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Advanced Workshop on Energy Transport in Low-Dimensional Systems: Achievements and Mysteries

15 - 24 October 2012

Heat Transport in Low-dimensional Systems with Asymmetric Inter-particle Interaction (Asymmetric Heat Conduction and Negative Differential Thermal Resistance in Nonlinear Systems)

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Transport and relaxation in one-dimensional models

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Recent works of our group

1. Breakdown of the power-law decay of current-current correlation in 1D lattices (Phys. Rev. E **85**, 060102(R) (2012); S. Chen et.al., arXiv:12**04**.5933)
2. Diffusion of heat, energy, momentum and mass in 1D systems (S. Chen et.al., arXiv:1106.2896)
3. Non-universal heat conduction of 1D momentum conserving lattices (D. Xiong et.al., PRE **85**, 020102(R) (2012))
4. How to correct finite-size effects in calculating the current-current correlation (S. Chen, et. al., arXiv:1208.0888)

Outline

Background & Problem

Models

Results

Possible mechanism

Background

Fluctuation-Dissipation-Theory

$$J_a = \sum_b L_{ab} F_b$$

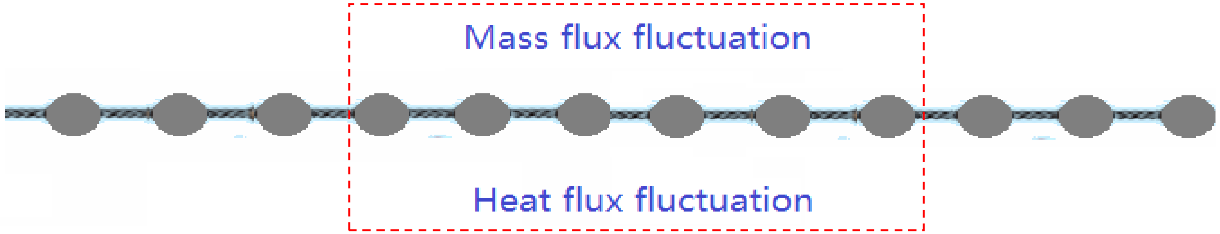
Onsager coefficients can be calculated by the Green-Kubo formula:

$$L_{ab} = \lim_{\tau \to \infty} \lim_{L \to \infty} \frac{1}{2} \int_0^{\tau} C_{ab}(t) dt$$

Where,

$$C_{ab}(t) =< J_a(t) J_b(0) >$$

Background



$$J_q = \sum \dot{x}_i \frac{\partial V(x_i)}{\partial x_i}$$

$$J_m = Mv$$

$$J_q = L_{qq} F_q + L_{qm} F_m$$

$$J_m = L_{mq} F_q + L_{mm} F_m$$

Problem I:

Onsager reciprocal relation:

$$L_{ab} = L_{ba}$$

But in what conditions we have

$$L_{ab} = L_{ba} \neq 0\,?$$

Background

$$L_{ab} = \lim_{\tau\to\infty} \lim_{L\to\infty} \frac{1}{2}\int_0^{\tau} C_{ab}(t)dt$$

- The conventional hydrodynamic approach assumes that the current correlation decay rapidly (i.e., exponentially) as

$$C_{ab}(t) \sim e^{-\gamma t}$$

which guarantees the convergence of the G-K formula

$$L_{ab} \sim const.$$

- However, after Alder (1970) numerically evidenced the ‘long time tail’

$$C_{ab}(t) \sim t^{-\gamma},$$

the G-K formula encounter the problem of divergence:

$$L_{ab} \sim L^{\alpha}$$

Background

In recent decades, the hydrodynamic analysis has been extended to lattice systems. At present, for momentum-conserving 1D fluids and lattices, it is actually believed that the current correlation should decay in the power-law manner, and resulting in a divergent thermal conductivity as

$$\kappa \sim L^{\alpha},$$

though some counterexamples with size-independent thermal conductivities have been found

Counterexamples: the rotator model [PRL. 84, 2144 (2000); PRL, 84, 2381 (2000)],
a 1D lattice in effective magnetic fields [J. Stat. Mech. P05009 (2005)],
the variant ding-a-ling model [PRE 82, 061118 (2010)],
lattice models with asymmetric inter-particle interactions [PRE 85, 060102(R) (2012)]

Problem II:

Does really the power-law decay so common in momentum-conserving 1D systems?

$$C_{ab}(t) \sim e^{-\gamma t} \quad or \quad C_{ab}(t) \sim t^{-\gamma}$$

Which one should be more general in real materials?

Models:

Lattices with asymmetric inter-particle interactions

$$H = \sum_i \frac{p_i^2}{2m} + V(q_i - q_{i-1} - a)$$

with

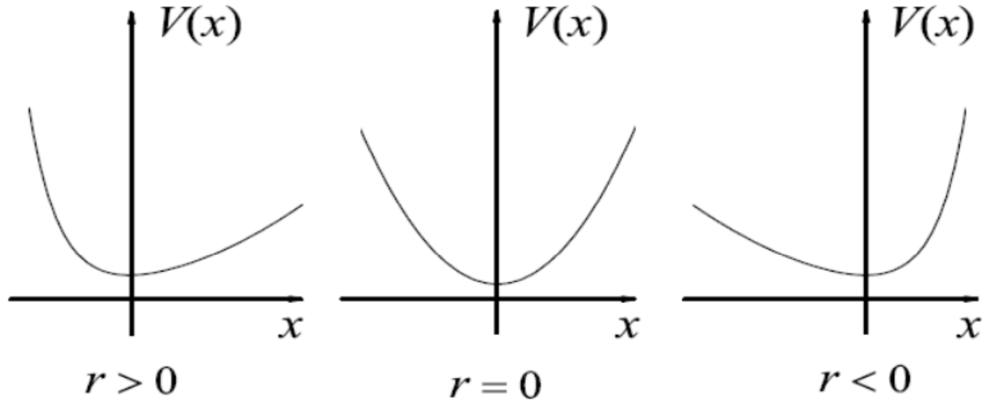
(a) $V(x) = \frac{1}{2}(x+r)^2 + e^{-rx}$

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

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

Models

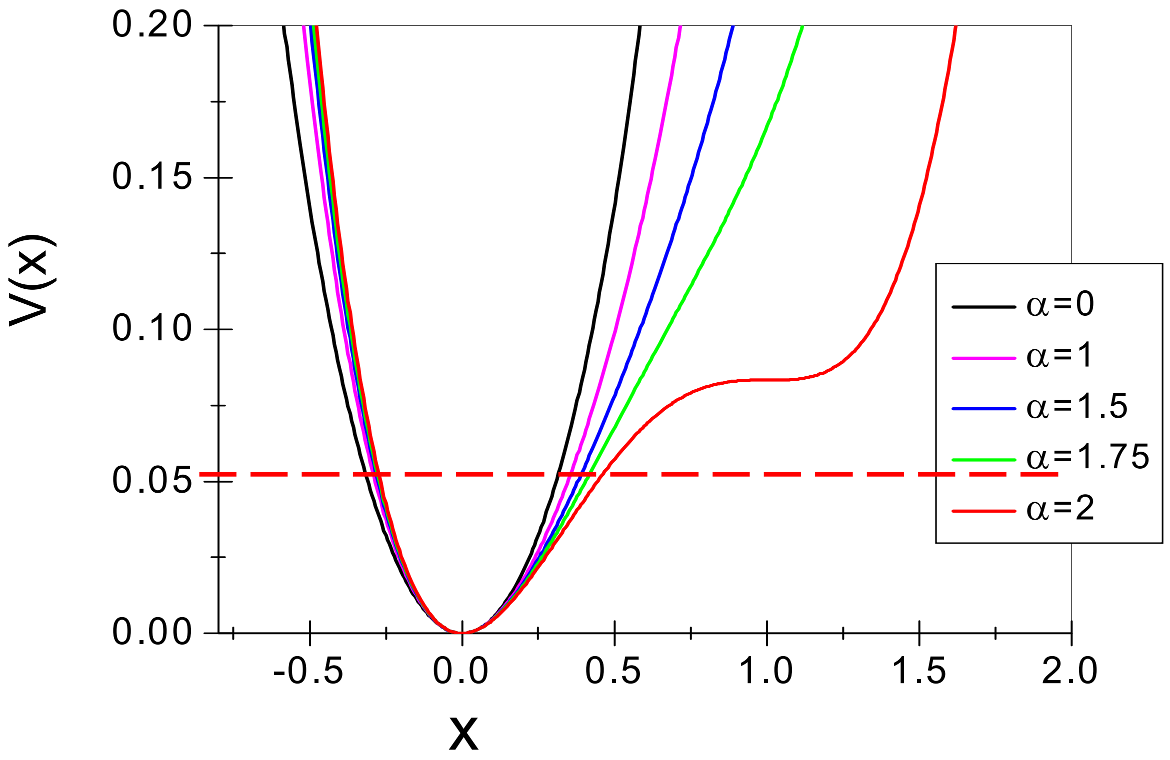
$$\text{(a)} \qquad V(x) = \frac{1}{2}(x+r)^2 + e^{-rx}$$



Thermal expansion   null thermal expansion   negative thermal expansion

Models

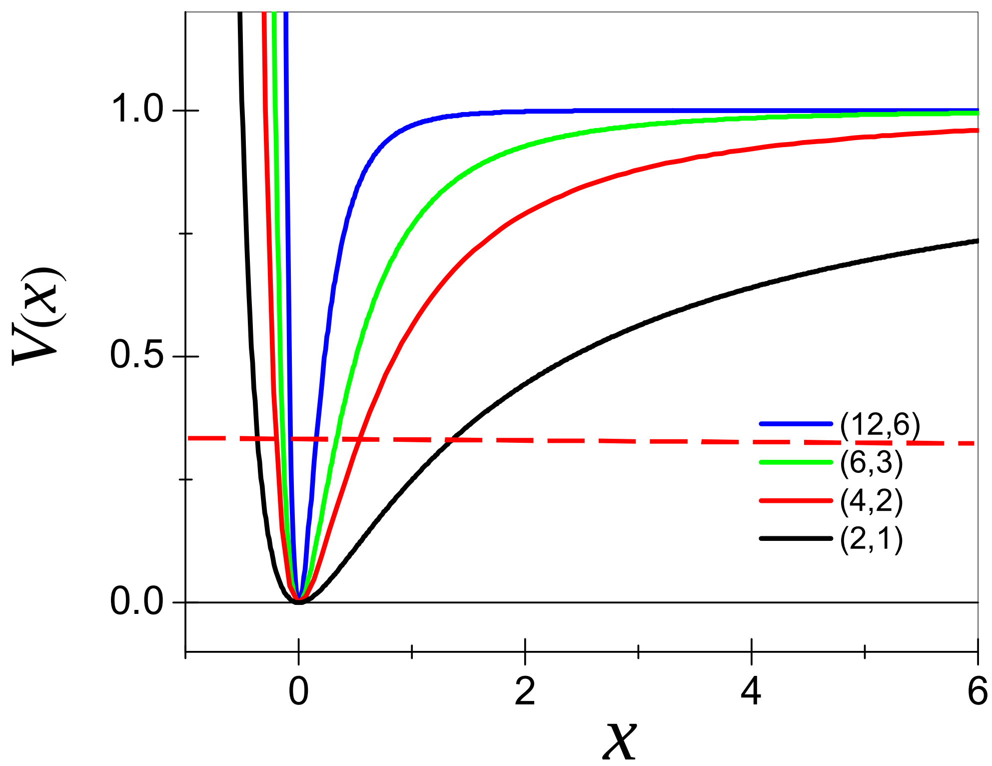
$$(b)\qquad V(x) = \frac{1}{2}x^2 - \frac{\alpha}{3}x^3 + \frac{1}{4}x^4 \quad \text{FPU} - \alpha\beta \text{ model}$$



Temperature~0.1

Models

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



Temperature~0.5

Methods: $c_{JJ}(t);\ \kappa;\ S(\omega)$

exponential decay:

$$C_{JJ}(t) \sim e^{-\gamma t} \Leftrightarrow \kappa = \text{cost.} \Leftrightarrow S(\omega) \sim \text{cos}\,t.(\omega \to 0)$$

power-law decay:

$$C_{JJ}(t) \sim t^{-\gamma} \Leftrightarrow \kappa = N^{\alpha} \Leftrightarrow S(\omega) \sim \omega^{-\delta}$$

Prof. Livi$:\alpha = \delta$

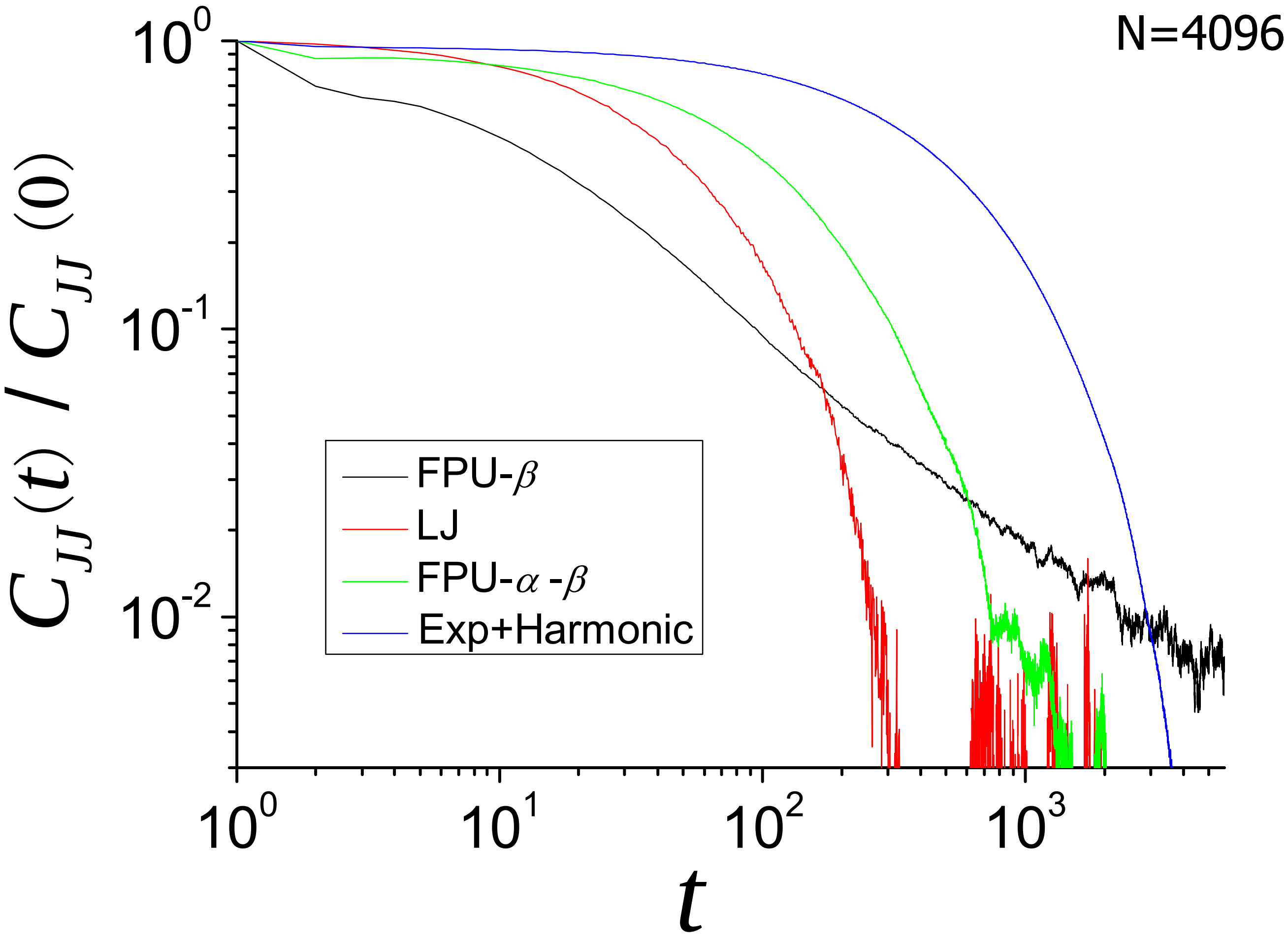
Note: the heat flux is equal to the energy flux in lattices

[S. Lepri, R. Livi, A. Politi, Physics Reports 377, 1 (2003)]

$$J_q = J_e = < \sum_i x_i \frac{\partial H}{\partial x_i} >$$

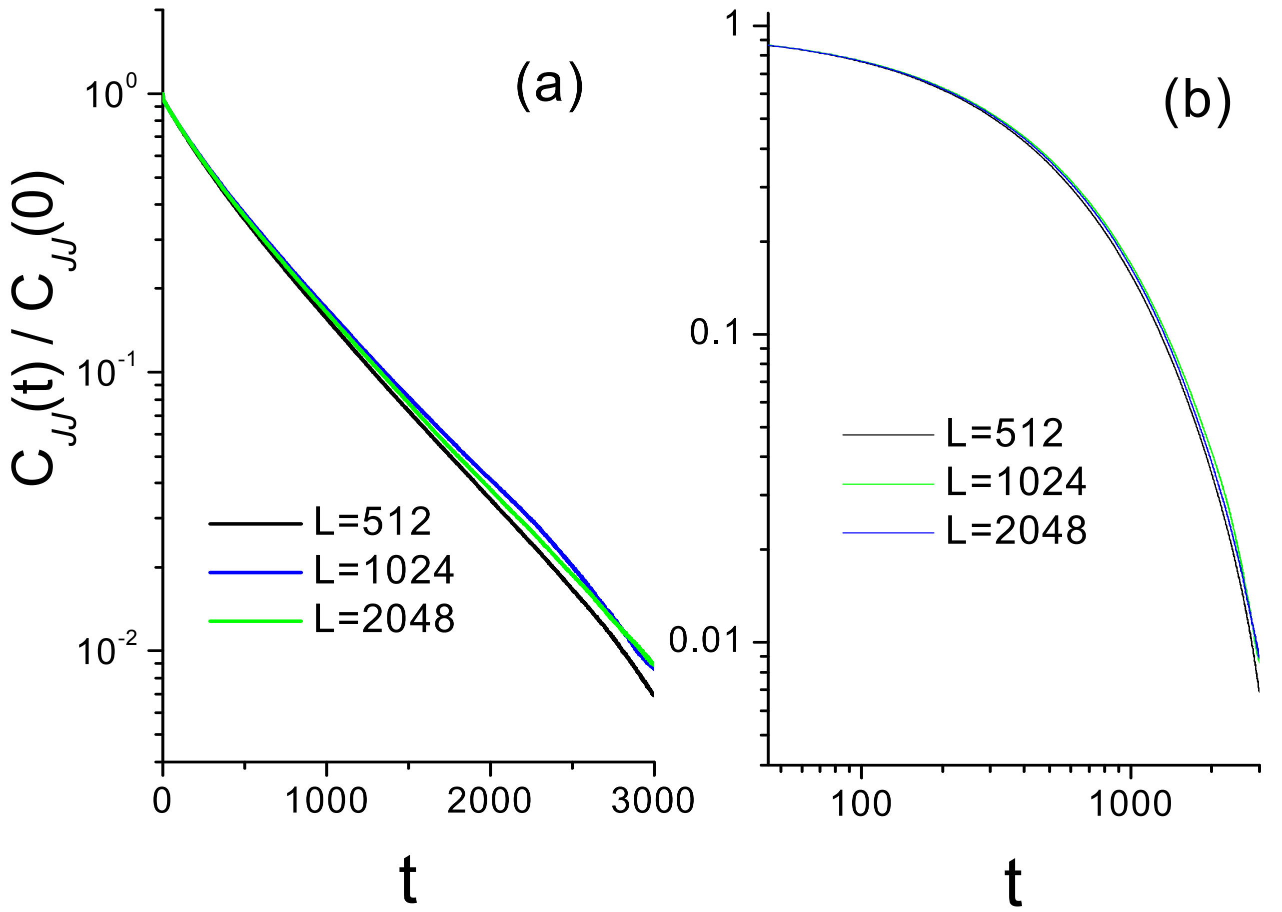
Results: (1) Equilibrium simulation

An overview for all of the three models



Results: (1) Equilibrium simulation

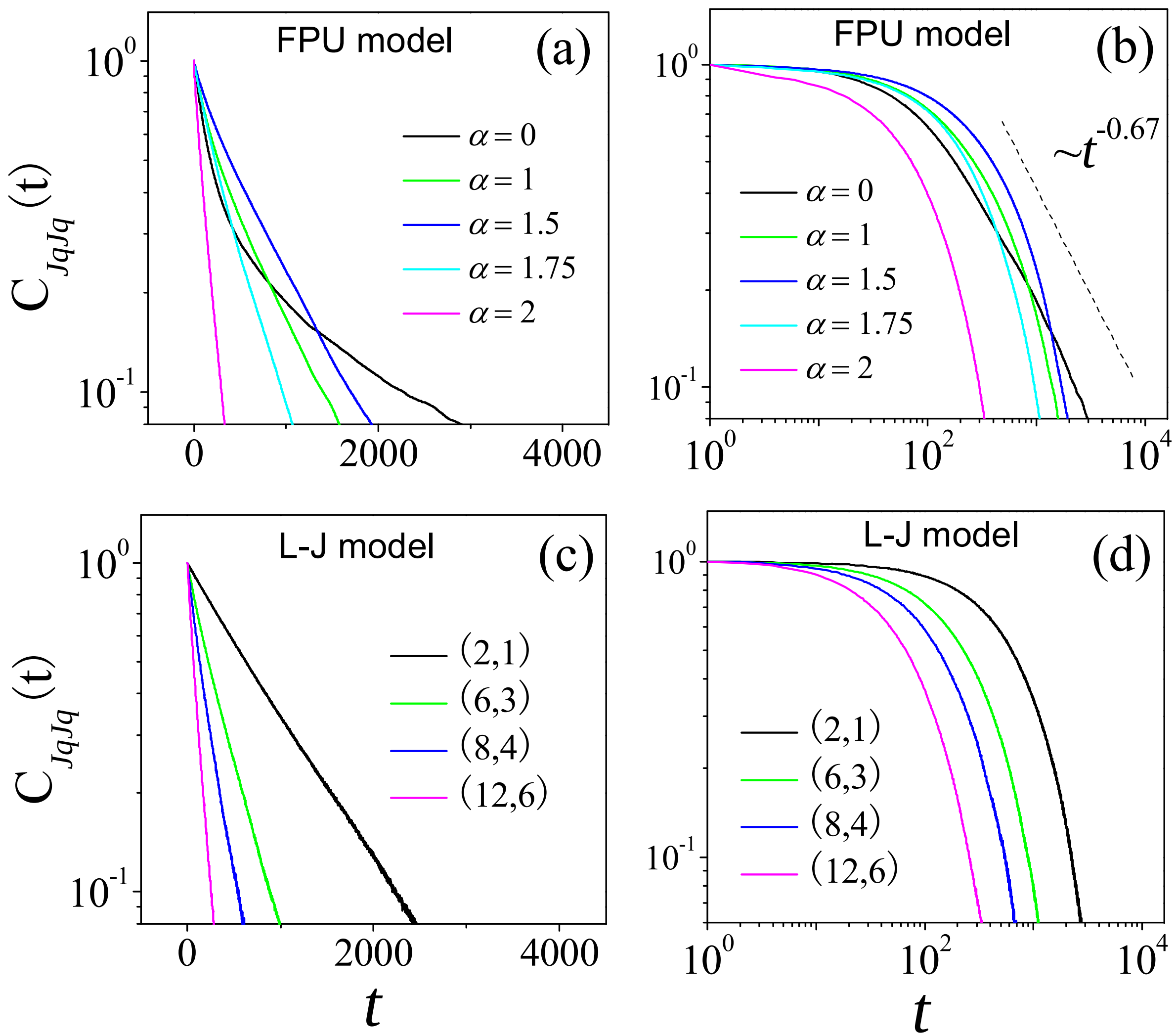
for model (a) with r=1.5:



Results: (1) Equilibrium simulation

for model (b) and (c)

Chen-fig.2

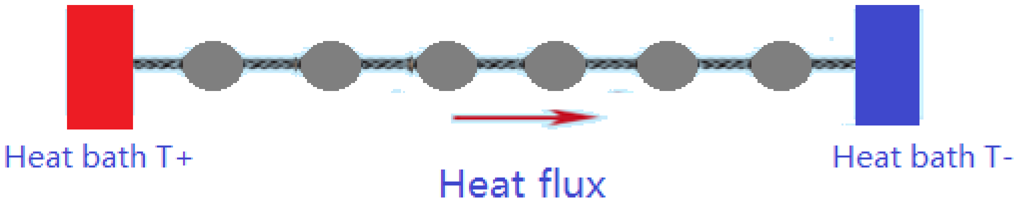


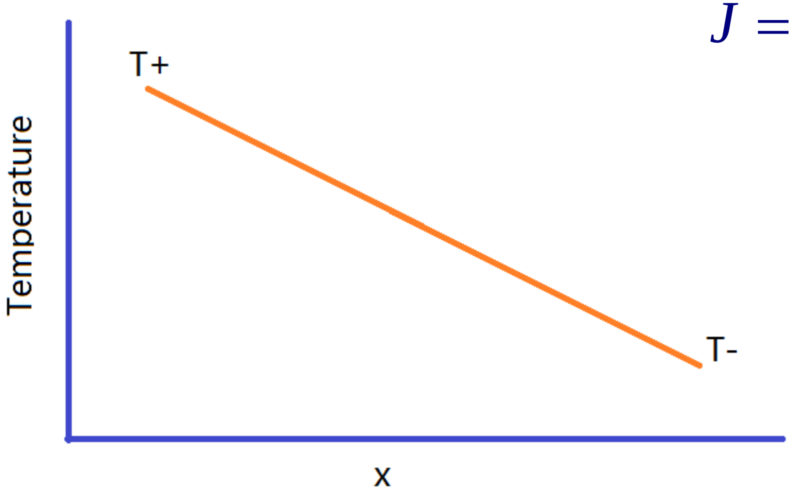
N=4096

Reliable time range is t<3000

S. Chen, et. al., arXiv:1204.5933

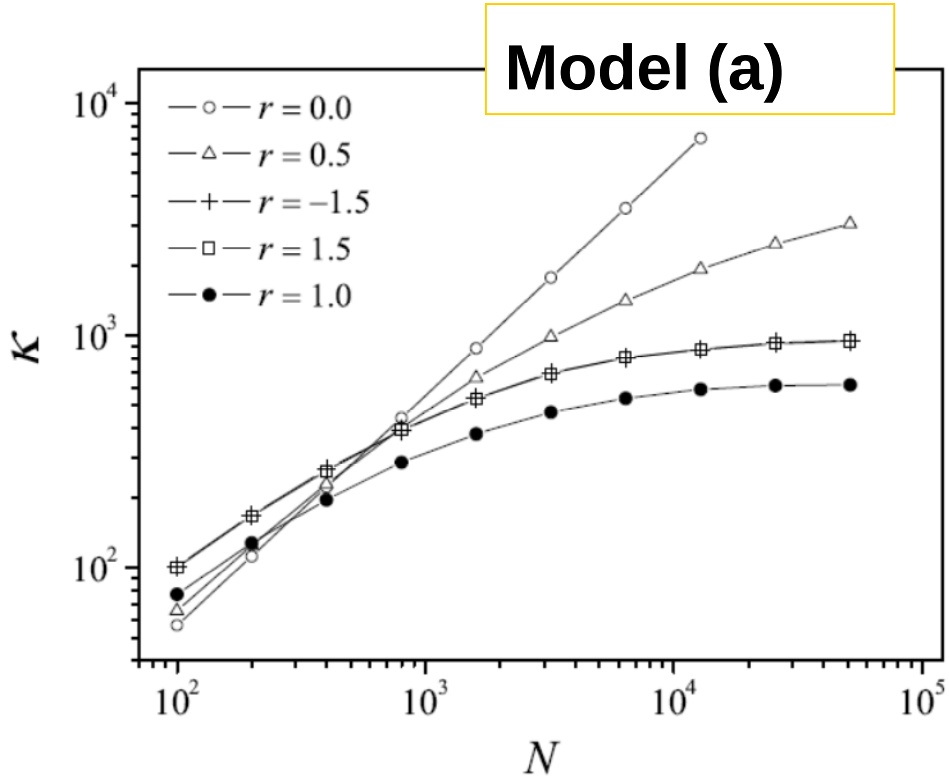
Results: (2) Nonequilibrium simulation



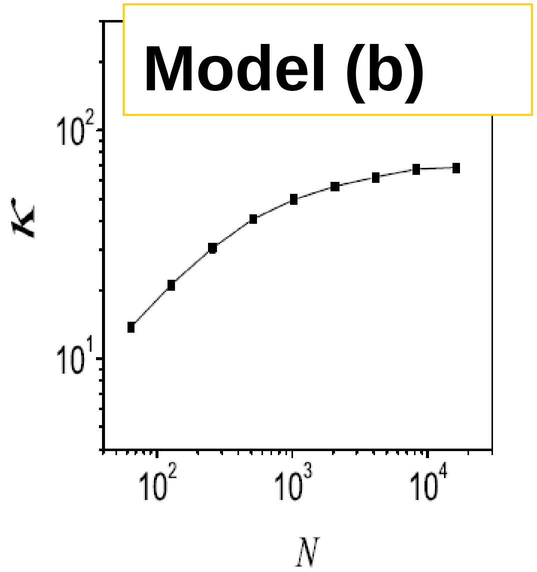


$$J = \kappa \frac{\Delta T}{\Delta x} \rightarrow \kappa \approx \frac{JL}{\Delta T}$$

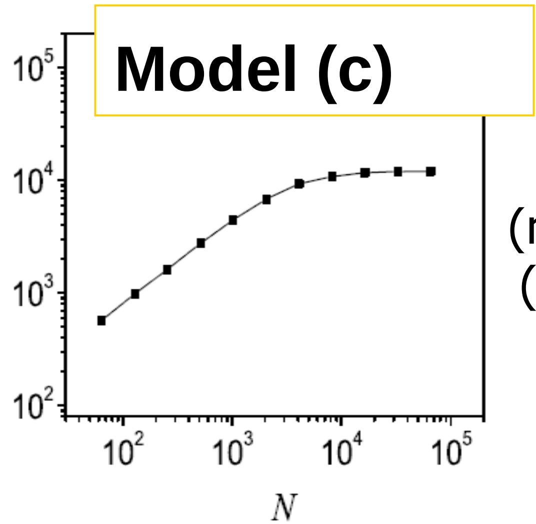
Results: (2) Nonequilibrium simulation



Y. Zhong *et al*, PRE **85**, 060102(R) (2012)



α=2

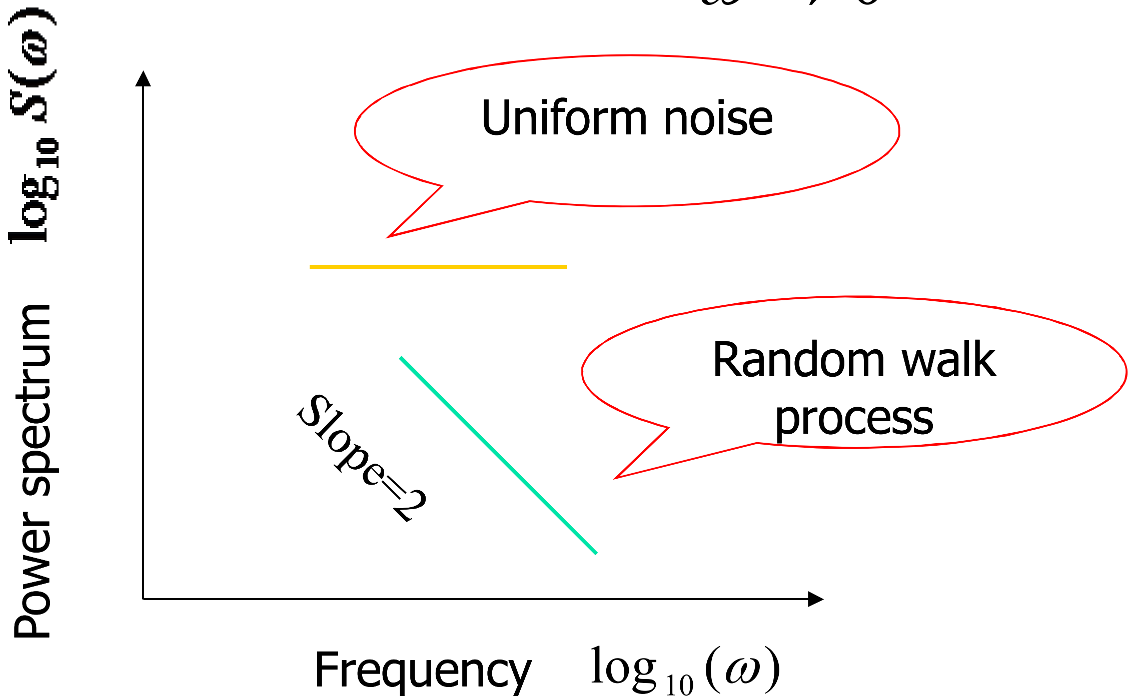


(m,n)=
(12,6)

S. Chen *et.al.*, arXiv:1204.5933

Results: (3) Spectrum analysis

$$S(\omega) \sim c$$
$$\omega \to 0$$



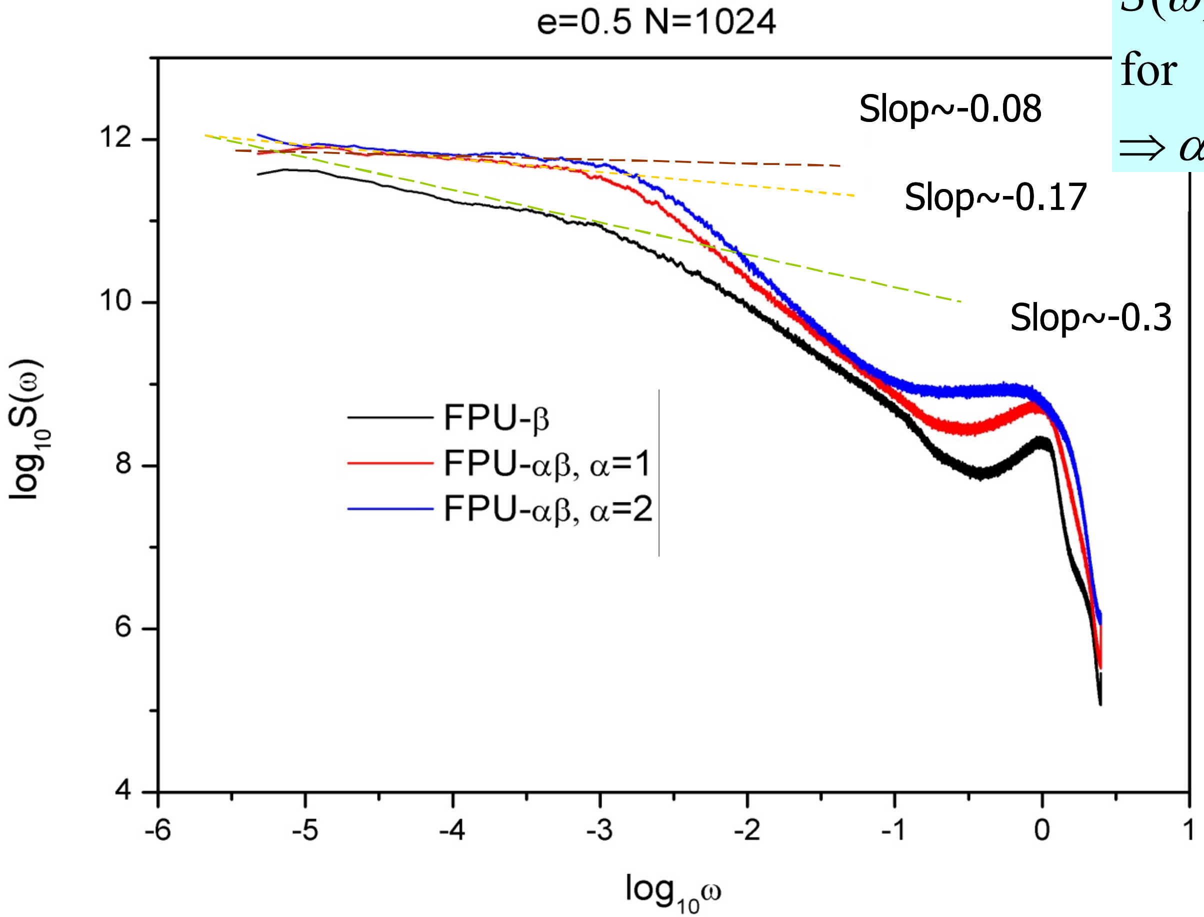
$$S(\omega) \sim \omega^{-2}$$
$$\omega \to 0$$

Prof. Livi: $$S(\omega) \propto \omega^{-\delta} (\omega \to 0) \Rightarrow \kappa \propto L^{\alpha}, \alpha = \delta$$

Results: (3) Spectrum analysis

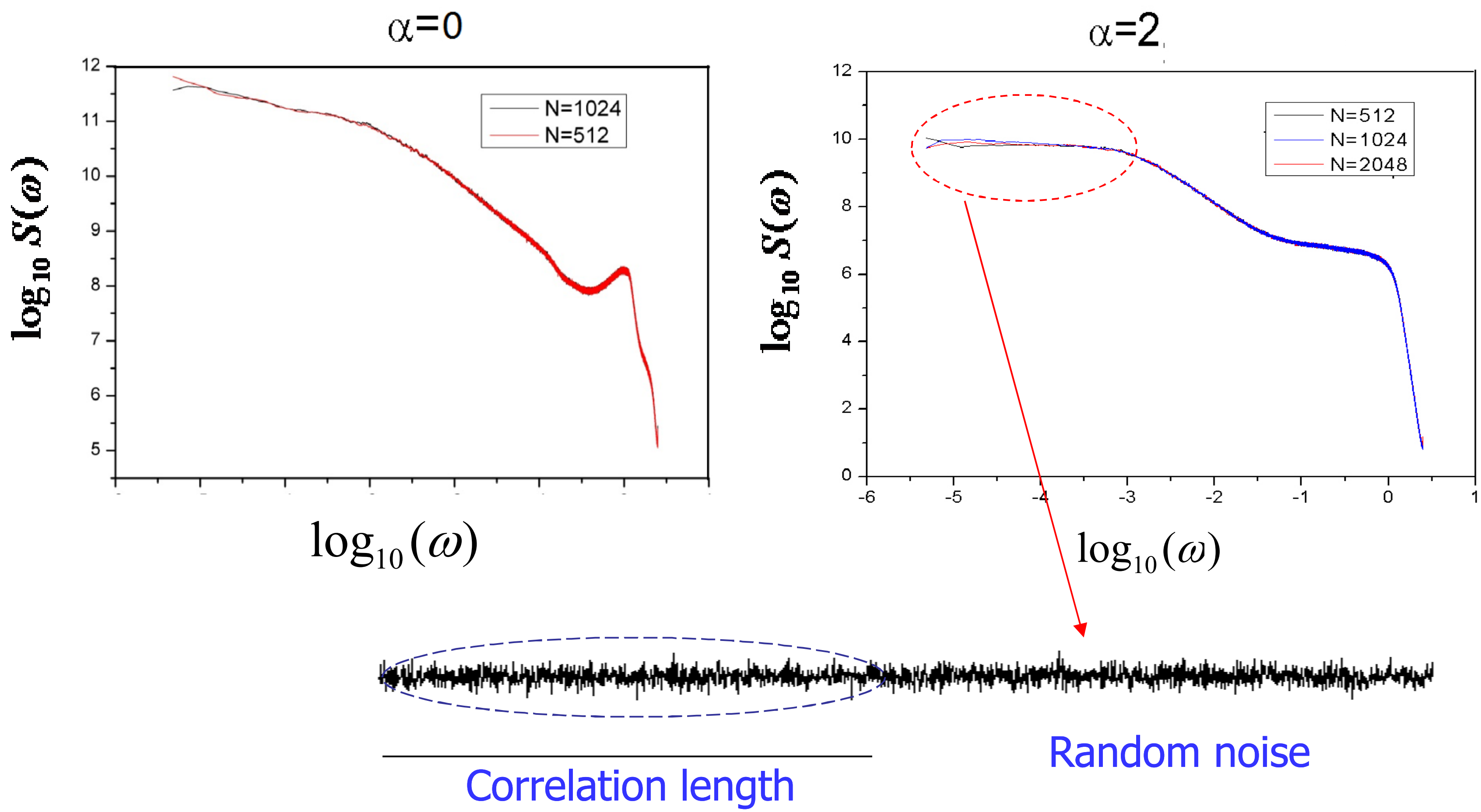
$\mathrm{FPU}-\alpha\beta$ model

$S(\omega) \sim \omega^{-0.3}$
for FPU − β model
$S(\omega) \sim \omega^{0}$
for FPU − α − β model
$\Rightarrow \alpha = \delta \sim 0$



Results: (3) Spectrum analysis

$\text{FPU}-\alpha\beta$ model:



Discussion: mechanism

Symmetry of inter-particle interactions is essential in determining physical properties of systems

$$U(x) = cx^2 - gx^3 - fx^4$$

$$g \neq 0: \quad \langle x \rangle = \frac{3g}{4c^2} k_B T$$

$$g = 0: \quad \langle x \rangle = 0$$

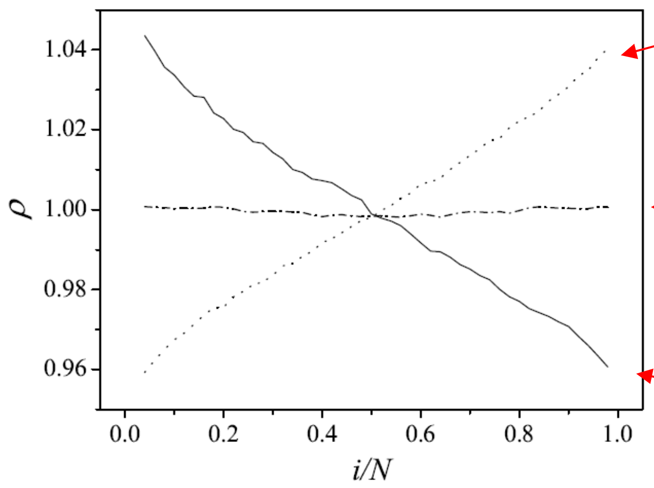
Asymmetric potential: $c_p \neq c_v, P_{\text{int}} \neq 0$, thermal expensive

Symmetric potential: $c_p = c_v, P_{\text{int}} = 0$, no thermal expension

C. Kittel, Introduction to Solid State Physics (7ed., Wiley, 1996), p130.

Discussion: mechanism

Nonequilibrium case: Thermal expansion can induce **Mass gradient,** which may provide additional scattering to the flux



thermal expansion.

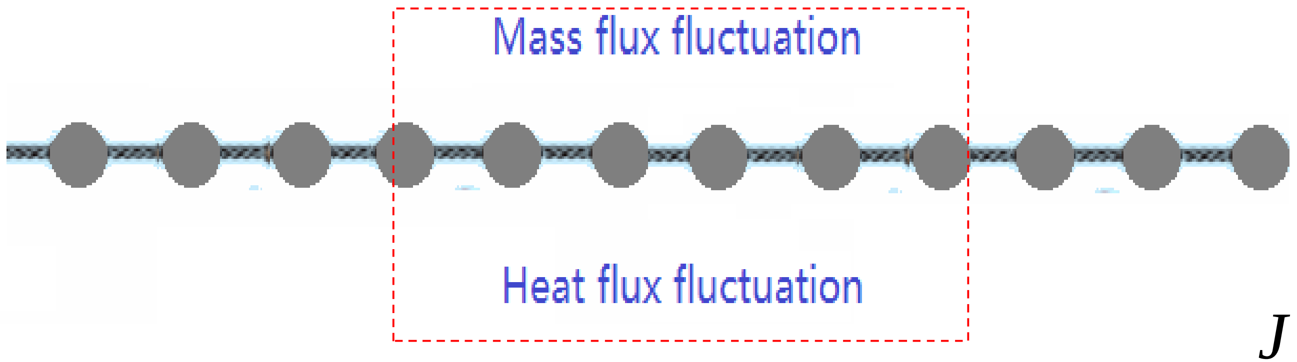
symmetry potential: no thermal expansion.

negative thermal expansion.

Phonon scattering + mass-gradient scattering

Discussion: mechanism

Equilibrium case: Thermal expansion can induce the coupling between heat current and mass current



$$J_q = \sum_i j_i^q$$

$$C_{qm}(t) = < J_q(t) J_m(0) >$$

$$C_{mq}(t) = < J_m(t) J_q(0) >$$

$$J_m(t) = M(t) v_M(t)$$

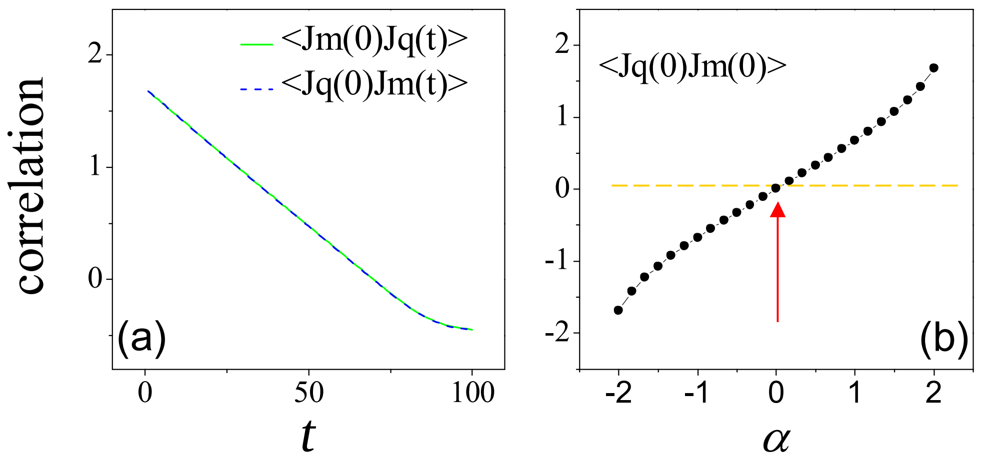
Discussion: mechanism

Coupling between the energy and mass currents

FPU $-\alpha\beta$ model:

$\alpha = 2$

Chen-fig.3



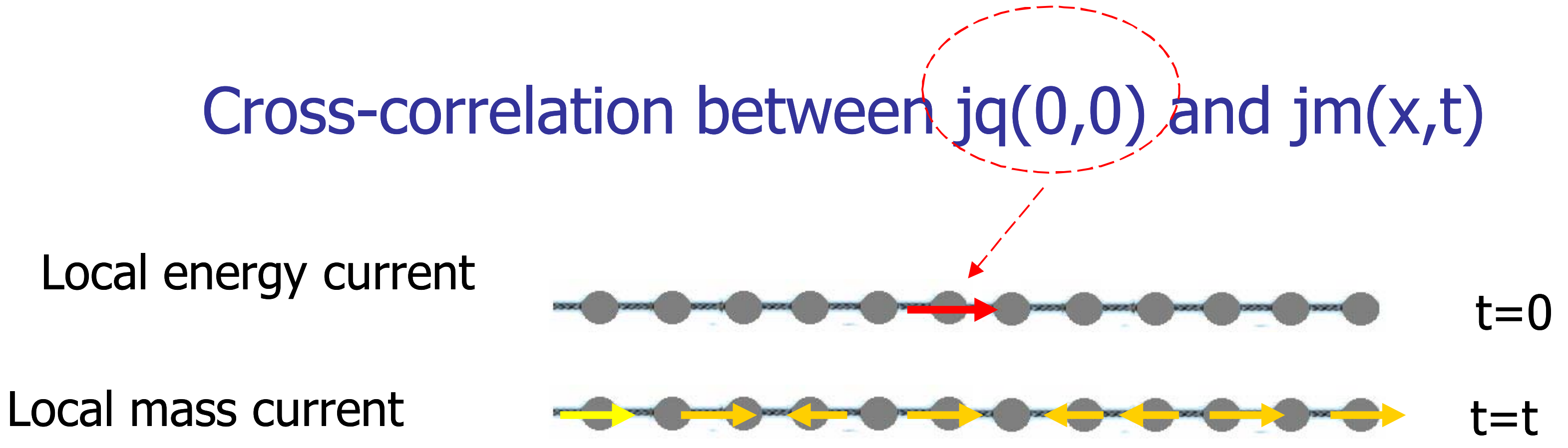
1. Onsager reciprocal relations $L_{qm} = L_{mq}$
2. Symmetry interaction $L_{qm} = L_{mq} = 0$
3. Asymmetry interaction $L_{qm} = L_{mq} \neq 0$

The asymmetry induce the coupling between the local currents of heat and mass

S. Chen *et.al.*, arXiv:1204.5933 (2012)

Discussion: mechanism

Cross-correlation between jq(0,0) and jm(x,t)

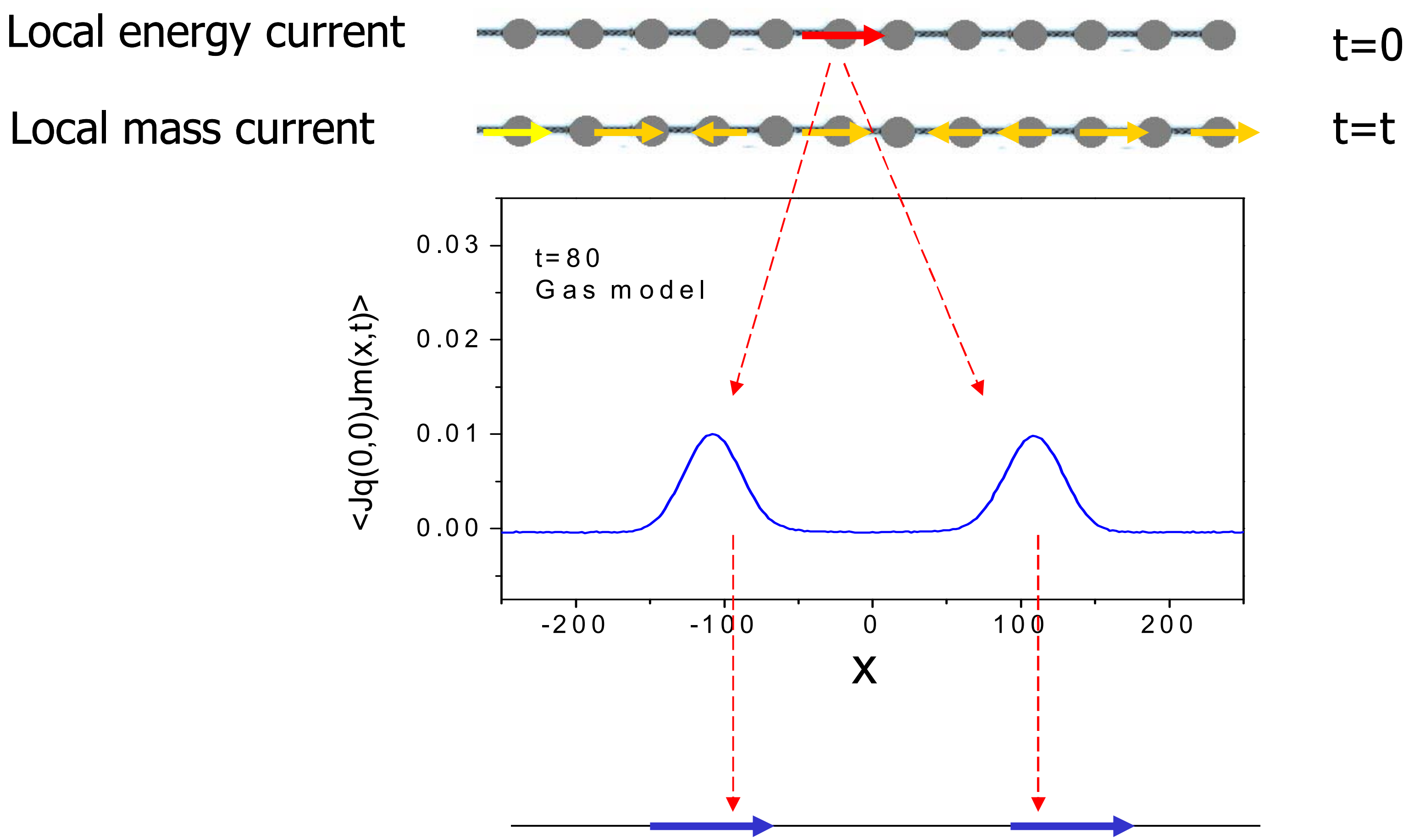


$$c(x,t) \equiv \left\langle j_q(0,0)\, j_m(x,t) \right\rangle$$

--spatiotemporal cross correlation between
the fluctuations of local energy currents and mass currents

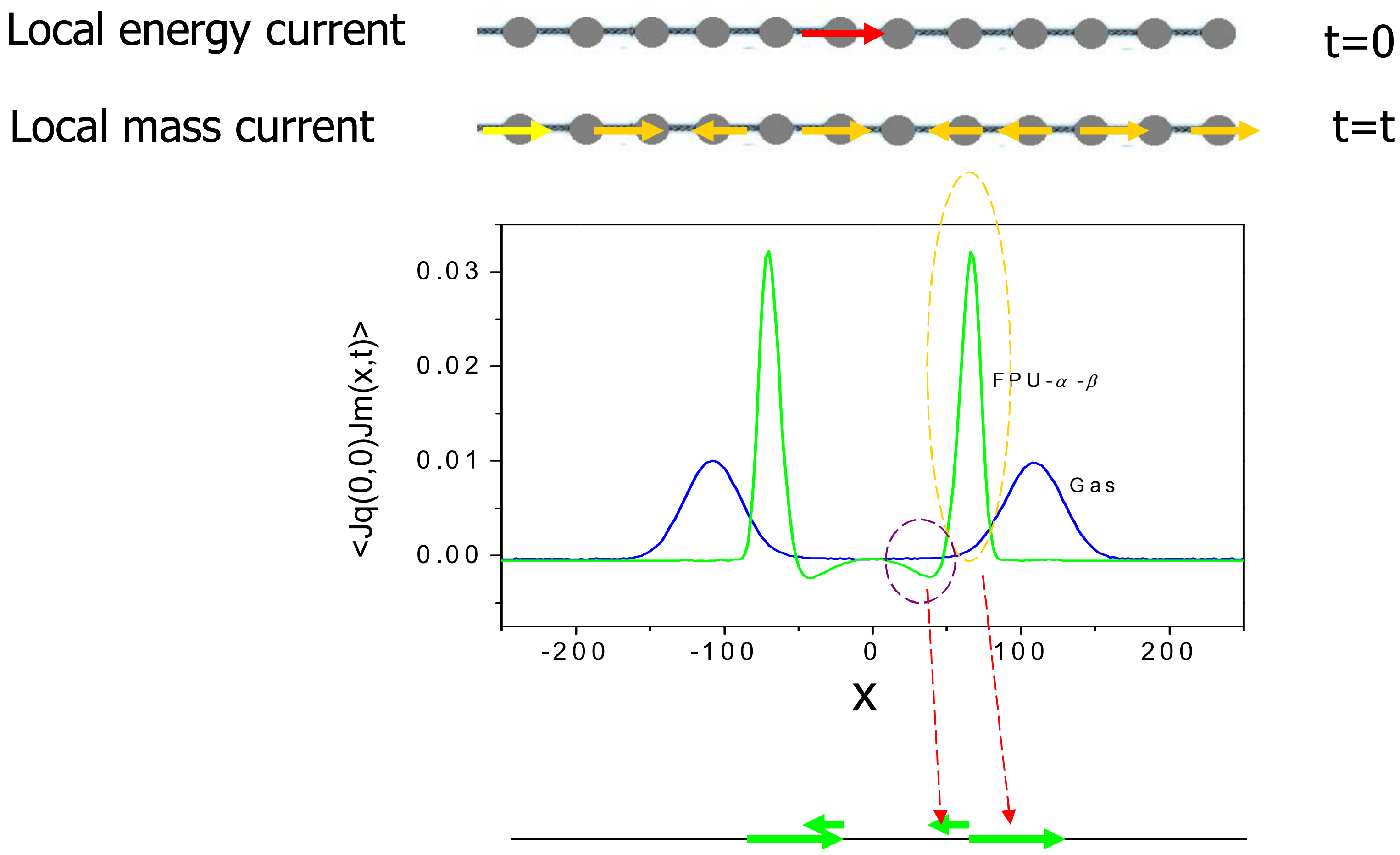
Discussion: mechanism

Cross-correlation between jq(0,0) and jm(x,t)



Discussion: mechanism

Cross-correlation between jq(0,0) and jm(x,t)



Additional scattering is induced by the lattice feature

Summary: results

For momentum conserving 1d lattice with proper degree of asymmetry:

(1) $L_{qm} = L_{mq} \neq 0$ while in the symmetric case $L_{qm} = L_{mq} = 0$

(2) for the heat conductivity:

(a) Equilibrium simulation: The current-current correlation decays faster than the power law;

(b) Nonequilibrium simulation: The thermal conductivity converges in the thermodynamic limit.

(c) Power spectrum analysis: A size-independent heat conductivity

Summary: Mechanism

$$\begin{cases} \text{symmetry} \Rightarrow \text{power} - \text{law decay} \\ \text{asymmetry} \Rightarrow \begin{cases} \text{rapid decay} & \text{for lattices} \\ \text{power} - \text{law decay} & \text{for fluids} \end{cases} \end{cases}$$

fluids: mass-current coupling

Lattice with asymmetric interactions

Mass-current coupling + lattice scattering + nonlinear interactions

Lattice with symmetric interactions

lattice scattering+ nonlinear interactions

Also guesses! We are trying to find more details….

a guess

The transport theories of hydrodynamics and kinetics may apply to

momentum conserving fluids &

momentum conserving lattice with symmetric interactions

but may not apply to

momentum conserving lattice with asymmetric interactions

Three Puzzles

(1) Why it deviates the hydrodynamic prediction?

(2) Does there exist a transition from the power-law decay to the rapid decay with the increase of the asymmetry? — open question

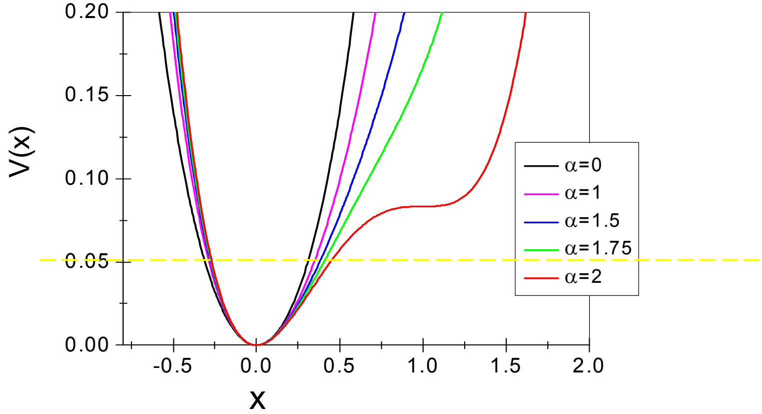
$$\text{FPU} - \alpha - \beta \text{ model, } \beta = 1$$

$$T = 1, \ \alpha = 1 \ \Rightarrow \text{power-law decay}$$

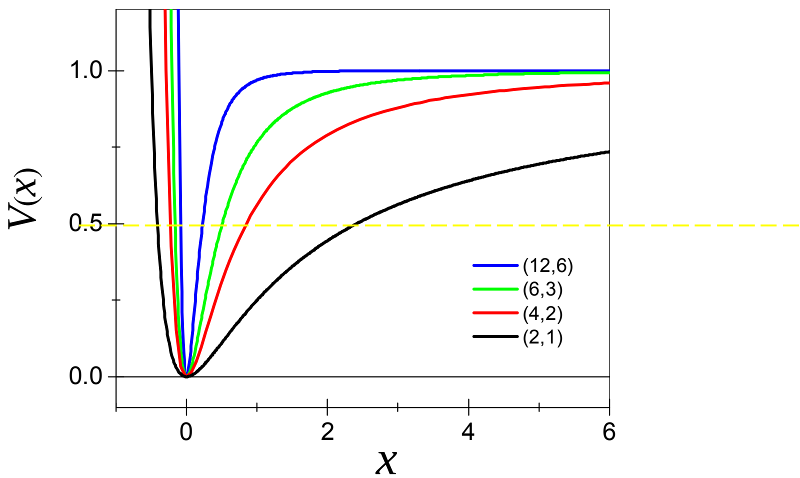
$$T = 1, \ \alpha = 2 \ \Rightarrow \text{exponential decay}$$

$$T = 0.1, \ \alpha = 1 \ \Rightarrow \text{exponential decay}$$

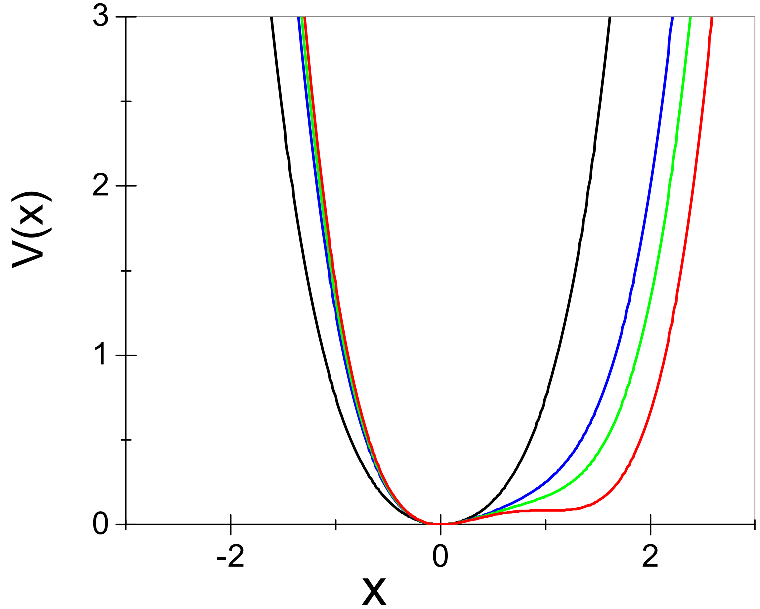
$$T = 0.1, \ \alpha = 2 \Rightarrow \text{exponential decay}$$



V(x)
x
0.00
0.05
0.10
0.15
0.20
-0.5
0.0
0.5
1.0
1.5
2.0
α=0
α=1
α=1.5
α=1.75
α=2

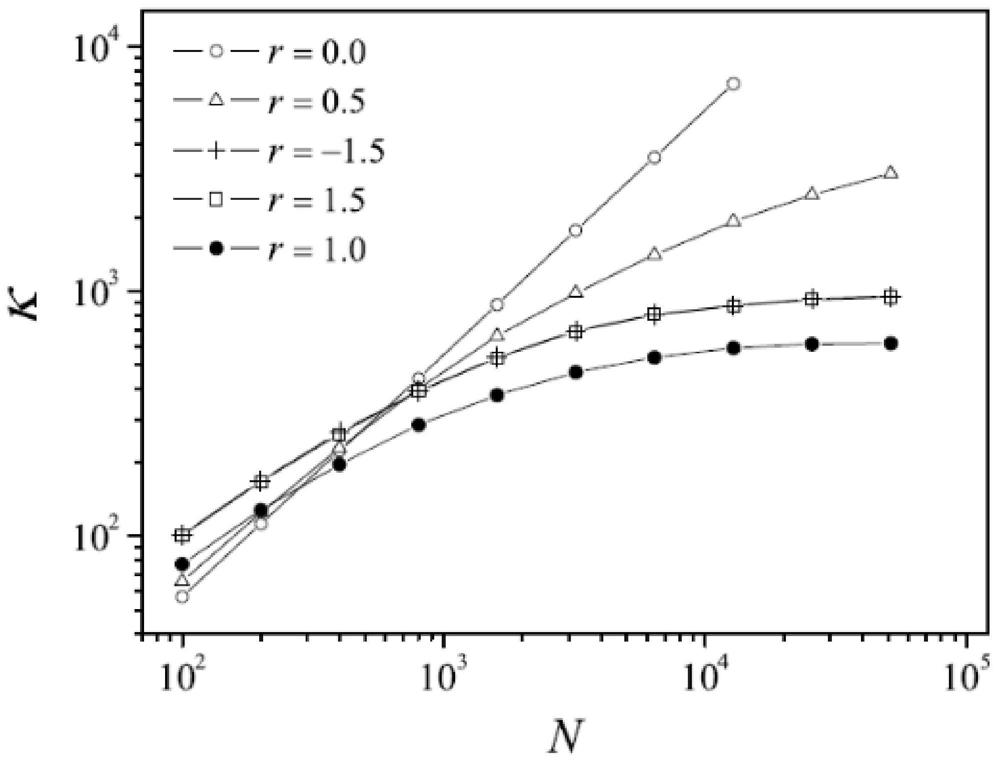


V(x)
x
0.0
0.5
1.0
0
2
4
6
(12,6)
(6,3)
(4,2)
(2,1)



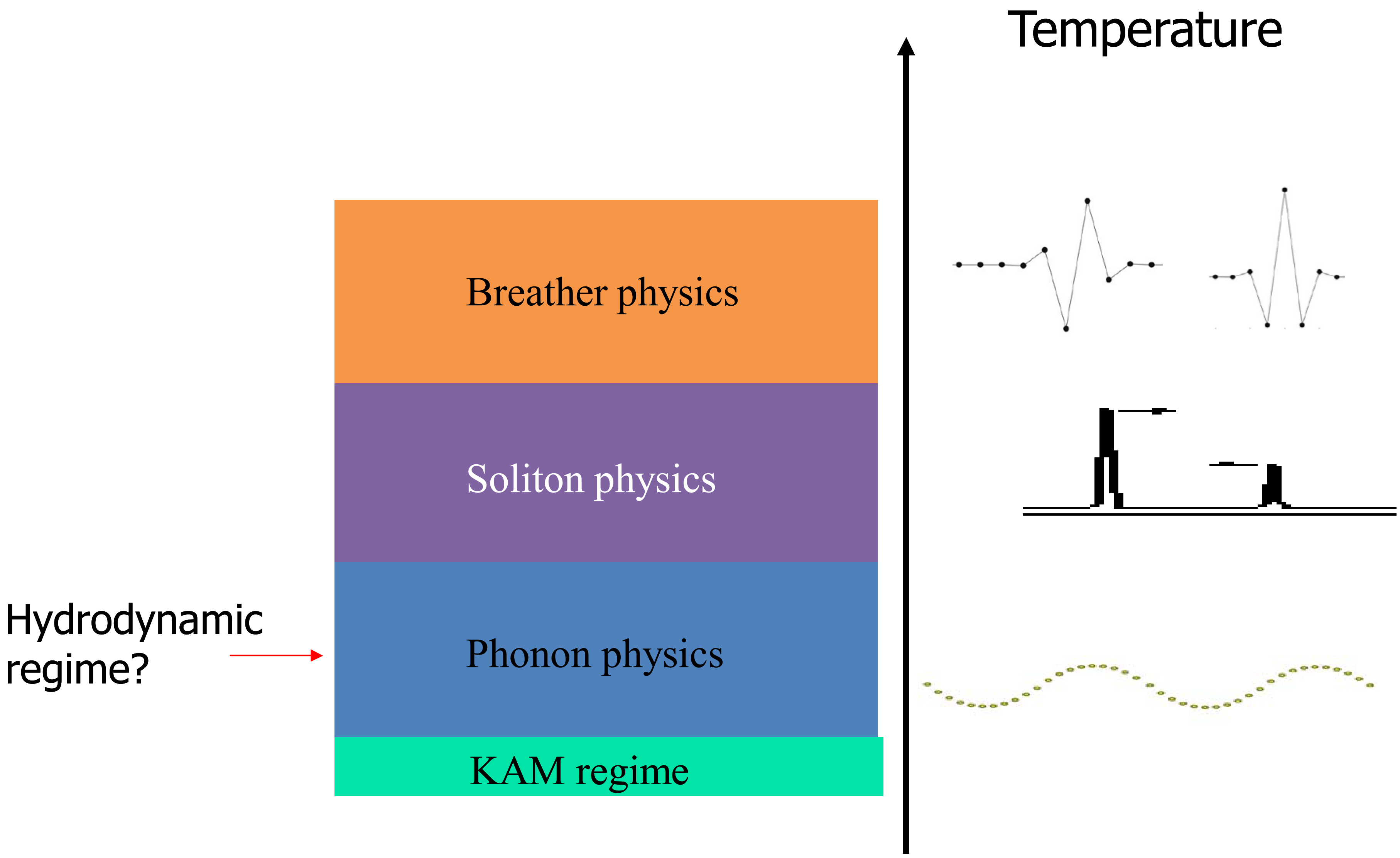
V(x)
x
0
1
2
3
-2
0
2

(3) The convergence length ?



If, say for graphene , the potential is near-symmetry, the convergence length should be quit long

A big guess


Temperature
Breather physics
Soliton physics
Phonon physics
KAM regime
Hydrodynamic regime?

Finally, I would like to thanks profs. S. Lepri, R. Livi, A. Politi for helpful discuss.
They pushed us keeping studying the mechanism of the observed phenomena

Thanks for your attention!

Part II. Diffusion of heat, energy, momentum and mass in 1D systems

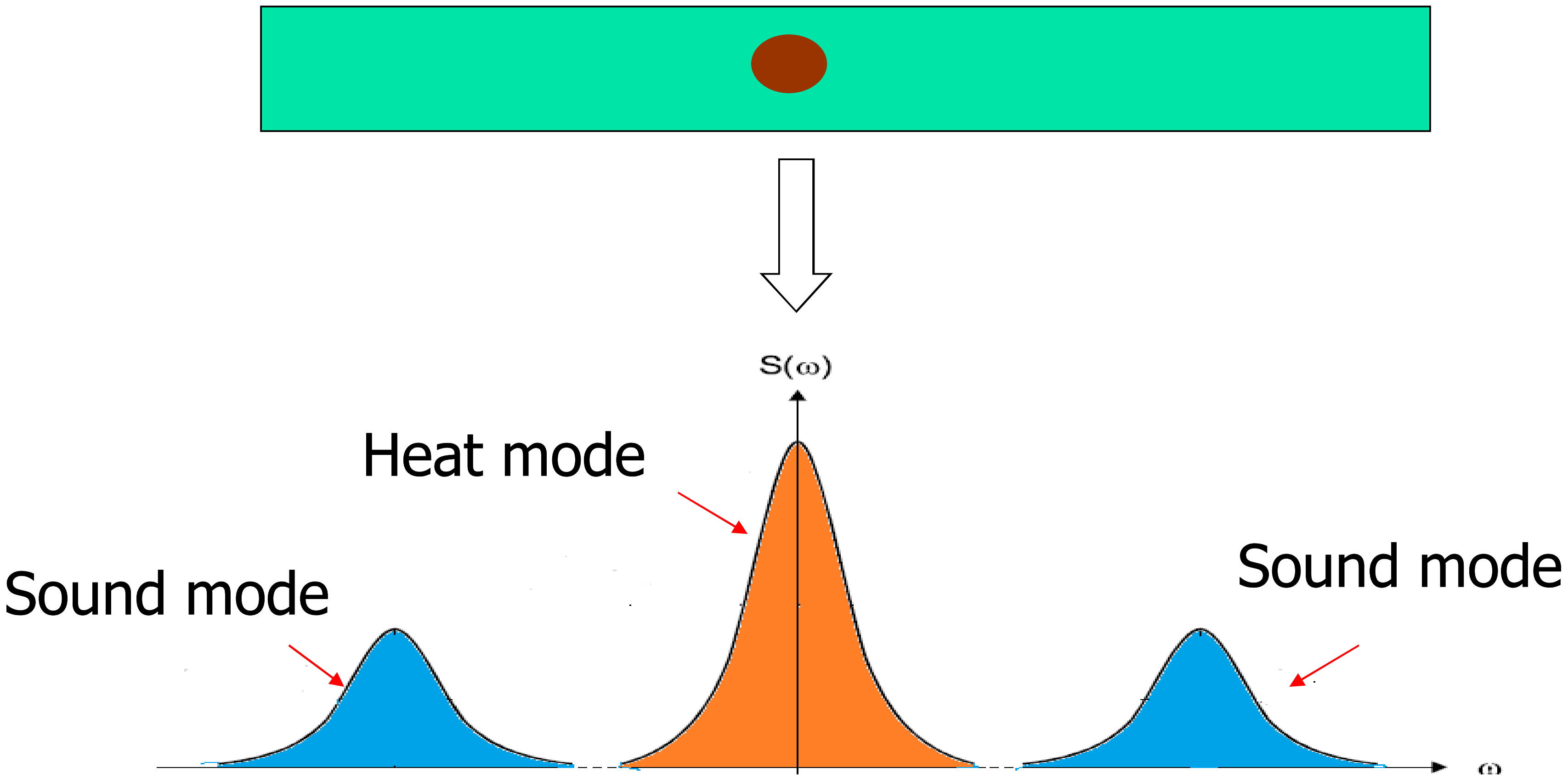
1. Problem & Background
2. Methods
3. Models
4. Results & Discussions

Question:

In equilibrium systems, a perturbation will induce fluctuations of energy, mass, momentum, heat , local flux and etc.

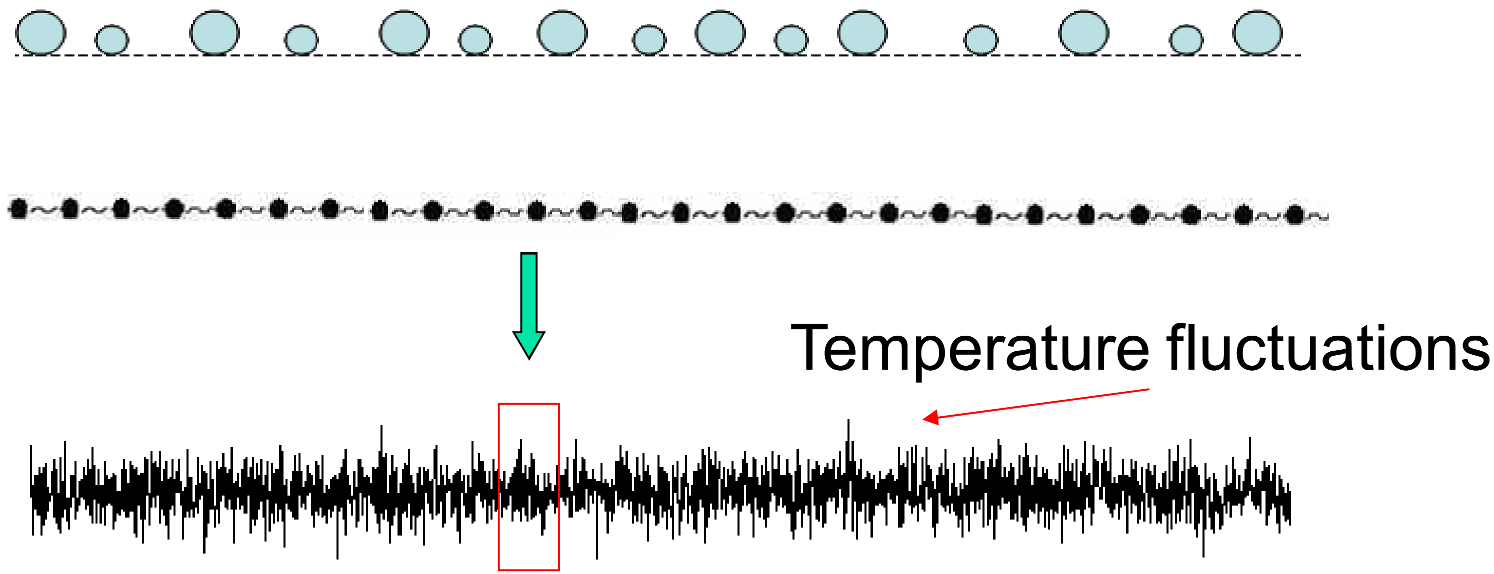
How does a local fluctuation spread or diffuse into other parts of the system?

Hydrodynamic prediction for the problem



JP Hansen, IR McDonald, Theory of Simple Liquids, 3rd edition, 2006.

Our aim



Explore the diffusion or relax behavior of local deviations by direct simulation

Background: Distribution function and diffusion classification

Probability distribution function (PDF) $\rho(r,t)$

$$\Longrightarrow \quad < r^2(t) >= \int r^2 \rho(r,t)dr \Longrightarrow < r^2(t) > \sim t^{\alpha}$$

$$\alpha < 1, \quad subdiffusion, \quad \alpha = 1, \quad normal\ diffusion$$

$$\alpha > 1, \quad superdiffusion, \quad \alpha = 2, \quad ballistic\ motion$$

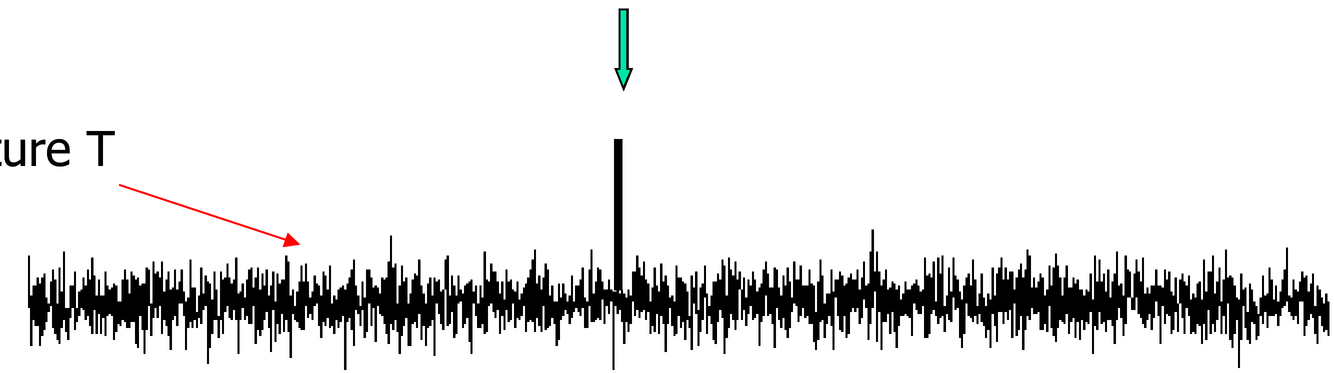
Diffusion can represent not only the diffusive motion but also regular motion

Methods

Methods:
Nonequilibrium extraction

Add a kick $\delta A = \tilde{A}(0,0) - A(0,0)$

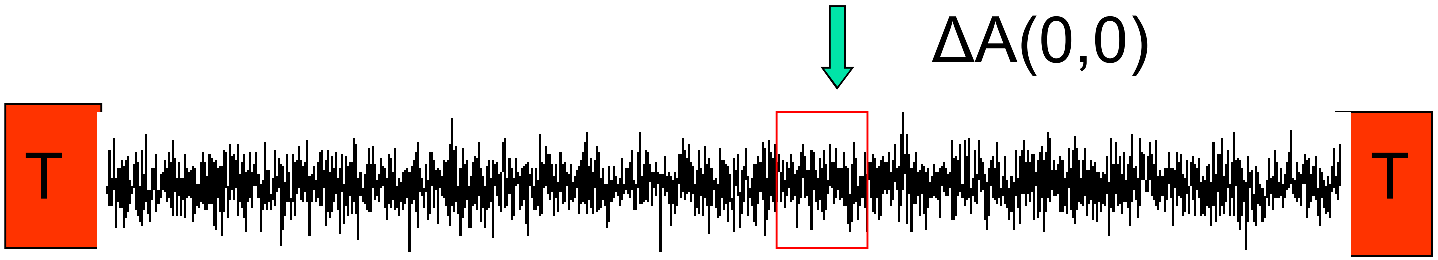
Temperature T



$$\rho(r,t) = \frac{<\tilde{A}(r,t) - A(0,0)>}{<\tilde{A}(0,0) - A(0,0)>}$$

B. Li and J. Wang, PRL 91 (2003);P. Cipriani, S. Denisov, and A. Politi PRL 94 (2005)

Methods:
Equilibrium extraction



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

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

H. Zhao, PRL 96, (2006);P.Huang and H. Zhao, arXiv:1106.2866v1;
S. Chen, Y. Zhang, J. Wang and H. Zhao, arXiv:1106.2896v2

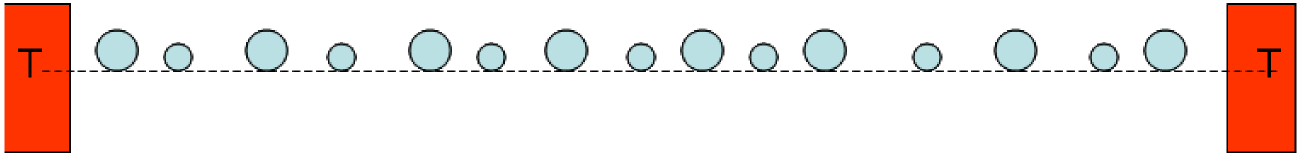
Equilibrium and nonequilibrium methods are equivalent

if the Fluctuation–Dissipation Relation (FDR) remains correct:

$$\frac{< \widetilde{A}(r,t) - A(r,t) >}{< \widetilde{A}(0,0) - A(0,0) >} = \frac{< \Delta A(0,0)\Delta A(r,t) >}{\int < \Delta A(0,0)\Delta A(r,0) > dr}$$

Models

1 1D gas with alternating masses



2 FPU lattice

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

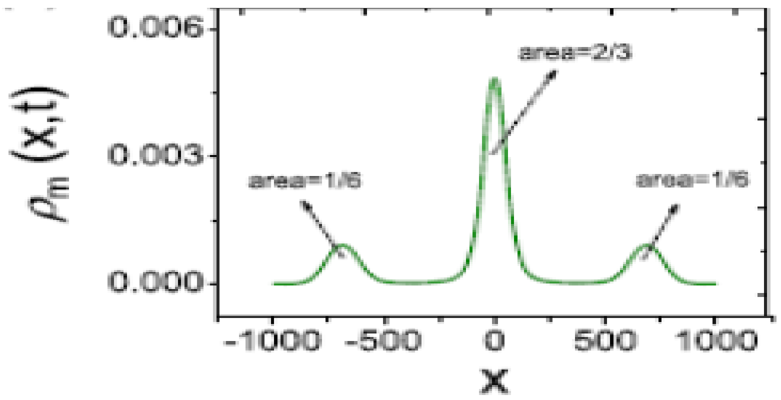
3 Lattice φ^4 model

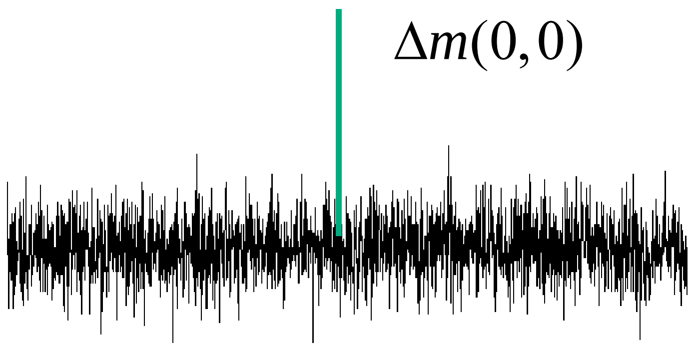
$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \frac{1}{2}\lambda(x_i - x_{i-1} - a)^2 + \frac{\beta}{4}(x_i - i)^4$$

Results

An example: the distribution function of mass-density fluctuations (The dynamic structure factor) of the 1d gas at t=300

$$\rho_m(r,t) = \frac{<\Delta m(0,0)\Delta m(r,t)>}{\int <\Delta m(0,0)\Delta m(r,0)>dr} + \frac{1}{N-1}$$

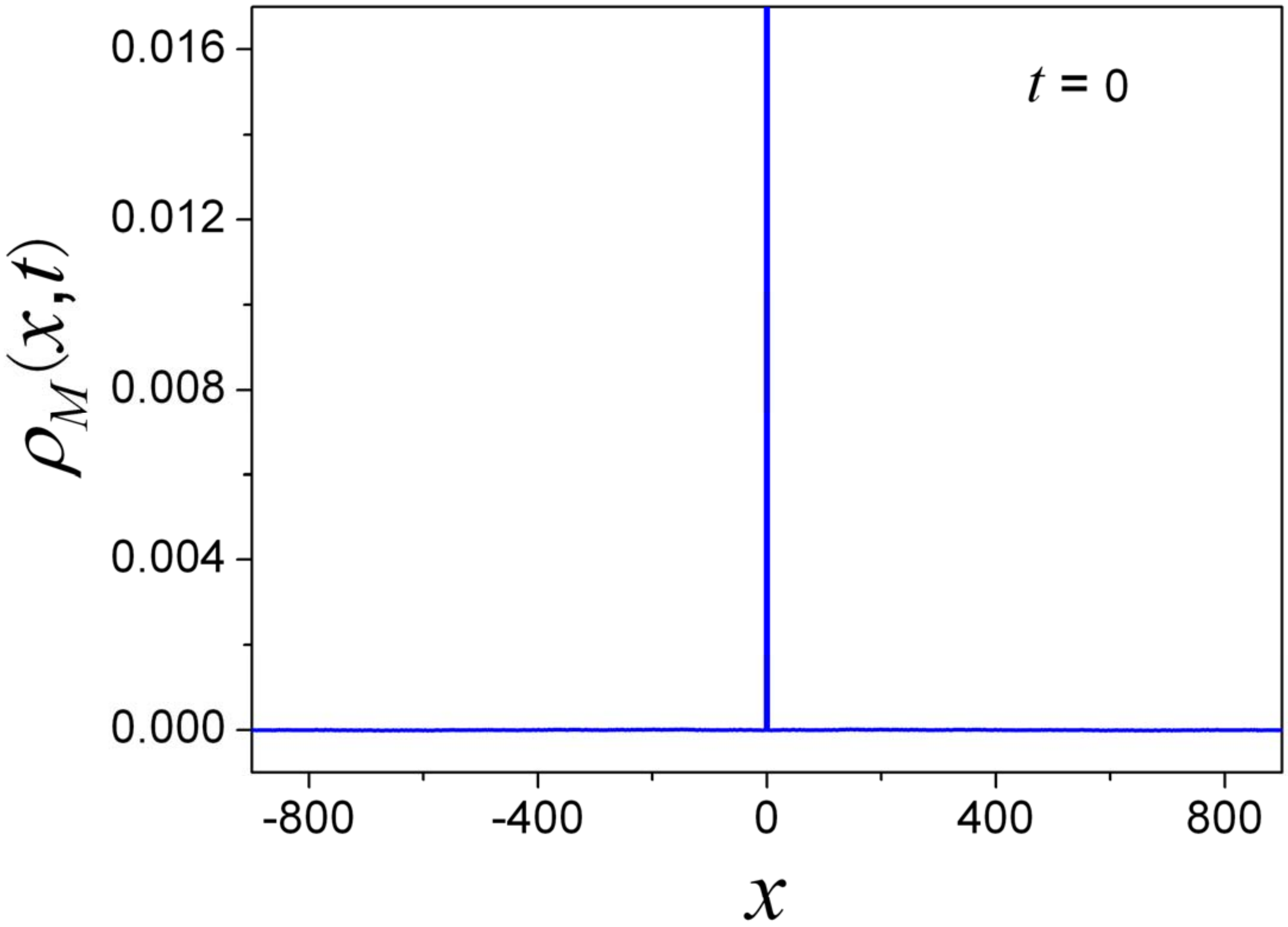




Temperature T=2

$$Landau - Placzek\ ratio = \frac{area\ of\ centrt\ peak}{area\ of\ side\ peaks} = 2$$

S. Chen, Y. Zhang, J. Wang and H. Zhao, arXiv:1106.2896v2

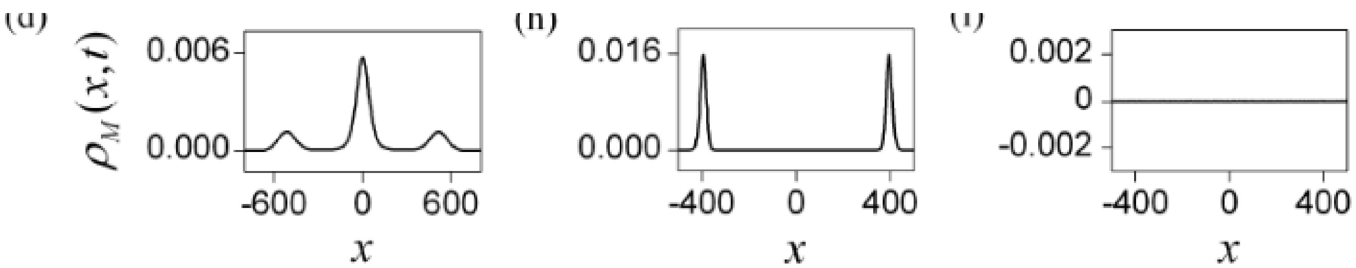


0.016
0.012
0.008
0.004
0.000
$\rho_M(x,t)$
t = 0
-800
-400
0
400
800
x

Diffusion distribution functions

(t=300)

1d gas　　FPU　　φ^4 Lattice

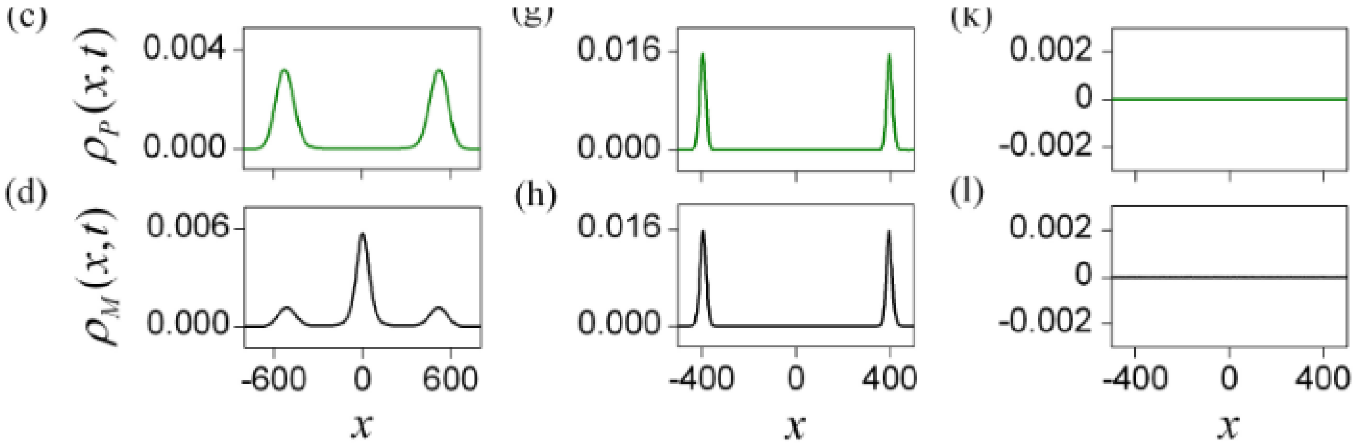


Mass density

Diffusion distribution functions

(t=300)

1d gas FPU φ^4 Lattice



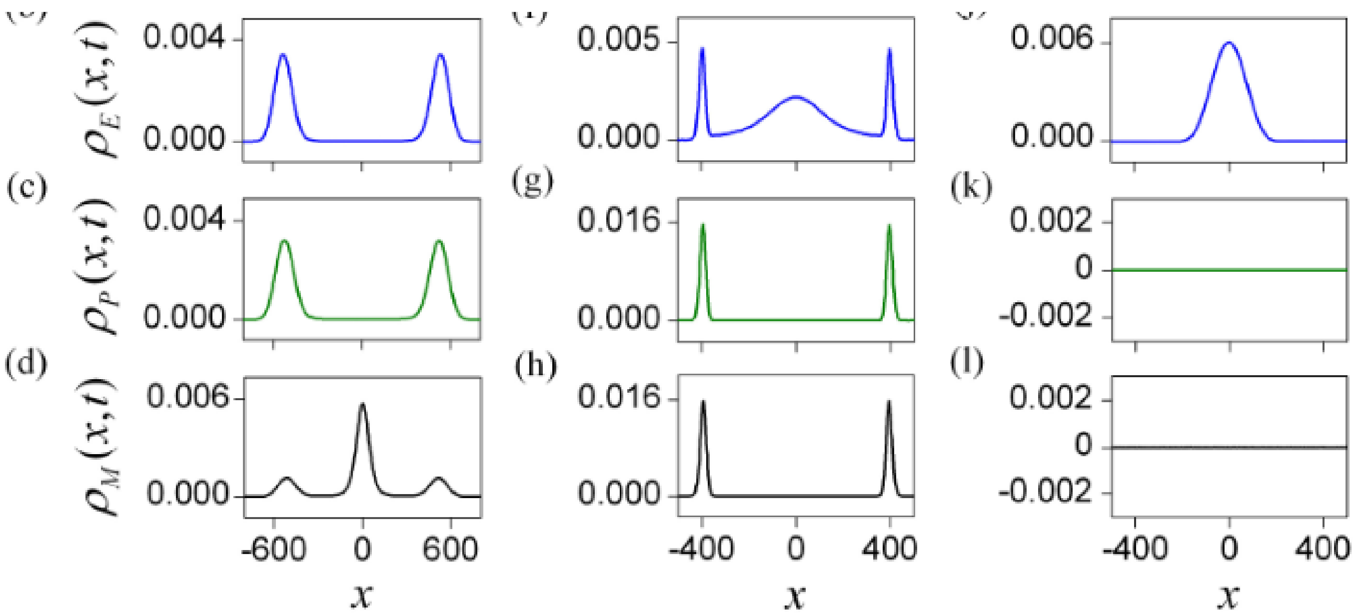
Momentum

Mass density

Diffusion distribution functions

(t=300)

1d gas FPU φ^4 Lattice



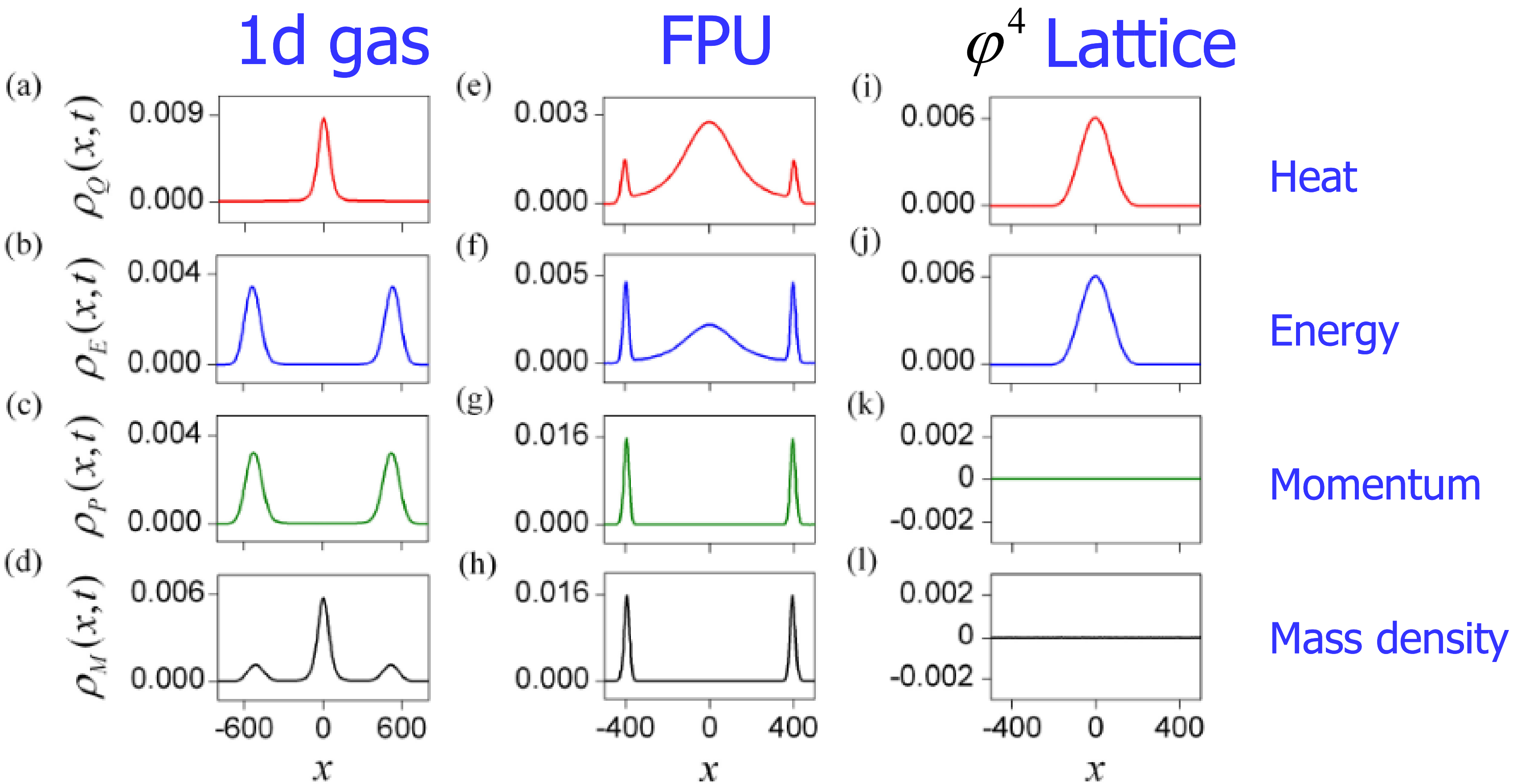
Energy

Momentum

Mass density

Diffusion distribution functions

(t=300)



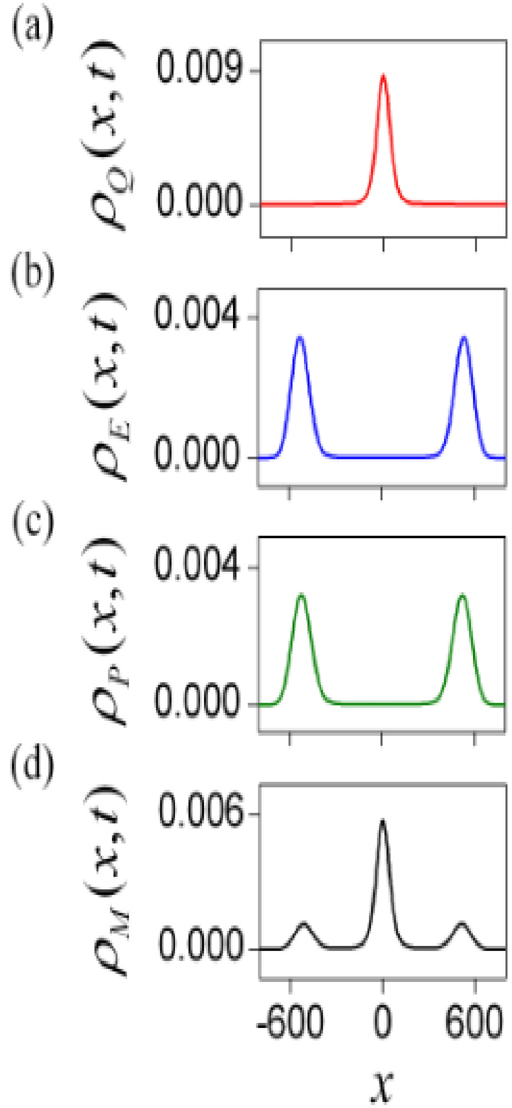
S. Chen, Y. Zhang, J. Wang and H. Zhao, arXiv:1106.2896v2

Summary for the gas model

(1) Sound mode carries the total momentum, energy, and 1/3 mass-density fluctuations and spreads outwards at the sound speed

(2) Heat mode diffuses superdiffusively

(3) Energy and heat are separated completely

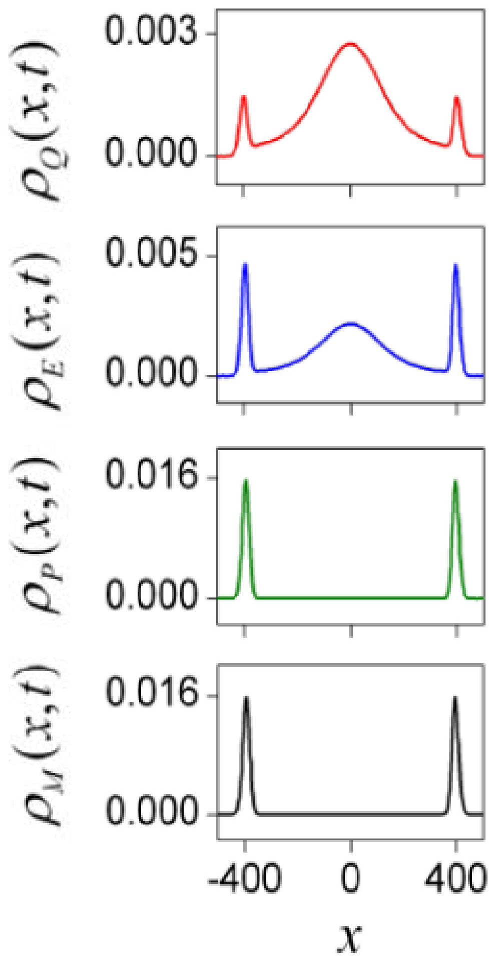


Summary for the FPU model

(1) Sound mode carries the total momentum, total mass-density, partial energy fluctuations

(2) Heat mode diffuses superdiffusively, its PDF shows a three-peak structure in a transient process, but asymptotically it will evolve into single-peak structure one

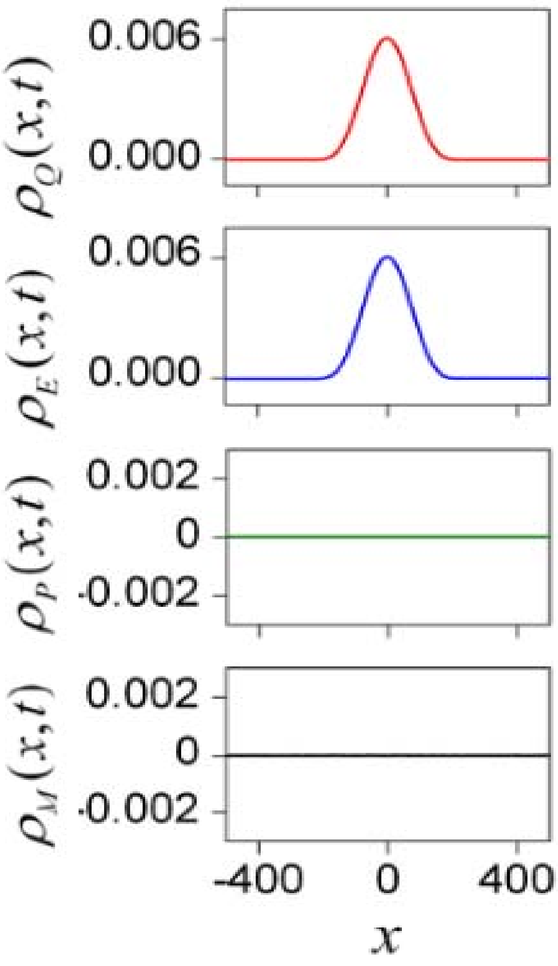
(3) The PDF of the energy always keep the three-peak structure.



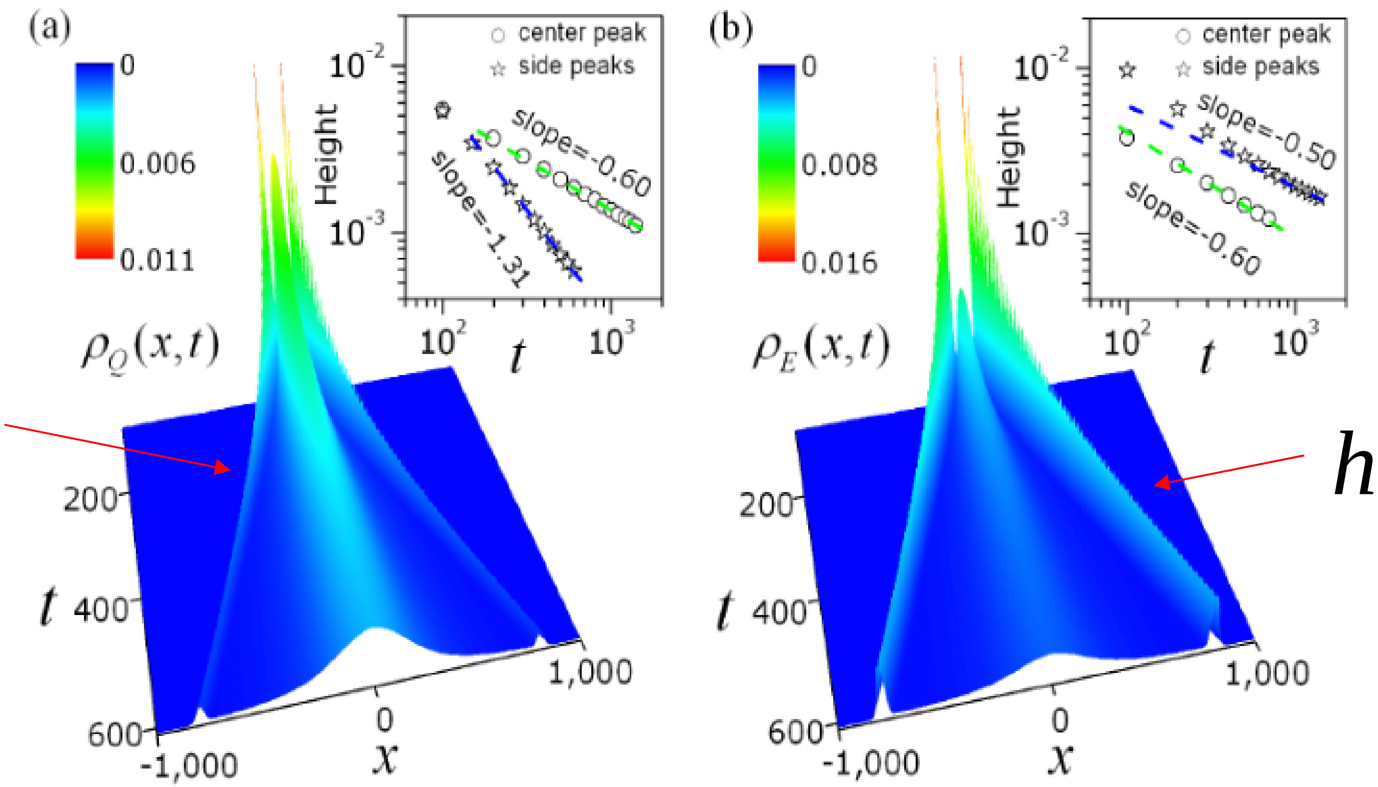
Summary for the φ^4 Lattice

(1) Sound mode disappears;

(2) The diffusion behavior of energy and heat are identical, they diffuse normally.



Discussion: the heat and energy diffusion in the FPU lattice



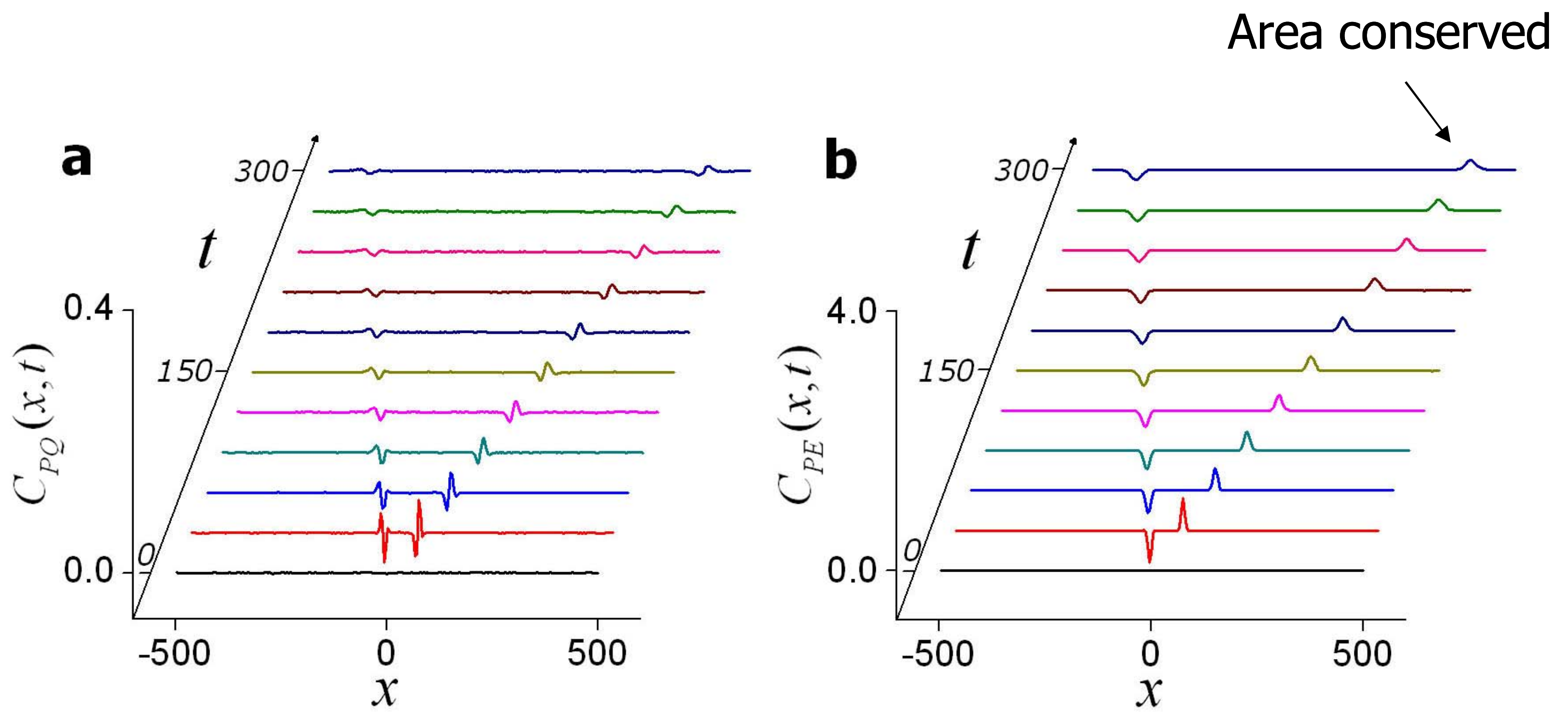
$h \sim t^{-1.33}$

$h \sim t^{-0.5}$

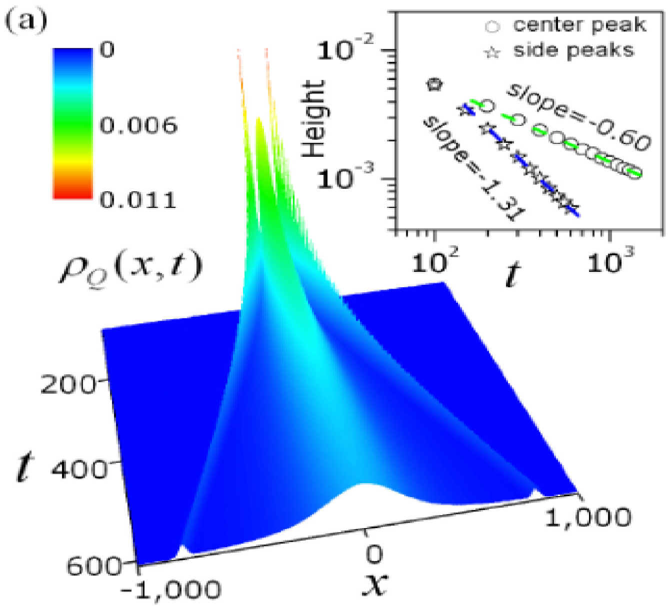
S. Chen, Y. Zhang, J. Wang and H. Zhao, arXiv:1106.2896v2

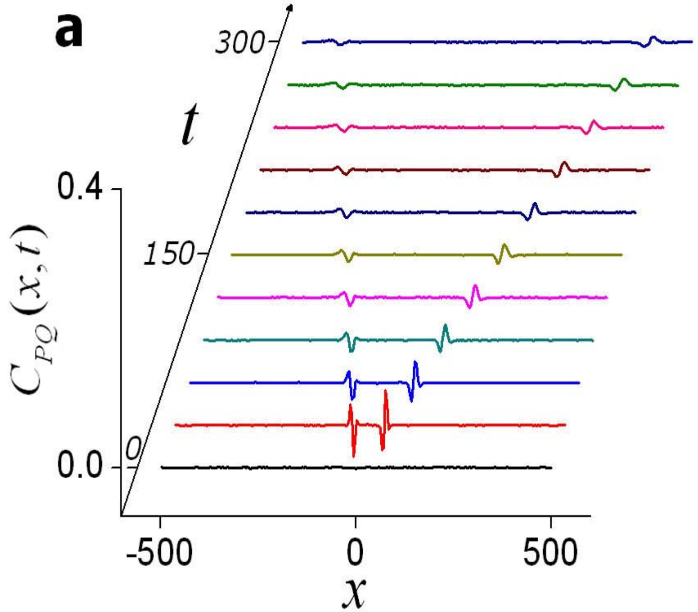
Discussion: the heat and energy diffusion in the FPU lattice

Cross correlation between Q-P and E-P



Discussion: What the side-peaks on $\rho_Q(x,t)$ are?



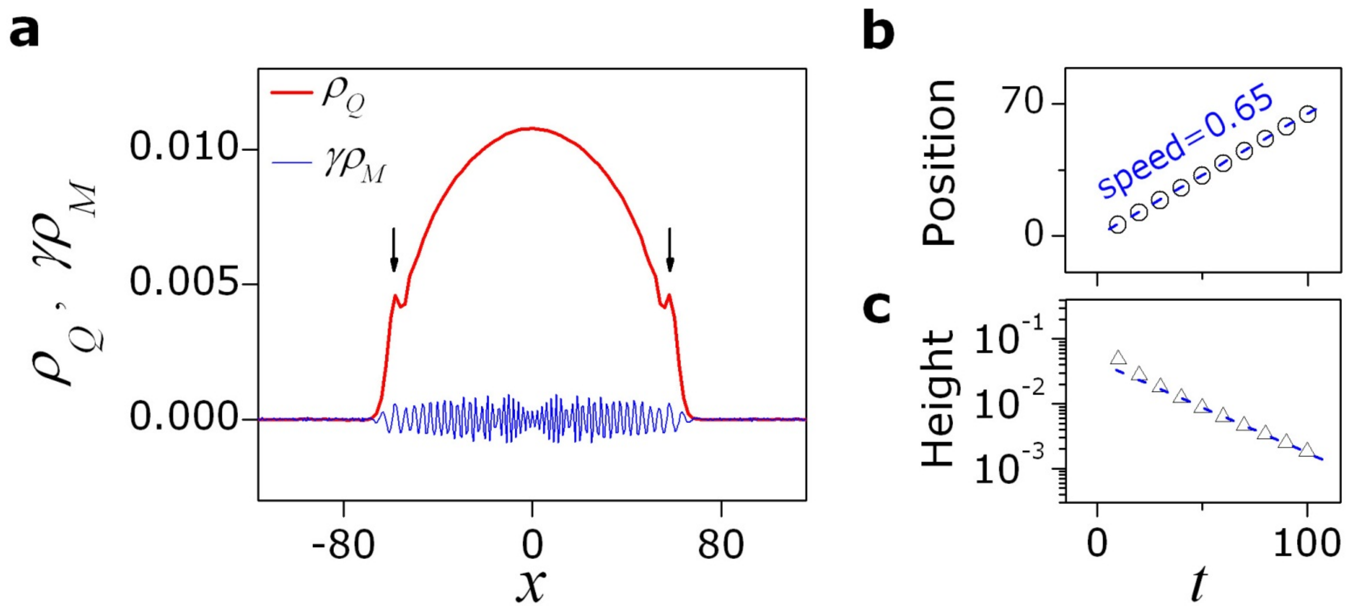


Move at a supersonic speed and decay in power-law;

They may be the long lived heat waves.

Discussion: Heat wave in short-time scale

φ^4 Lattice



Moves at a 2/3 sound speed, decays exponentially.

Discussion: connection to heat conduction

Can we establish the universal connection between heat conduct and energy diffusion?

No!

(1) By definition, they are different quantities

$$q(\mathbf{r},t) = e(\mathbf{r},t) - \left(\frac{e+P}{\rho}\right)\rho(\mathbf{r},t)$$

(2) Practically, we have shown that energy diffusion may have any connection to that of heat in the case of the gas model

Discussion: connection to heat conduction

It has been found that the heat conductivity of 1D momentum conserved systems goes as:

$$\kappa \sim L^{\alpha}$$

It has been declared that the energy in these systems diffuse as:

$$\left\langle x^2(t) \right\rangle \sim t^{\beta}$$

Tow formula connecting the exponents are presented

$$\beta = \alpha - 1$$

B. Li and J. Wang, Phys. Rev. Lett. 91, (2003)

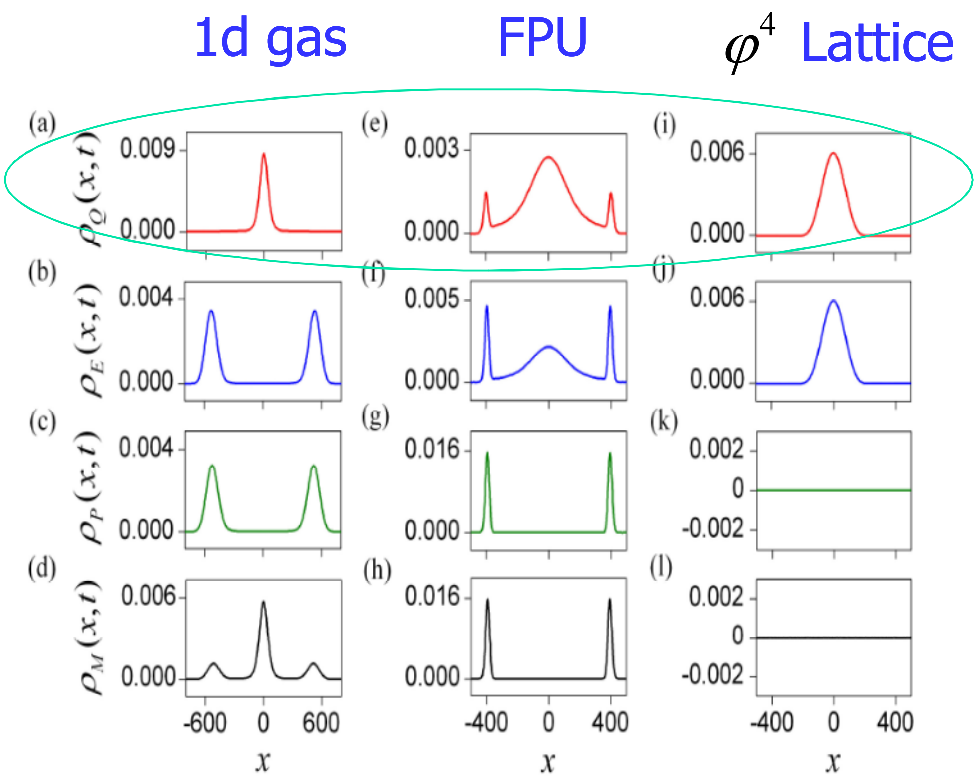
$$\beta = 2 - 2/\alpha$$

S. Denisov et. al. Phys. Rev. Lett. 91, (2003

P. Cipriani, S. Denisov and A. Politi, Phys. Rev. Lett. 94, (2005); B. Li, J. Wang, L. Wang and G. Zhang, Chaos 15, (2005); H. Zhao, Phys. Rev. Lett. 96, (2006); L. Delfini, at.al, Eur. Phys. J. Special Topics 146, (2007)

Discussion: connection to heat conduction

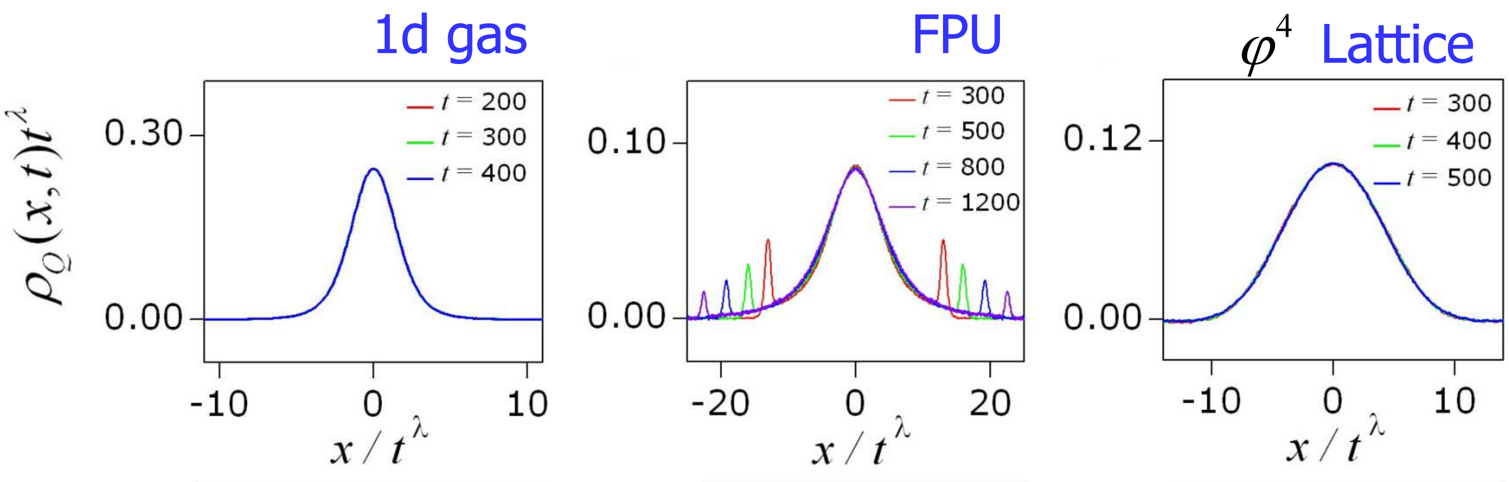
Connection between the heat diffusion
and heat conductivity may exist



$$\langle x^2(t) \rangle \sim t^{\beta}$$

Discussion: connection to heat conduct

The function $\rho_Q(x,t)$ is invariant upon rescaling $x \to t^{\lambda} x$



→ $\beta = 2\lambda = 1.176,\ 1.201, 1.000$

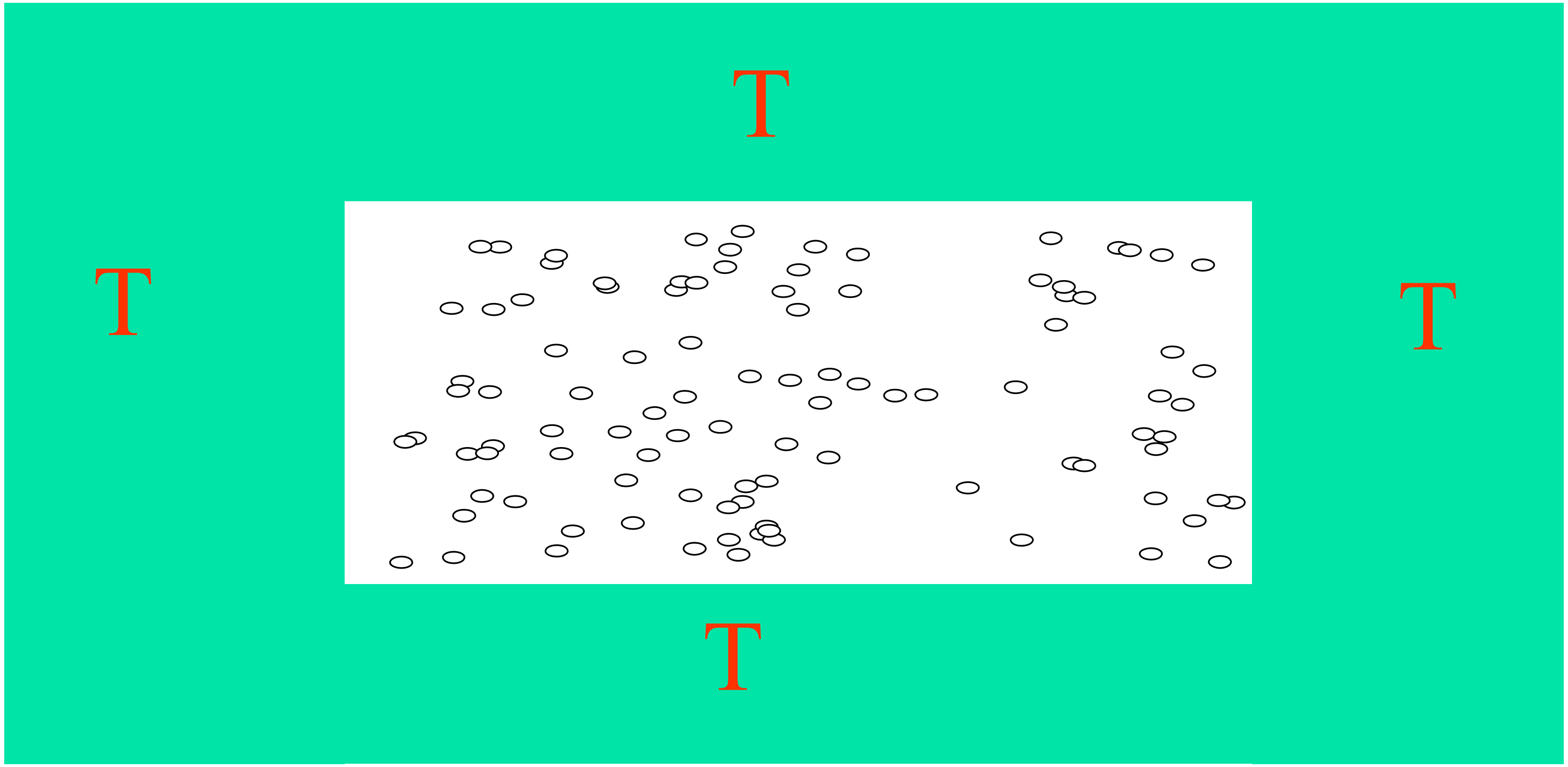
→ $\beta = \alpha - 1$

$\beta = 2 - 2/\alpha$ √

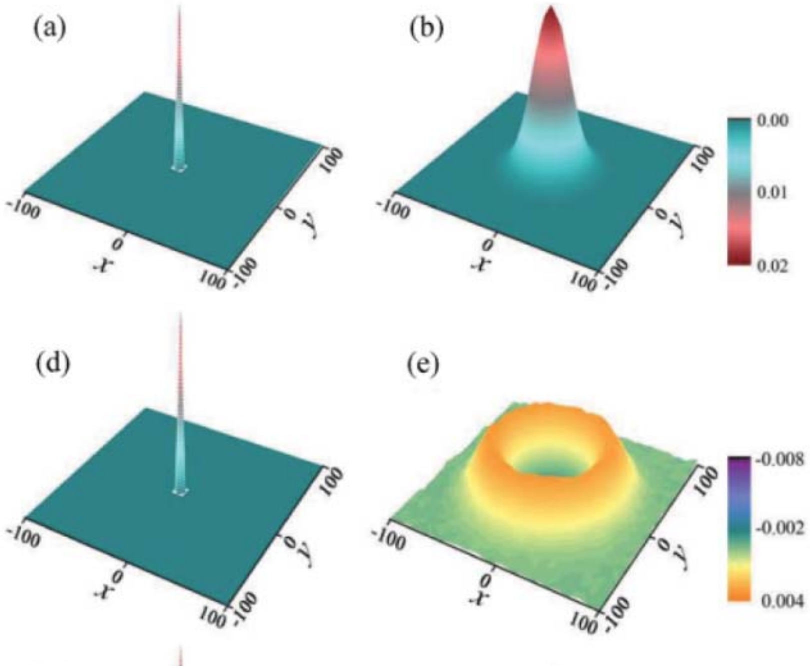
S. Chen, Y. Zhang, J. Wang and H. Zhao, arXiv:1106.2896v2

Discussion: Two-dimensional systems:

2D Gas with L-J potential



Discussion: Two-dimensional systems:

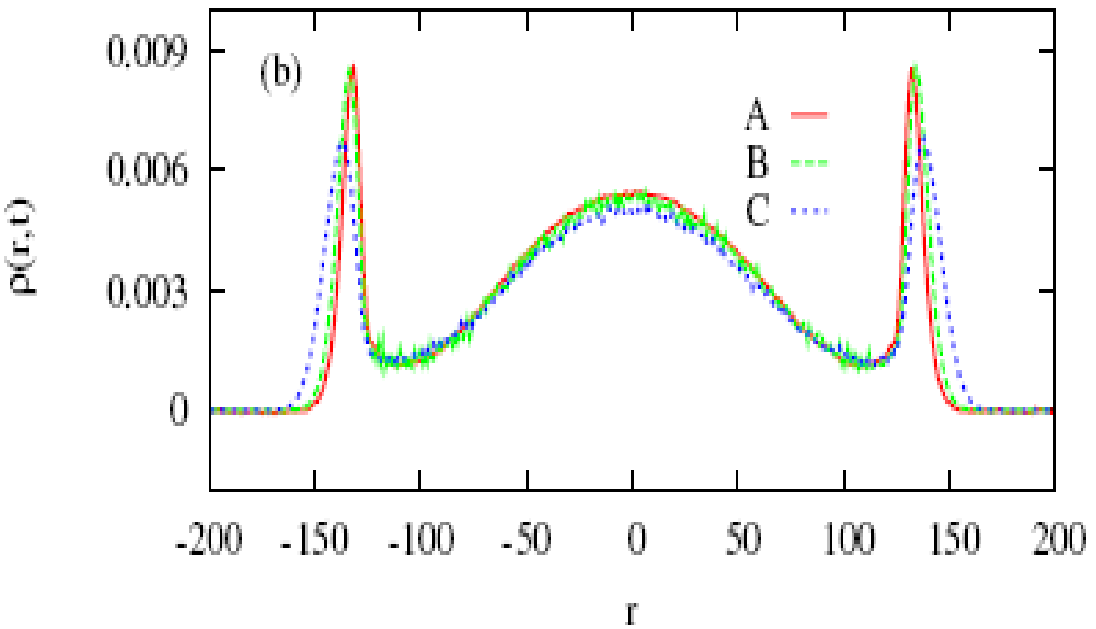


Diffusion of a particle

Diffusion of the energy and momentum

J.H. Yang *et al*, PRE 83, 052104 (2011)

Check of the FDR

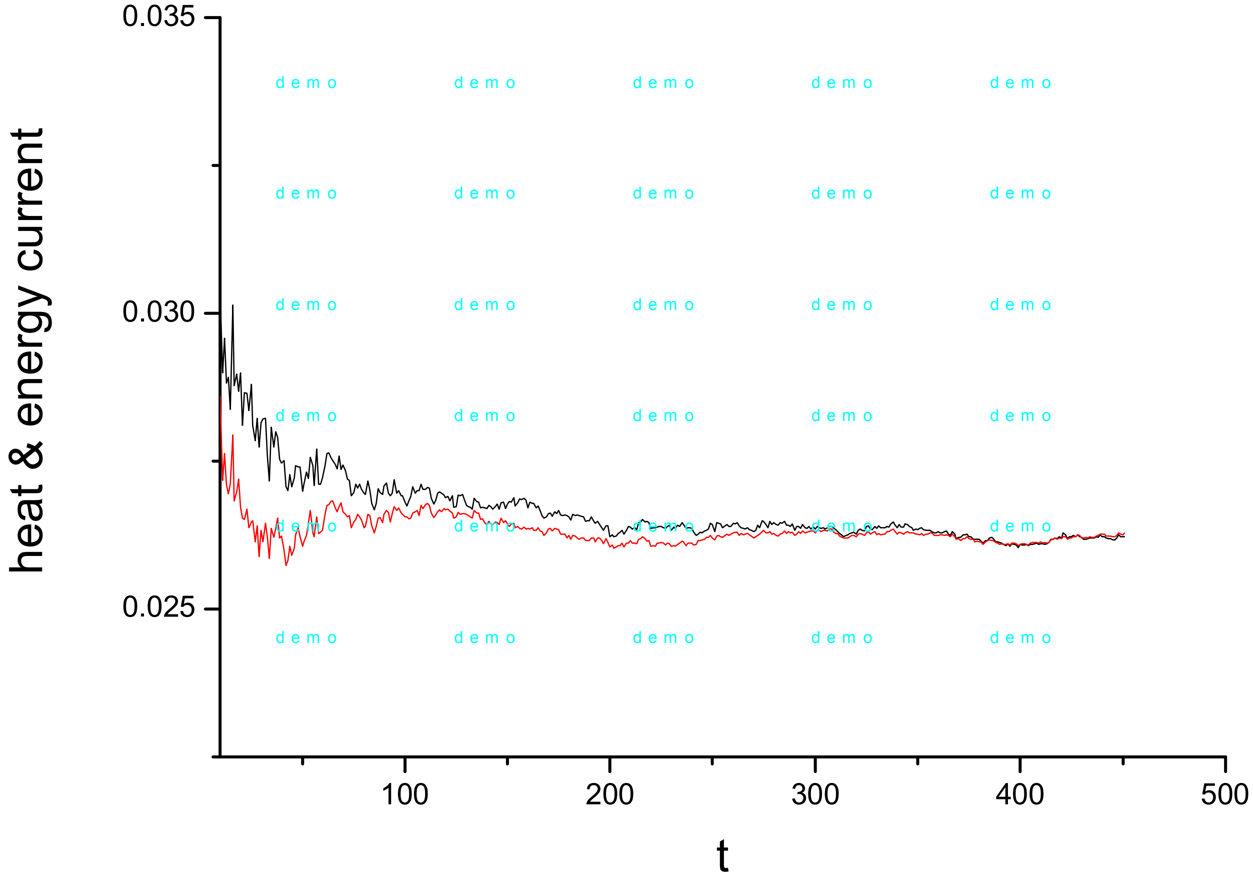


A: equilibrium method

B &C: nonequilibrium method, B: δH=5E C: δH=2E

P Hwang and H Zhao, arXiv:1106.2866v1;

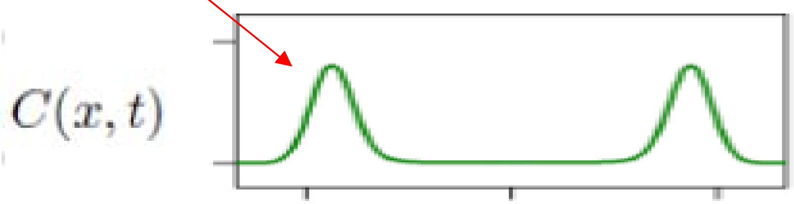
The heat and energy flux in 1D gas model



Discussion: diffusion of the local-flux fluctuations and how to approach the autocorrelation function of the global flux

$$C(x,t) = < j_n(0) j_m(t) >$$

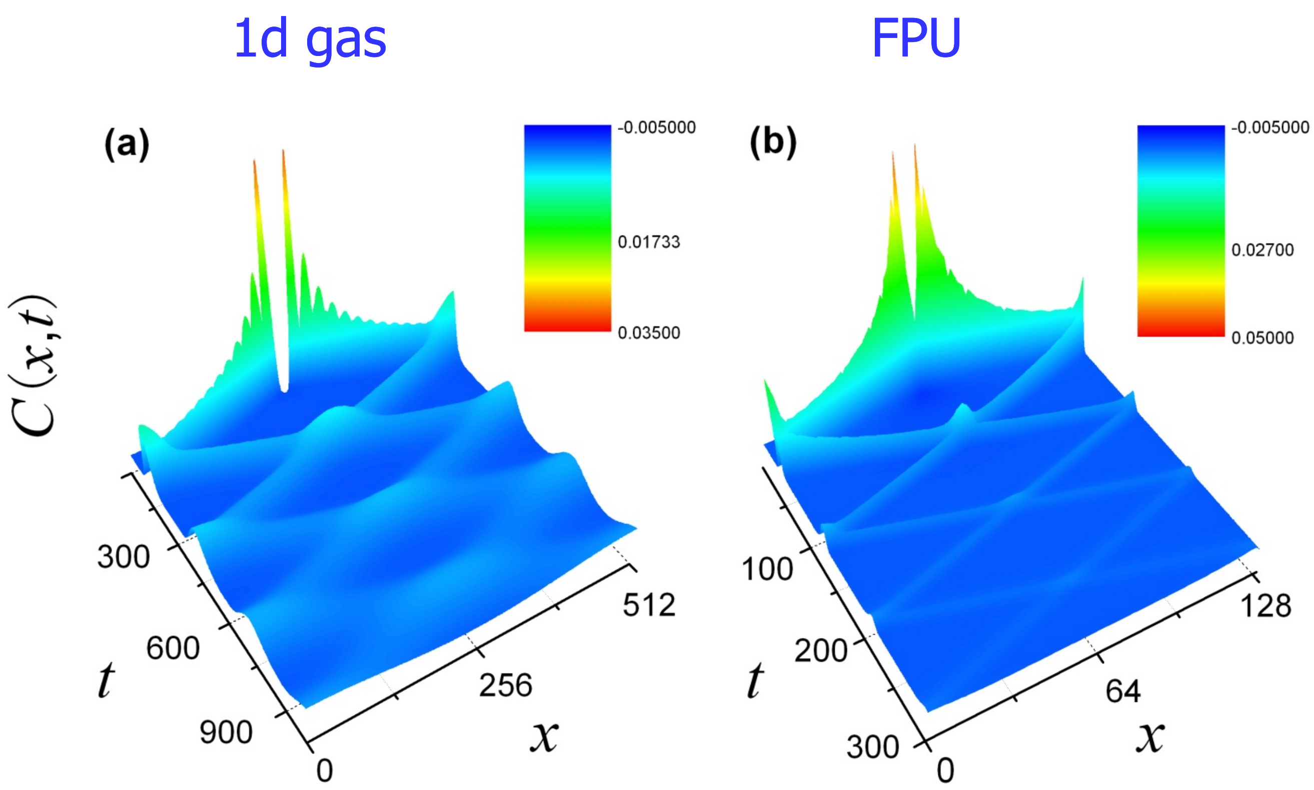
The area decay with time



1d gas FPU φ^4 Lattice

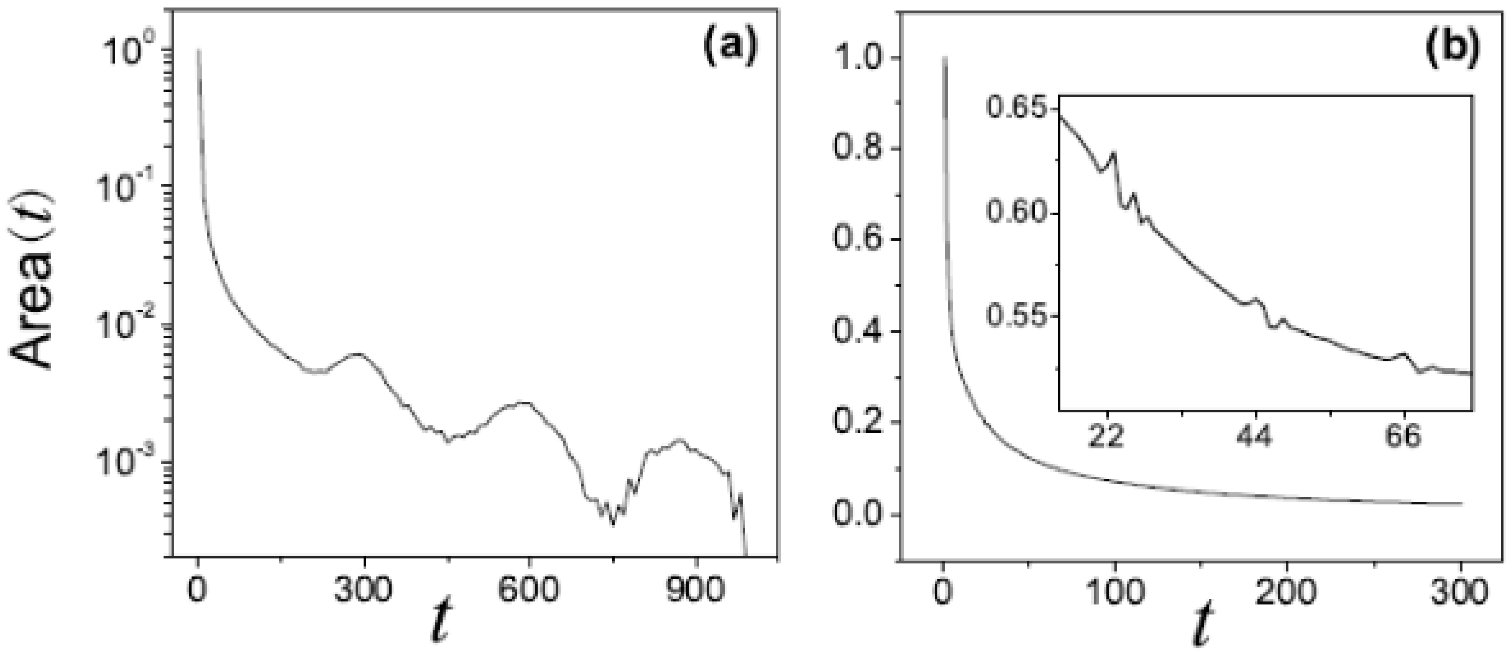
Diffusion:

The diffusion of local-flux fluctuations in systems with periodic boundary conditions



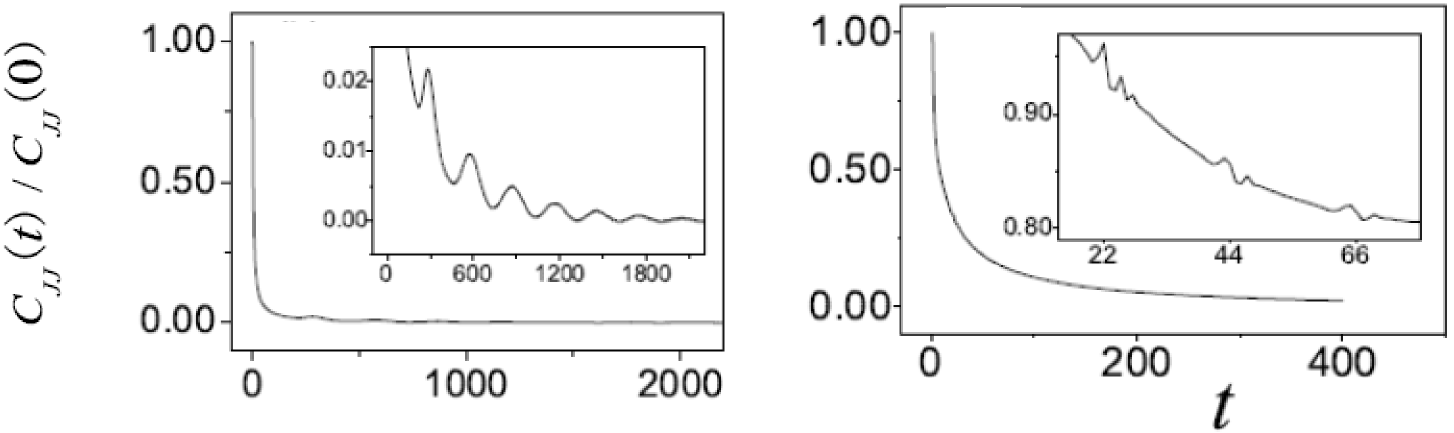
Diffusion:

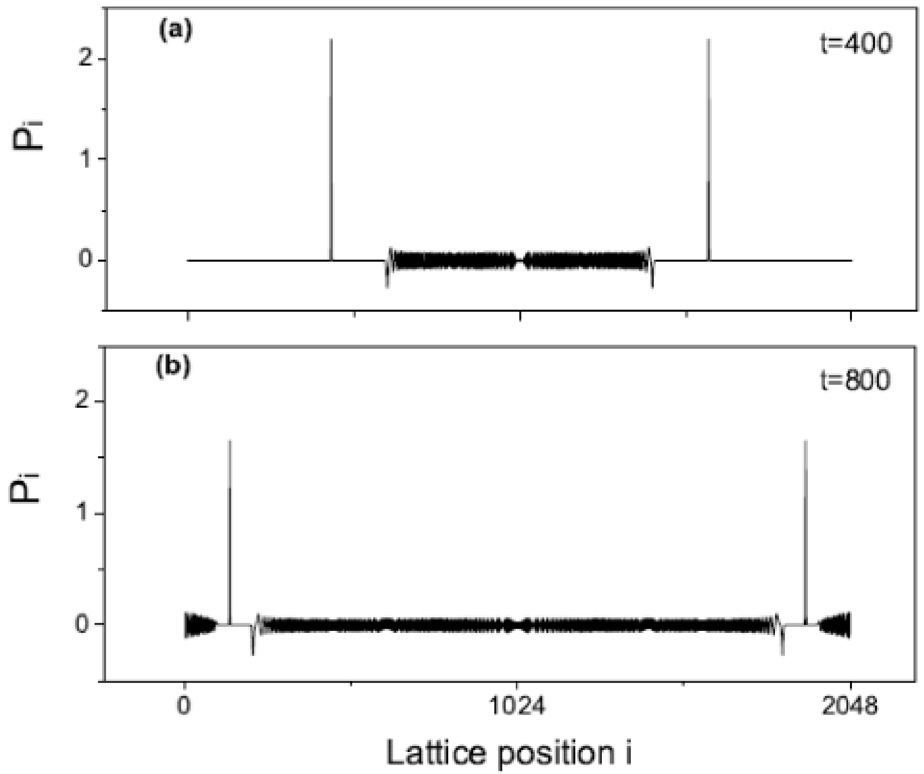
The area decays as a function of time



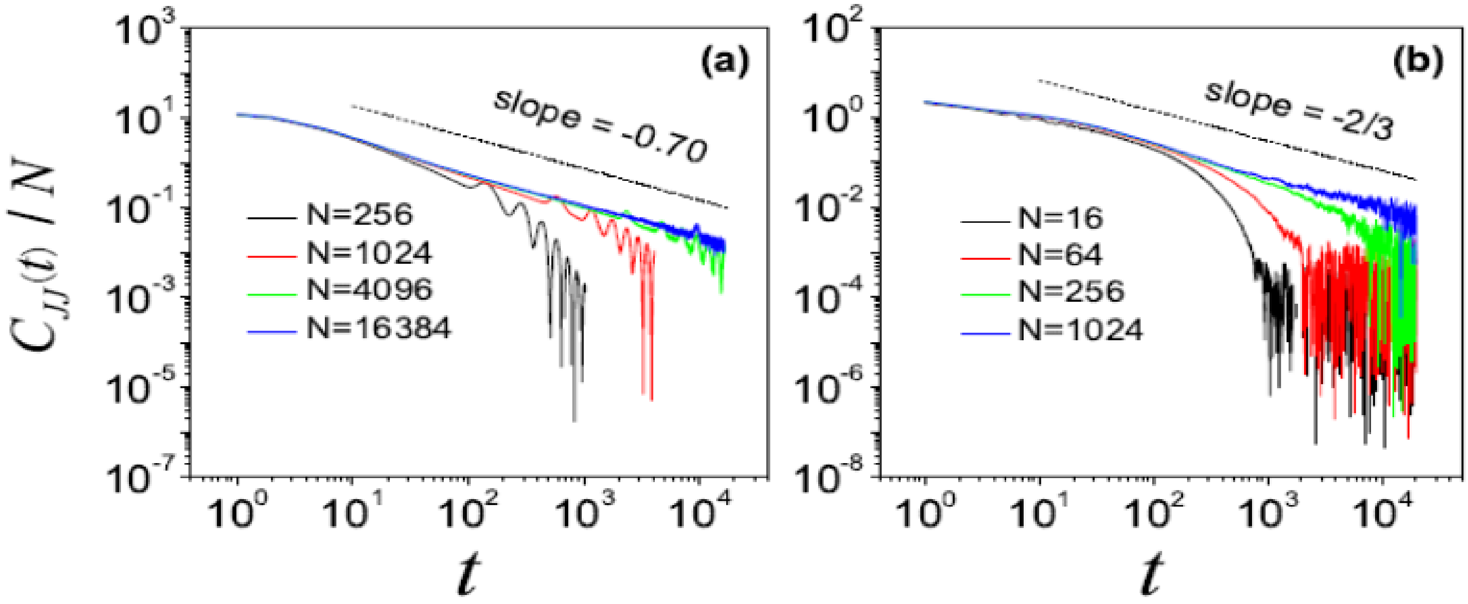
Diffusion:

Periodic behavior of the autocorrelation function of the global flux.




(a)
t=400
P_i
2
1
0
(b)
t=800
P_i
2
1
0
0
1024
2048
Lattice position i

Diffusion:



The autocorrelation function of the global flux is reliable only for

$$t \leq \frac{L - l}{2v}$$

L:system size, l: the width of the peaks,
v: the speed of the peaks

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

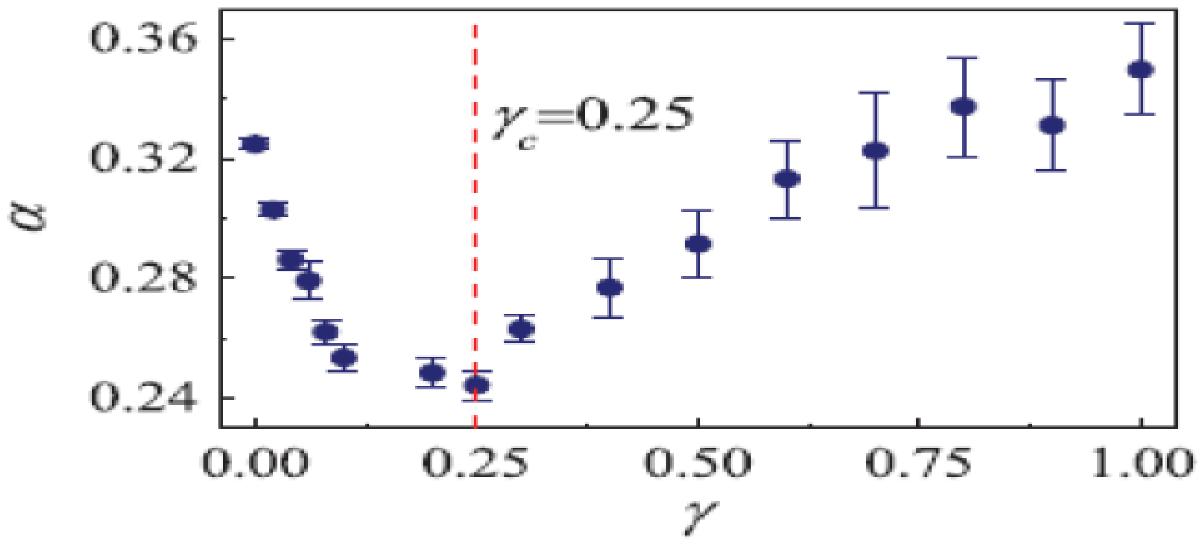


Fig. 5 The dependence of α on the parameter γ [4].