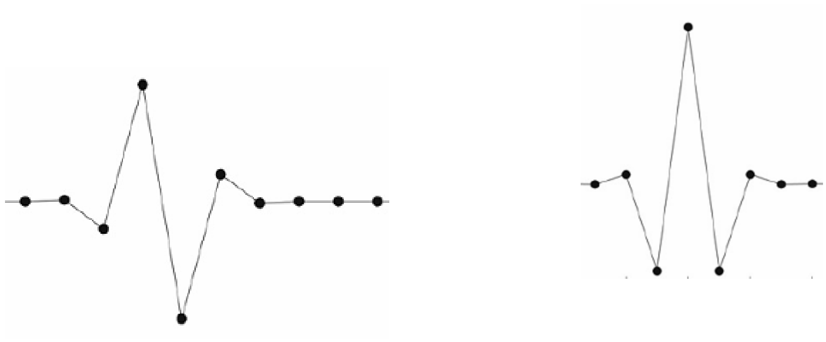
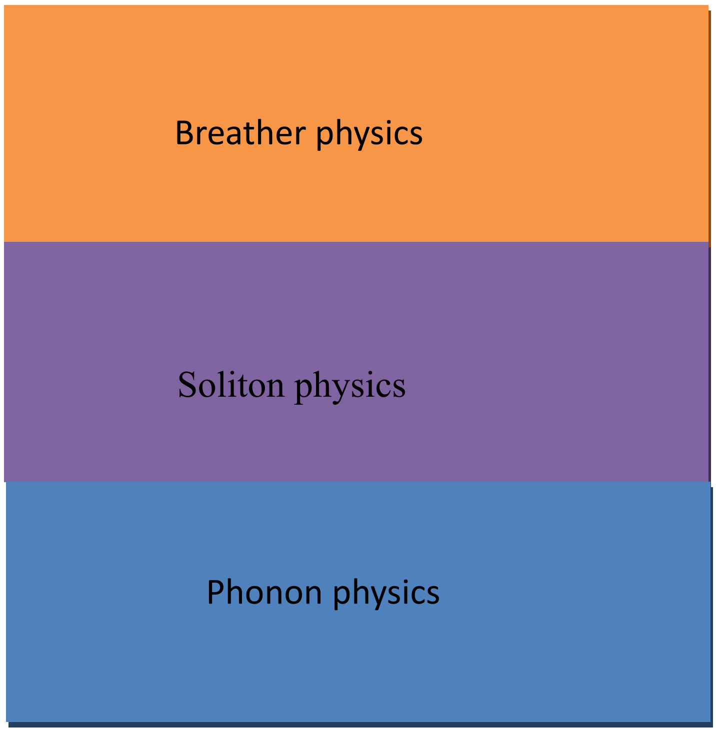


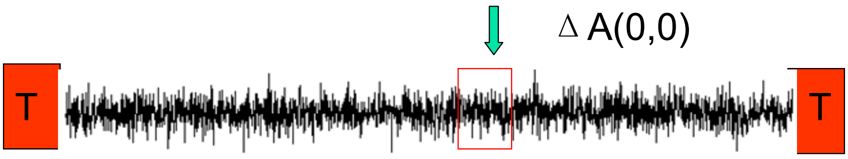
Fig.7 Tow types of breathers in the next-nearest-neighbor FPU-β model. Their density change with the parameter γ



Part III: Diffusion of heat, energy, momentum and mass in one-dimensional systems

Relaxation is crucial for understanding various nonequilibrium processes. Here we demonstrate by simulations the relaxation processes of fluctuations of heat, energy, momentum and mass in several paradigmatic one-dimensional systems. It is shown that the fluctuations of different quantity may have dramatically distinct relaxation features in a system and vary from system to system. In particular, we find that in a gas model, while heat fluctuations undergo a superdiffusive relaxation, energy fluctuations may propagate ballistically instead. But in clear contract, in a lattice model, energy fluctuations may develop into two parts; one part propagates ballistically and another relaxes superdiffusively. These results suggest that generally the fluctuation-evolving behavior of a given physical quantity can not be extracted from that of other quantities. In addition, previous studies trying to establish a universal connection between relaxation of energy fluctuations and heat conduction should be revisited. [3,6,7]

Method: Equilibrium extraction of spatial-temporal correlation functions



$$\textit{Canonical system}: \rho_a(r,t) = \frac{<\Delta A(0,0)\Delta A(r,t)>}{\int <\Delta A(0,0)\Delta A(r,0)> dr}$$

$$\textit{Microcanonical system}: \rho_a(r,t) = \frac{<\Delta A(0,0)\Delta A(r,t)>}{\int <\Delta A(0,0)\Delta A(r,0)> dr} + \frac{1}{N-1}$$

Models:

1 1D gas with alternating masses

2 FPU lattice

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \frac{1}{2}(x_i - x_{i-1} - a)^2 + \frac{1}{4}(x_i - x_{i-1} - a)^4$$

3 Lattice φ^4 model

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \frac{1}{2}(x_i - x_{i-1} - a)^2 + \frac{1}{4}(x_i - i)^4$$

Results: different quantity may obey different law of diffusion.

(t=300)

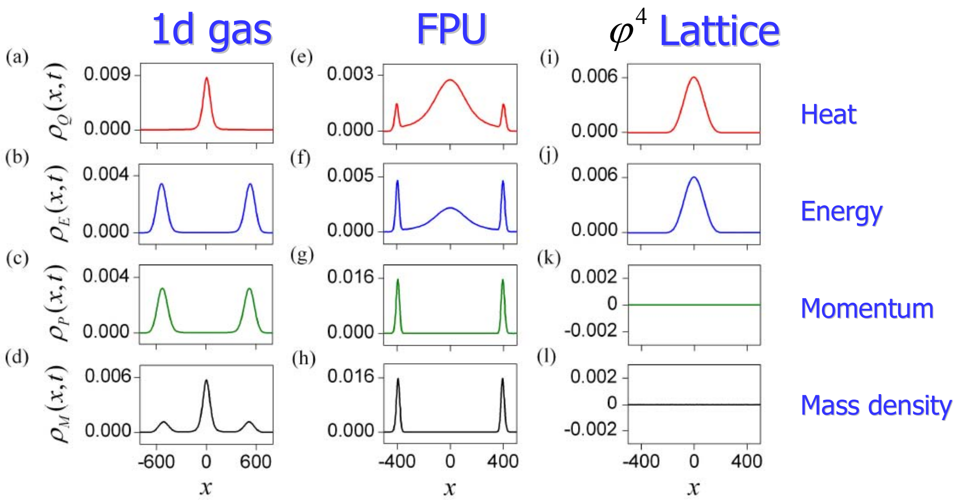


Fig.8 Diffusion of fluctuations of heat, energy, momentum and mass density

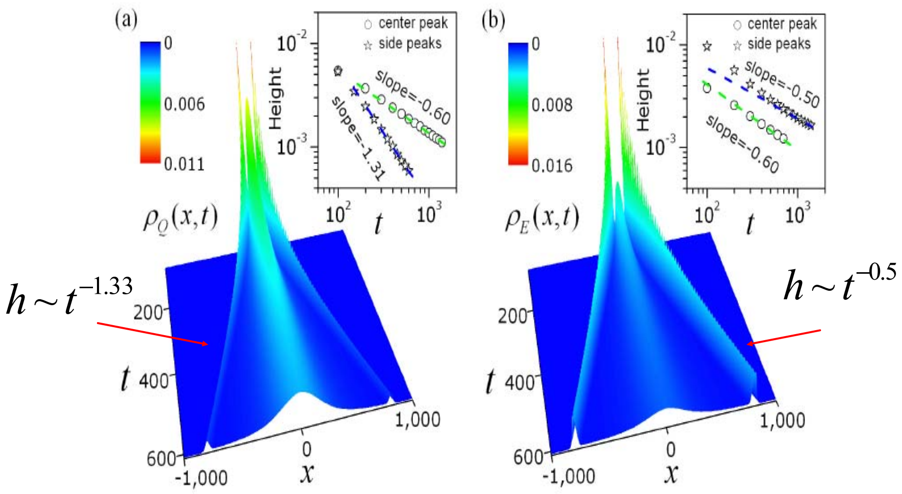


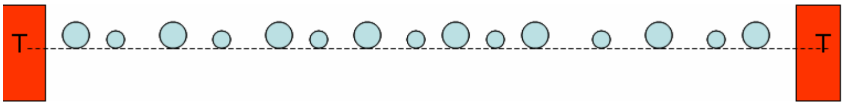
Fig.9 Temporal heat and energy diffusion processes in the FPU lattice.

Part IV: Finite-size effect in calculating the auto-correlation function of current

We study the finite-size effect in calculating the autocorrelation function of the global current using periodic boundary conditions. It is shown that the elastic and inelastic scattering may take place when the sound modes of the local current meet after they travel across the system. The elastic scattering induces periodic oscillations or periodic pulses depending on the fact that the system is a gas model or a lattice model, and the inelastic scattering may result in additional decay of the current for both kinds of systems. We illustrate that before the collision of the sound modes, the autocorrelation function obtained with a finite system size is identical to that of the infinite system, but after the collision remarkable deviation may arise. We further suggest a criterion to determine the time of collision, and find that it is much shorter than the time range adopted in previous studies for best fitting the decay of the autocorrelation functions. [1]

Models:

1. 1D gas with alternating masses



2 FPU lattice

$$H=\sum_{i=1}^{N}\frac{p_i^2}{2m_i}+\frac{1}{2}(x_i-x_{i-1}-a)^2+\frac{1}{4}(x_i-x_{i-1}-a)^4$$

Results: Both show periodic features in autocorrelation functions

Gas model: the function shows periodic oscillations

Lattice model: the function shows periodic pulses

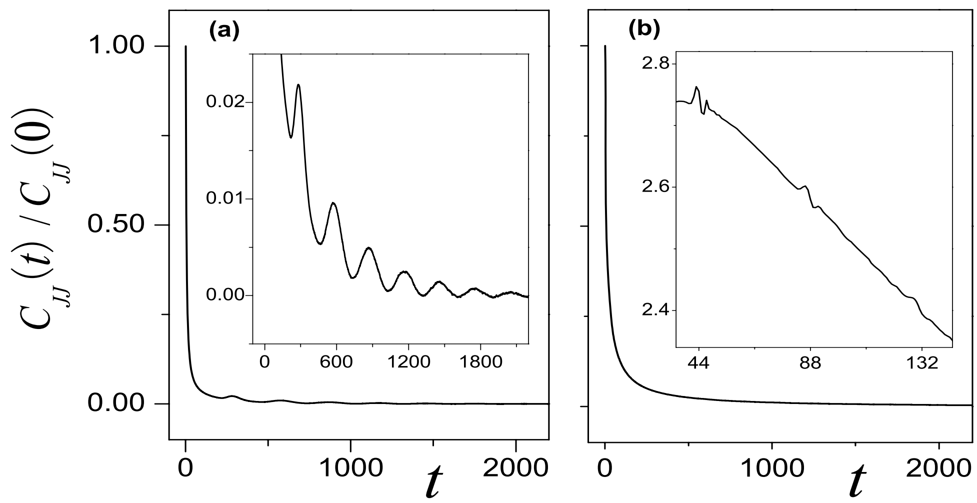


Fig.10 Autocorrelation functions of total current for gas (a) and lattice (b).

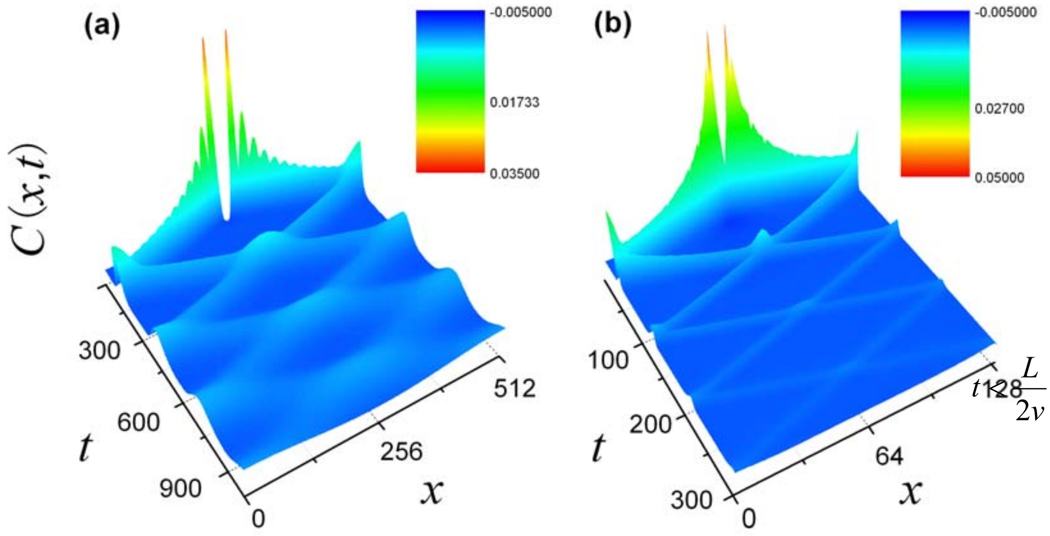


Fig. 11 Evolution process of the correlation functions of local currents for the gas (a) and the lattice (b). The gas and lattice models have different mechanism for their size effects.

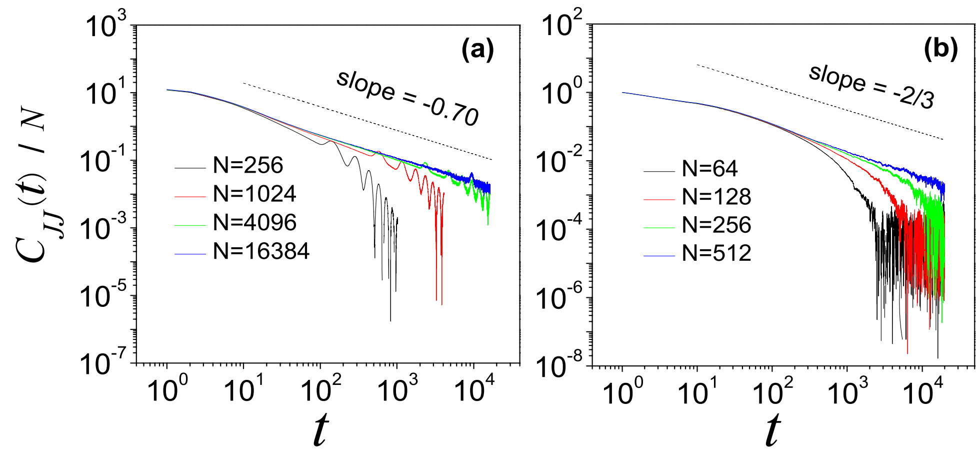


Fig. 12 Finite-Size effect of the autocorrelation functions for the gas (a) and the lattice (b).

As a Consequence, the confidence interval for extracting the correlation function is

$$t < \frac{L - l(\tau)}{2v}$$

Where L is the system size, l is the width of peaks of C(x,t) before the collision, v is the speed of the transport mode.