Iran-2015/4/15

Transport and diffusion in Low-D system:
First part—transport behavior
Relaxation of current fluctuations in low-dimensional momentum conserving systems：Power-law decay or exponential decay?

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Outline

1. **Relax behavior of current fluctuations—the role of asymmetric interaction potential**
   (a) Background
   (b) Results
   (c) Mechanism
   (d) Conclusion & Discussion
2. **Relax behavior of densities fluctuations— relation to curren decay**
   (a)Background
   (b)Results
   (c)Discussion

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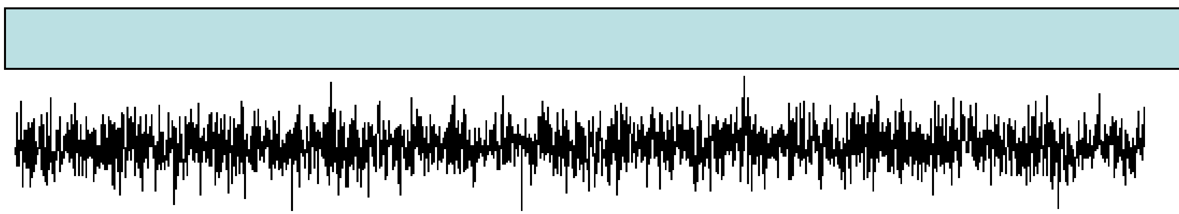
Background

Problem

Equilibrium system with temperature T:



temperature fluctuations

current fluctuations

$J(t)$

$$C(t) = < J(t) J(0) >$$

$$C(t) \sim e^{-\gamma t} \quad \textbf{or} \quad C(t) \sim t^{-\beta}$$

The non-equilibrium transport coefficients can be calculated by the Green-Kubo formula:

$$\kappa = \lim_{\tau\to\infty} \lim_{L\to\infty} \frac{1}{2k_B T^2}\int_0^{\tau} C(t)dt$$

$$C(t) \sim \mathrm{e}^{-\gamma t} \to \kappa = \text{constant}$$

$$C(t) \sim \mathrm{t}^{-\gamma} \to \kappa \sim \text{infinite } if \;\; \gamma < 1$$

$$C(t) \sim \mathrm{t}^{-\gamma} \Longrightarrow \kappa = \frac{1}{2k_B T^2}\int_0^{\tau} C(t)dt, \tau = \frac{L}{v} \Longrightarrow \kappa \sim L^{1-\gamma}$$

J.Stat.Mech.P02007(2007)

- **Before 1970** it assumes correlation function decays rapidly (i.e., exponentially) as

$$C(t) =< J(t)J(0) > \sim e^{-\gamma t}$$

- **After 1970**, Alder & Wainwright numerically evidenced the 'long time tail' , now, it is actually believed that the current correlation should decay in a power-law manner

$$C(t) =< J(t)J(0) > \sim t^{-\gamma}$$

for momentum-conserving systems.

B. J. Alder and T. E. Wainwright, Phys. Rev. Lett. 18, 988 (1967); J. R. Dorfman, E. G. D. Cohen, Phys. Rev. Lett. 25, 1257 (1970); M. H. Ernst, E. H. Hauge, and J. M. J. van Leeuwen, Phys. Rev. Lett. 25, 1254 (1970); S. Lepri, et.al, Physics Reports 377, 1 (2003); O. Narayan et.al, Phys. Rev. Lett. 89, 200601 (2002); J. P. Hansen et.al, Theory of Simple Liq-uids, 3rd ed. (Academic, London, 2006).

Hydrodynamic approach by momentum, energy, particles conservation

$$C(t) = < J(t)J(0) > \sim t^{-\gamma} \quad with\ \gamma = \begin{cases} \frac{1}{2} & (1D) \\ 1 & (2D) \\ \frac{3}{2} & (3D) \end{cases}$$

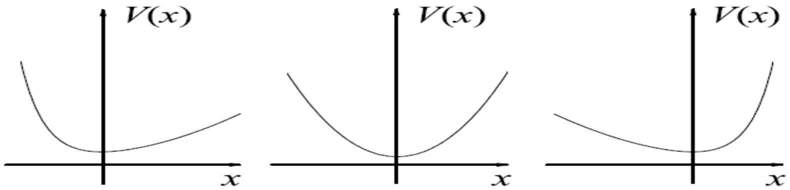
$$\begin{cases} \kappa = L^{0.5} & (1D) \\ \kappa = \ln(L) & (2D) \\ \kappa = \text{constant} & (3D) \end{cases}$$

Livi R, Lepri S. Nature, 2003, 421: 327

Approaches by considering inter-particle interactions

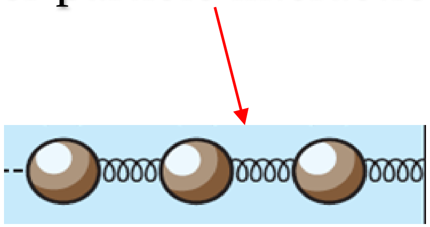
Recent theories predict that for heat current correlation it has

$$C(t) = < J(t)J(0) > \sim t^{-\gamma}$$



$$\gamma = \begin{cases} 2/3 & \text{for asymmetric potential} \\ 1/2 & \text{for symmetric potential} \end{cases}$$

Inter-particle interaction



L. Delfini, S. Lepri, R. Livi, A. Politi. J Stat Mech, P02007 (2007).
H. van Beijeren. Phys Rev Lett, 108, 180601 (2012).
H. Spohn, PRL (2014)

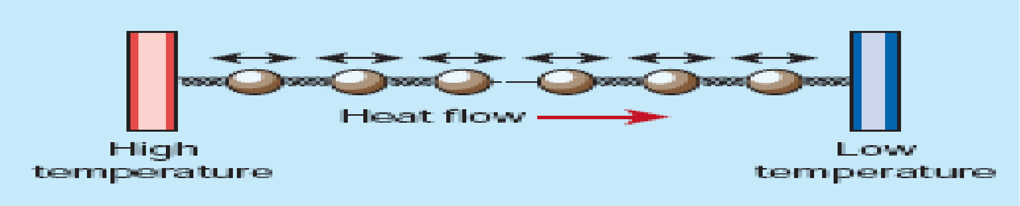
Another line of heat conduct study

1808 **Fourier's Law:**

$$J = \kappa \frac{dT}{dx}$$

The micro-mechanism of this law?

A Challenge to Theorists, F. Bonetto, J. L. Lebowitz, and L. Rey-Bellet, *Mathematical Physics* (Imperial College Press, London 2000)



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

1967: The exact solution for harmonic lattice

[Z. Rieder, J. L. Lebowitz, and E. Lieb, *J. Math. Phys.*8, 1073 (1967).]

$$T = \frac{T_+ + T_-}{2}, \text{ J is a constant, } \kappa \sim L,$$

1984：*ding-a-ling* model Chaos may responsible to the law

[G. Casati *et al*., *Phys. Rev. Lett*. 52, 1861 (1984)]

κ is a constant

1997： Fermi-Pasta-Ulam（FPU）model, it is chaotic, but the thermal conductivity diverges with the system size

[S. Lepri *et al. Phys. Rev. Lett*. 78, 1896 (1997)]

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

1998: ϕ^4 model, κ is a constant

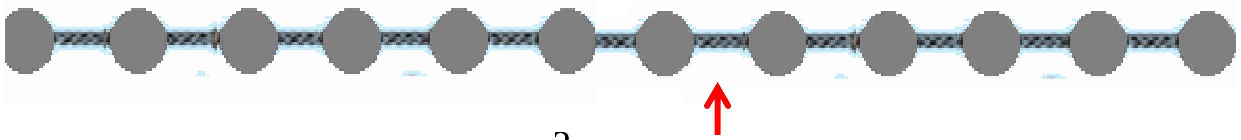
$$\begin{cases} \text{momentum conservating systems } \kappa \sim L^{\delta} \\ \text{momentum non-conservating systems } \kappa \sim \text{constant} \end{cases}$$

B.B. Hu, B.W. Li and H. Zhao, *Phys. Rev. E* 57, 2992(1998)

for momentum conservating 1D systems $\Rightarrow \kappa \sim L^{\delta}$

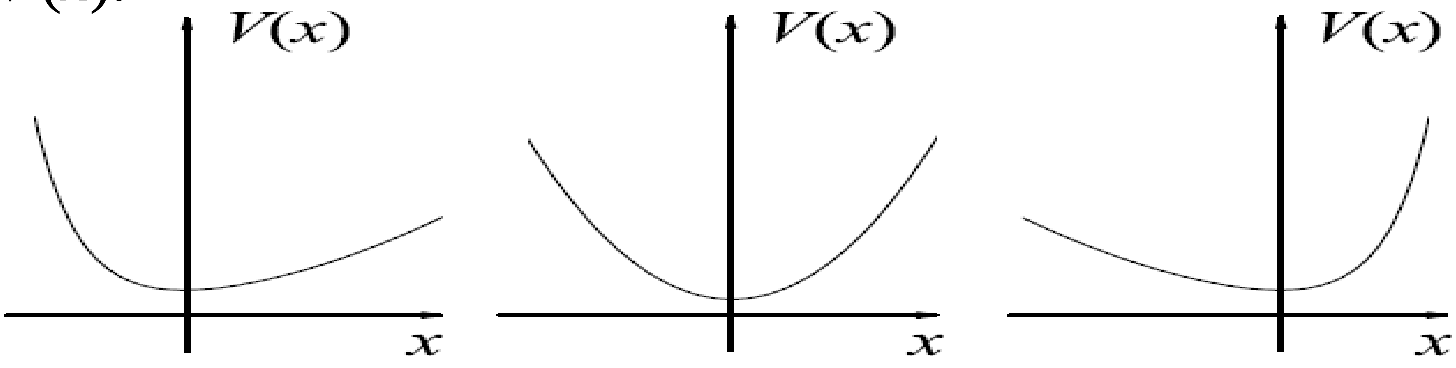
1D lattice models and the symmetry of potential

L=Na=N



$$H = \sum \frac{p_i^2}{2m} + V(x_{i+1} - x_i)$$

$V(x)$:



Thermal expansion　　null thermal expansion　　negative thermal expansion

Heat and energy

$$\frac{\partial}{\partial t}[e(x,t) - \frac{(e+P)\rho(x,t)}{\rho}] + \frac{\partial}{\partial x} j^q(x,t) = 0,$$

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

Basically they are conceptually different quantities

The local heat current and local energy current:

$$j_i^q(t) = j_i^e(t) - \frac{(e+P)}{\rho}\rho_i(r,t)v_i$$

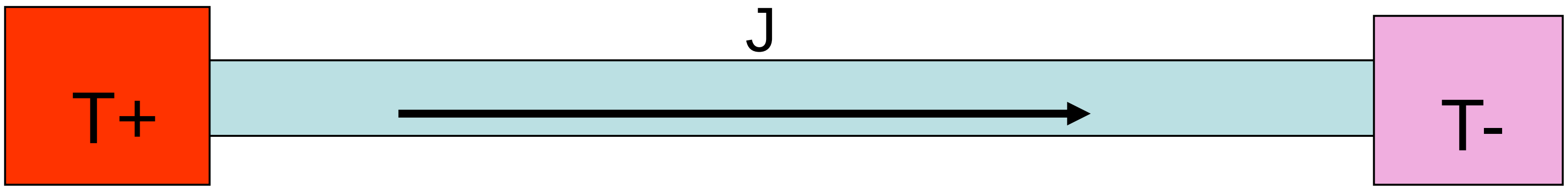
$$J^q(t) = J^e(t)$$

Two ways to calculate the thermal conductivity

Equilibrium simulation:

$$\kappa = \lim_{\tau\to\infty} \lim_{L\to\infty} \frac{1}{2k_B T^2}\int_0^{\tau} C(t)dt, \quad \tau = \frac{L}{v}$$

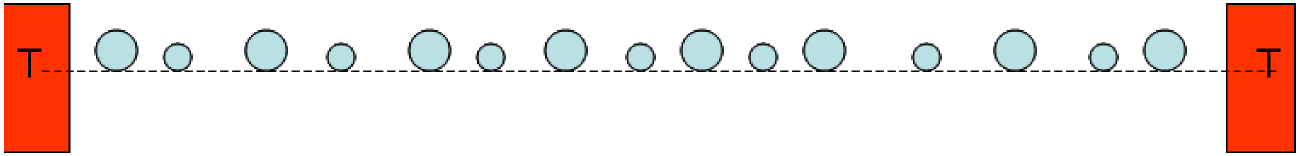
Non-equilibrium simulation:



$$J = \kappa(L)\frac{dT}{dx}$$

Models consistent to theoretical prediction

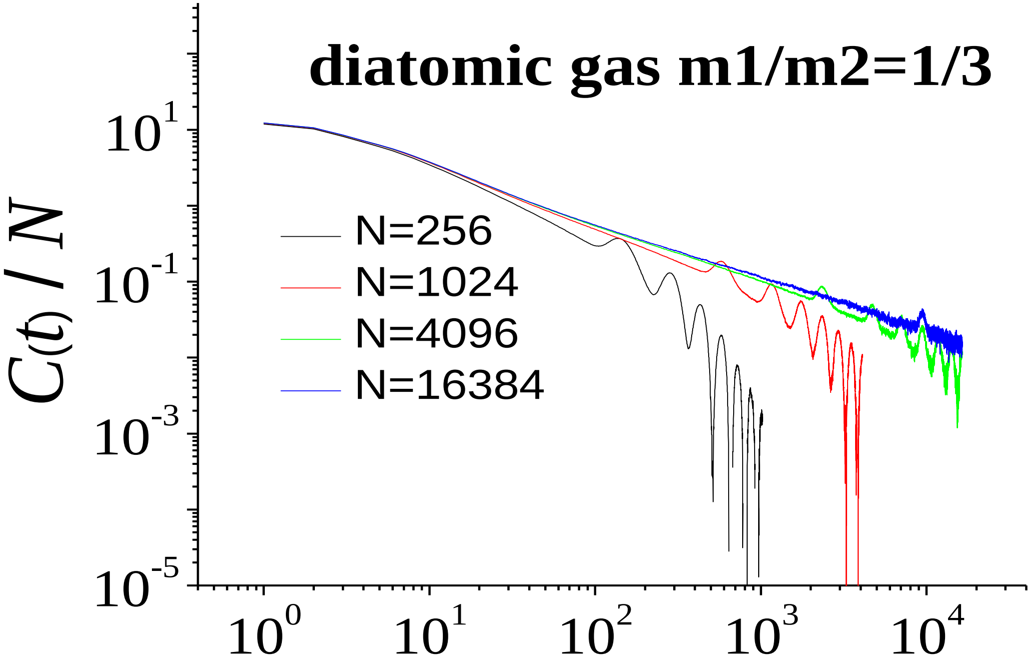
（a） 1D gas with alternative masses (asymmetric, m1/m2=1/3)



(b) The FPU $-\beta$ model (symmetric)

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

Finite-size effect in calculating the current autocorrelation



$$\tau \le \frac{L - l}{2v}$$

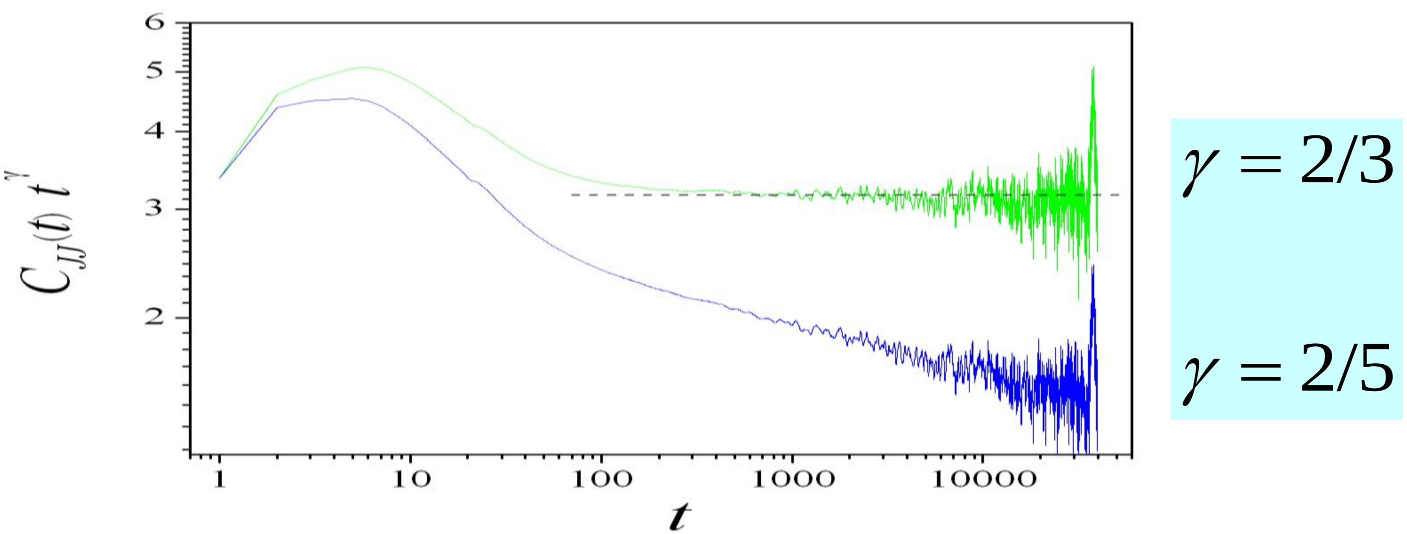
S. Chen et. al, Phys. Rev. E 87, 032153 (2014).

Models consistent to theoretical prediction

（1） 1D gas with alternating masses

$$C(t) = < J(t)J(0) > \sim t^{-\gamma}$$

simulation size	L	4096	8192	16384	32768	65536
gas model($t_0 = 100$)	γ	0.725	0.699	0.683	0.679	0.672
gas model($t_0 = 1000$)	γ	0.762	0.704	0.691	0.681	0.675



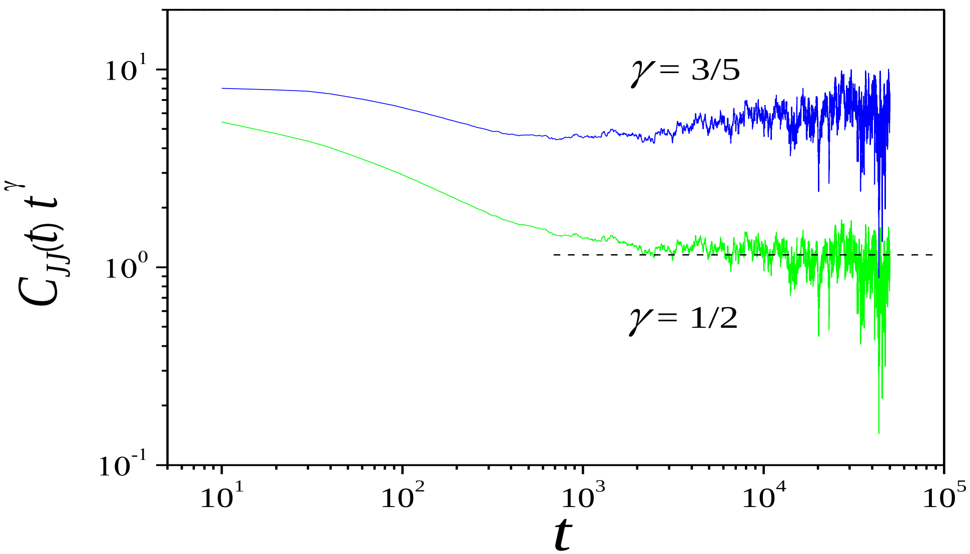
S. Chen et. al, Phys. Rev. E 87, 032153 (2014).

Models consistent to theoretical prediction

(2) The FPU $-\beta$ model

$$C(t) = < J(t)J(0) > \sim t^{-\gamma}$$

Simulation size	L	4096	8192	16384	32768	65536
FPU (t_0=1000)	γ	0.628	0.611	0.578	0.546	0.522
FPU (t_0=2000)	γ		0.565	0.583	0.532	0.518



L=131072

S. Chen et. al, Phys. Rev. E 87, 032153 (2013).

For 1D momentum-conserved systems, at present, it is actually believed that the current correlation should decay in the power-law manner, and resulting in a divergent thermal conductivity

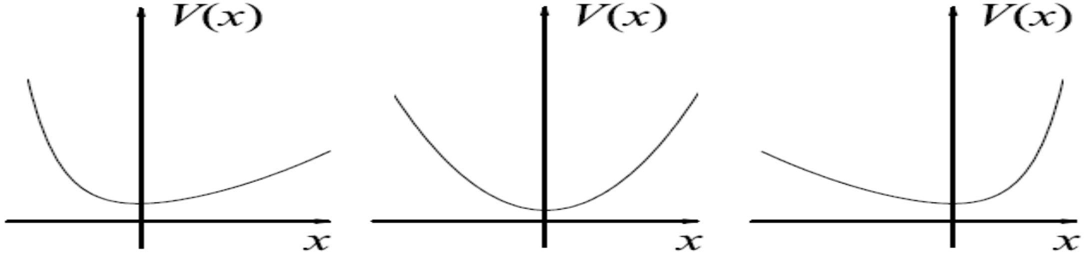
L. Delfini, S. Lepri, R. Livi, A. Politi. J Stat Mech, P02007 (2007).
H. van Beijeren. Phys Rev Lett, 108, 180601 (2012).
H. Spohn, PRL (2014)

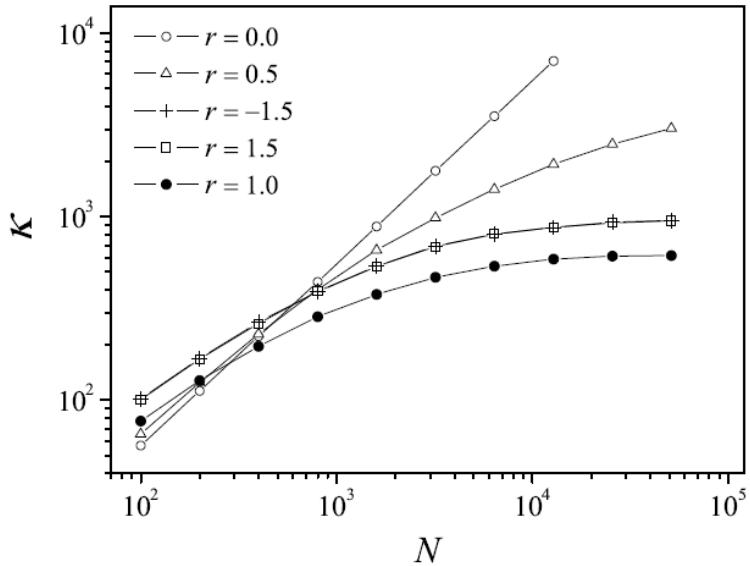
Results

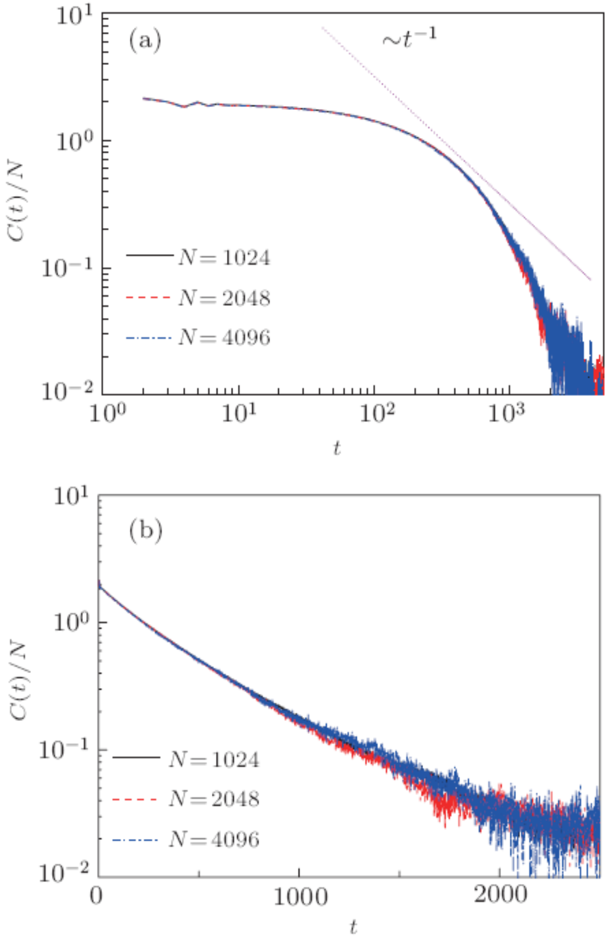
(1) Models inconsistent to theoretical predictions
(2) Asymmetric potential can make difference
(3) Why violates the theoretical predictions

A Challenge to this common belief

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





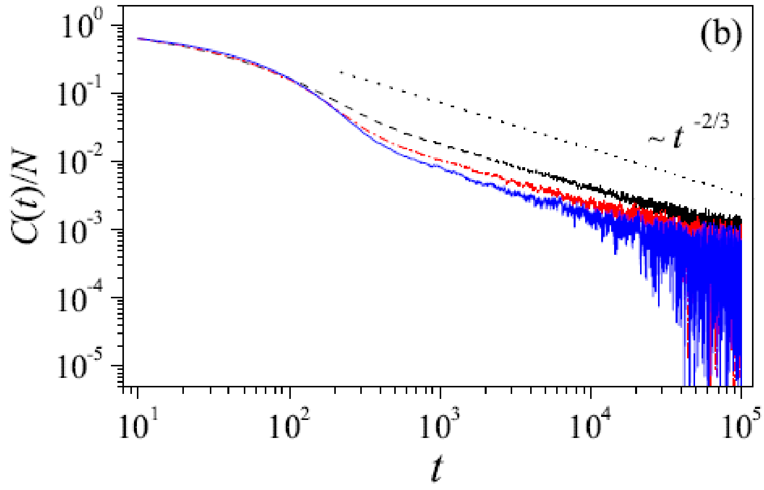


Y. Zhong Y. Zhang, J. Wang and H. Zhao, PRE 85, 060102(R) (2012)

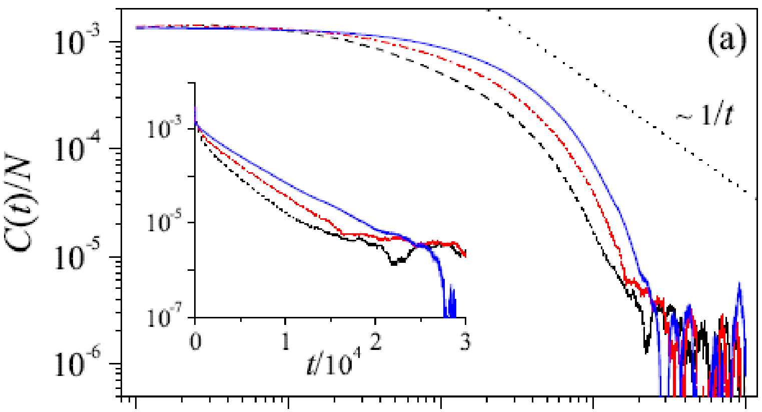
Models in contradiction with predictions

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

$\alpha = 0.5, \quad 1, \quad 1.5$



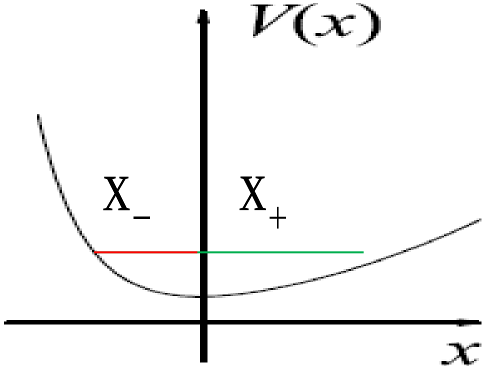
High temperature T=0.4



Low temperature
T=0.01

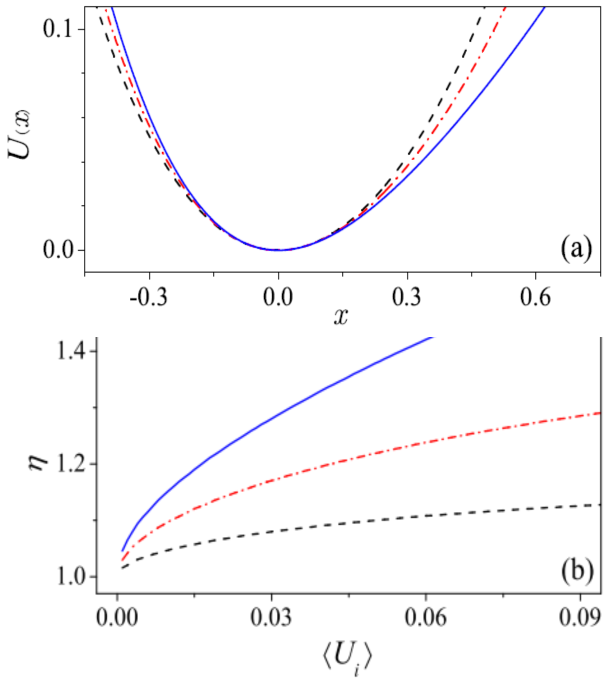
S. Chen Y. Zhang, J. Wang and H. Zhao,
arXiv:1204.5933(2012)

The asymmetry degree of potentials



$$\eta = \frac{x_+ - |x_-|}{x_+ + |x_-|} \quad ? \quad \text{no!}$$

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



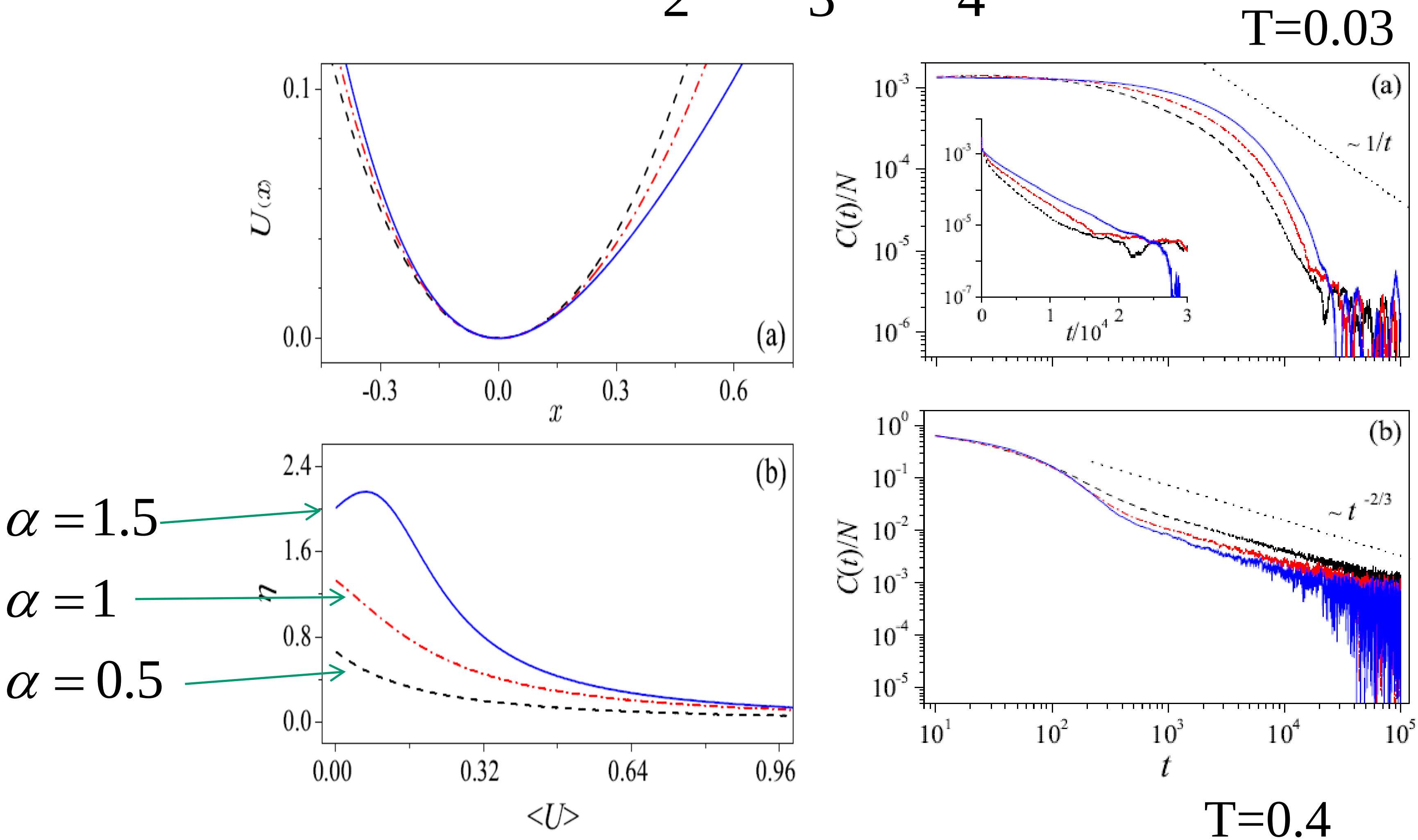
Asymmetry degree:

$$\eta \equiv \frac{d}{d\langle U \rangle}(x_+ - |x_-|)$$

Corresponding to the thermal expansion rate

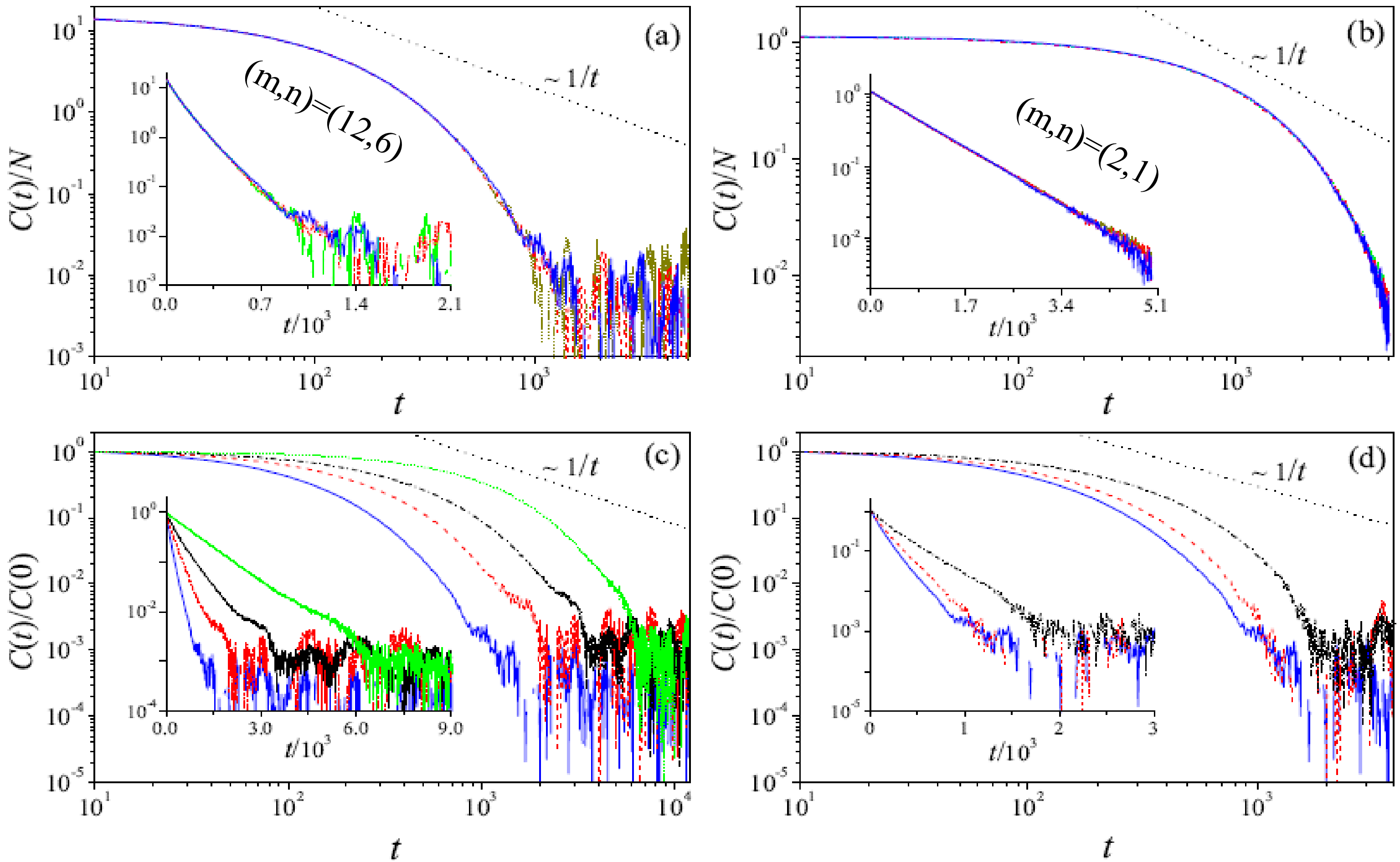
Correlation to the asymmetry degree

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



Models in contradiction with predictions

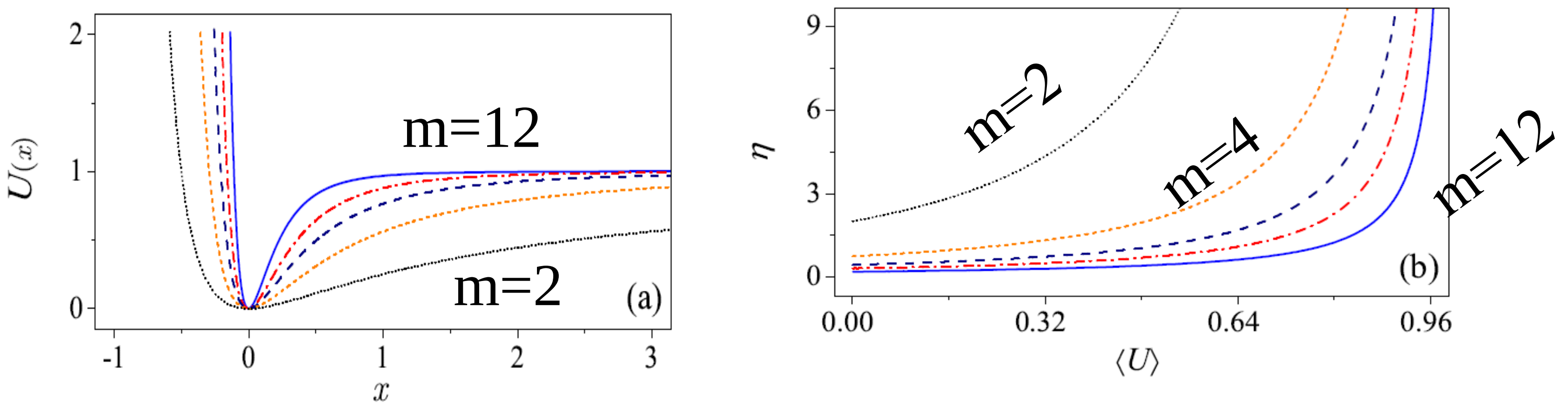
(b) L-J model: $V(x)=[(\frac{x_c}{x+x_c})^m-2(\frac{x_c}{x+x_c})^n+1]$



S. Chen Y. Zhang, J. Wang and H. Zhao, arXiv:1204.5933(2012)

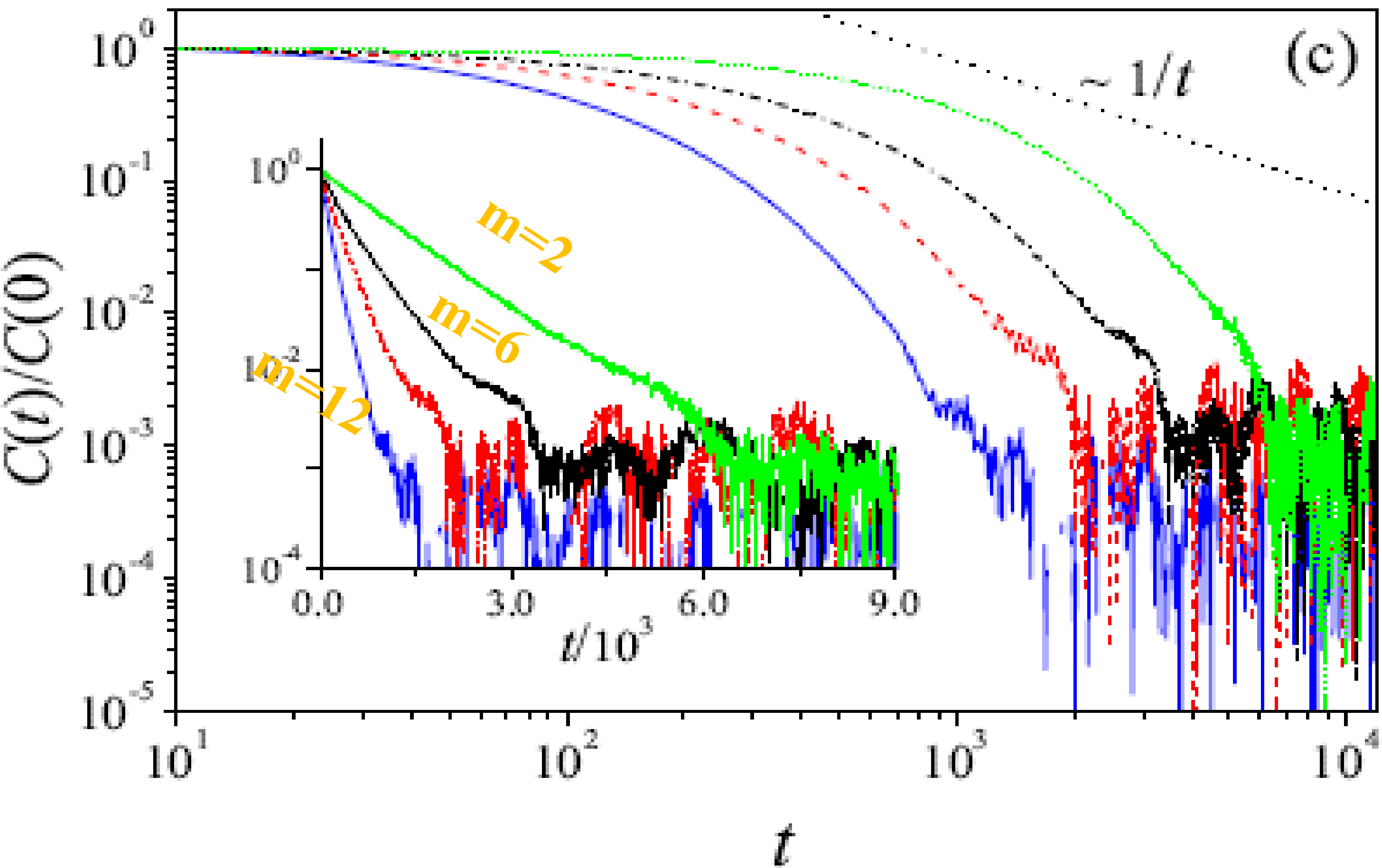
Correlations with the asymmetry degree of potentials

$$V(x)=[(\frac{x_c}{x+x_c})^m-2(\frac{x_c}{x+x_c})^n+1]\quad m=2,\ 4,\ 6,\ 8,\ 12$$



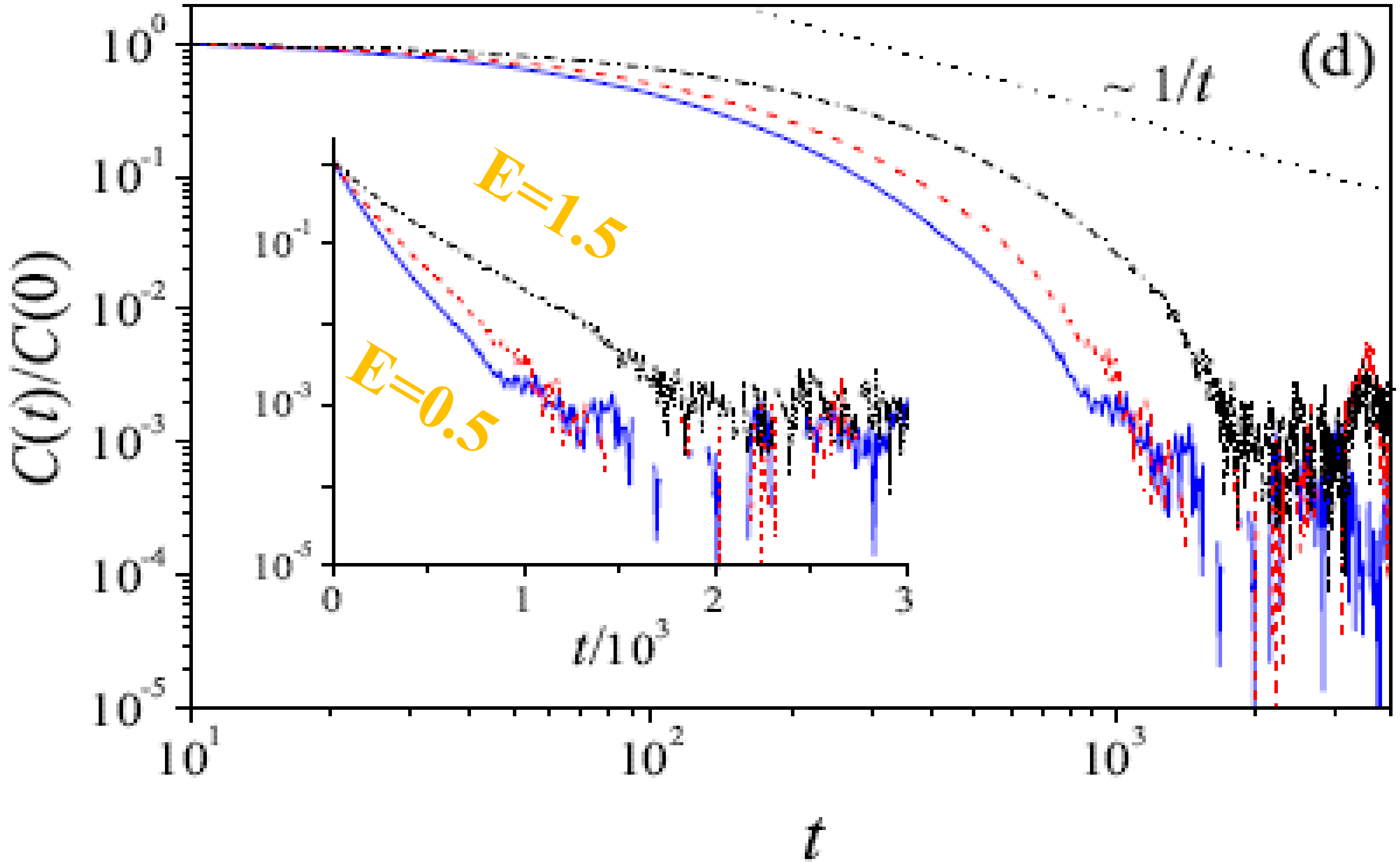
$$\eta(2)>\eta(4)>\eta(6)>\eta(8)>\eta(12)$$

Correlations with the asymmetry degree of potentials



m=12,8,6,2 (from bottom to top) with N=16384 and E=0.5

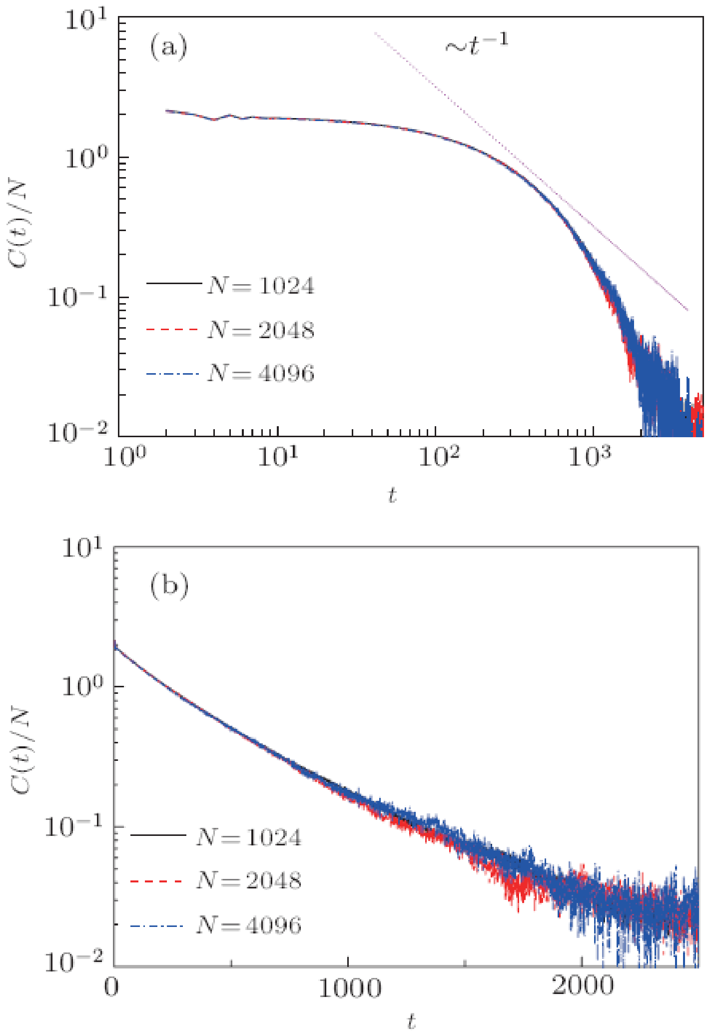
Correlations with the asymmetry degree of potentials

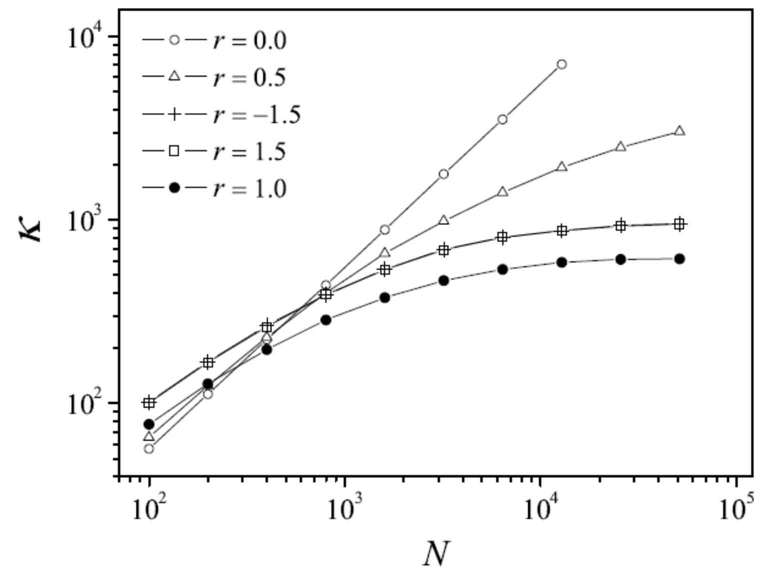


E=0.5, 1, 1.5 (from bottom to top) with N=16384 and m=12

Models in contradiction with predictions

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

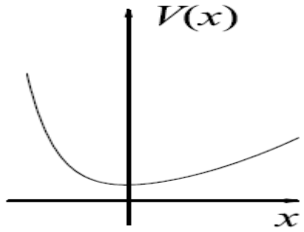


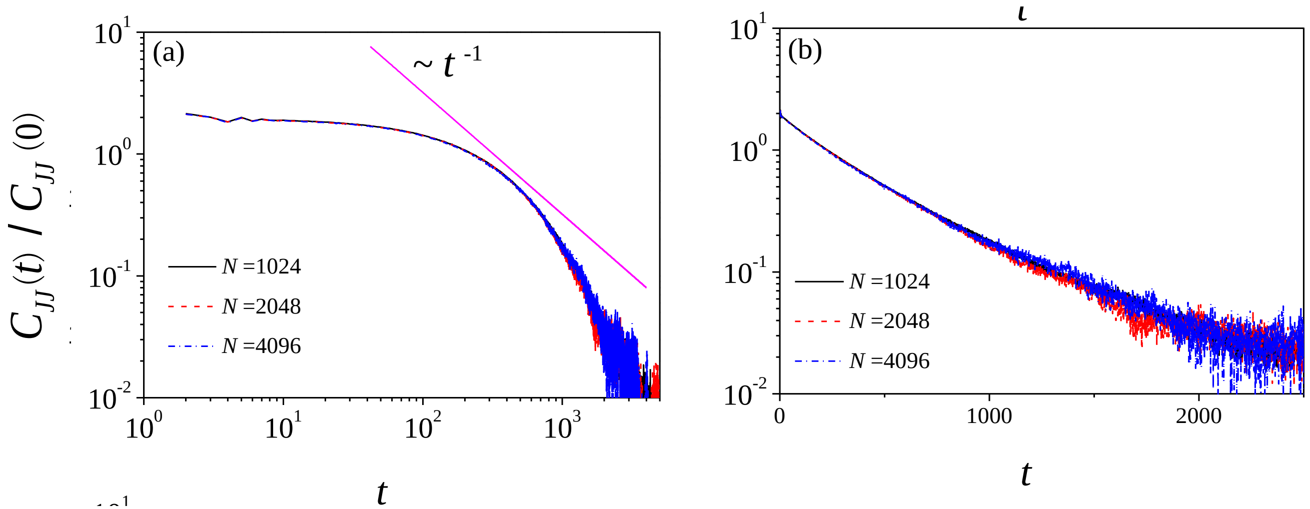


Y. Zhong Y. Zhang, J. Wang and H. Zhao, PRE 85, 060102(R) (2012)

Models in contradiction with predictions

(d) $V(x)=\begin{cases}0.5(1+r)x^2 & x<0\\ 0.5(1-r)x^2 & otherwise\end{cases}$

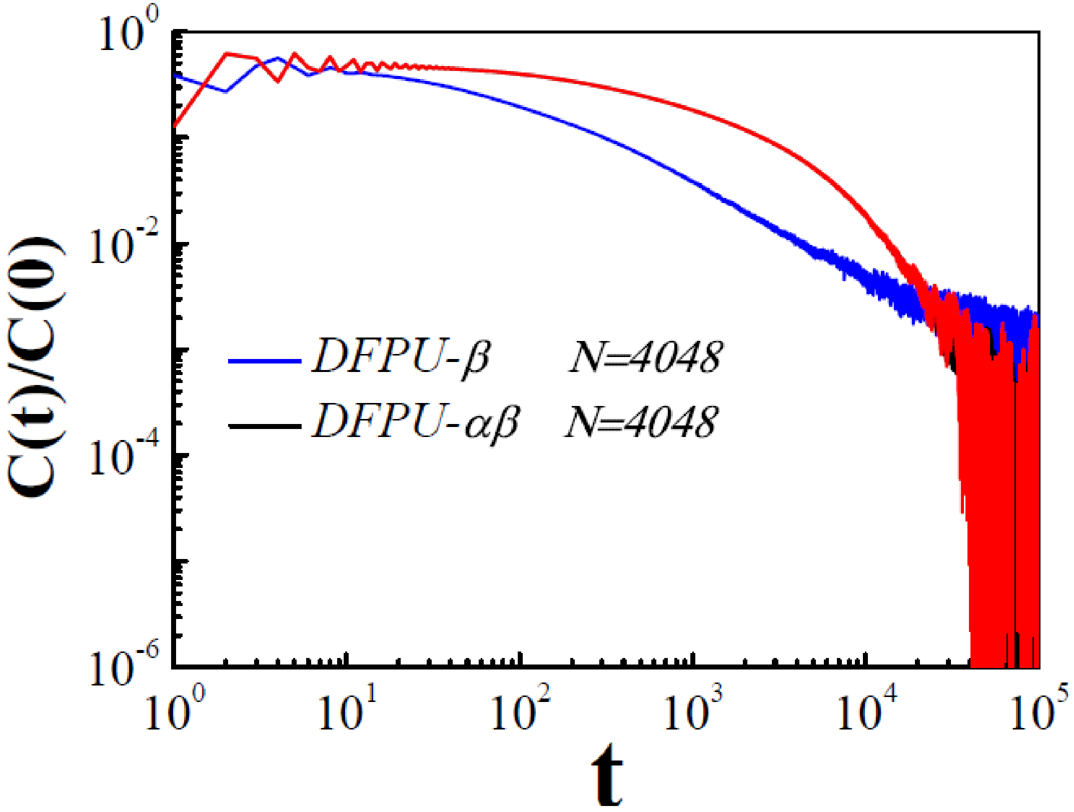




Y. Zhong, Y. Zhang, J. Wang and H. Zhao
Chin. Phys. B 22, 070505(2013)

Models in contradiction with predictions

$$\text{(e): Disordered FPU}-\alpha\beta \text{ model}: H=\sum \frac{p_i^2}{2m_i}+V(x_{i+1}\text{-}x_i)$$

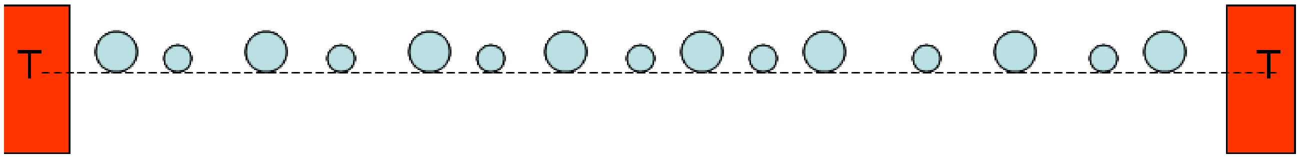


J. J. Wang, D.H. He, Y. Zhang, J. Wang and H. Zhao

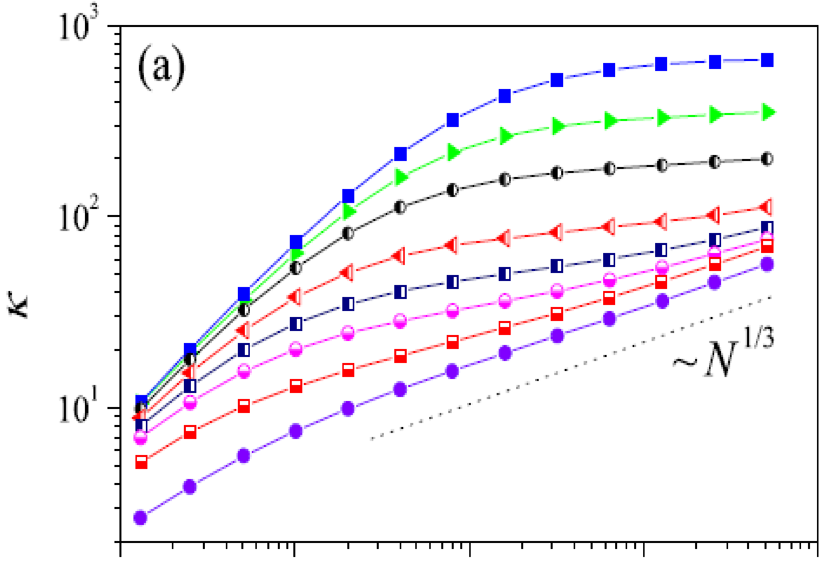
Models in contradiction with predictions

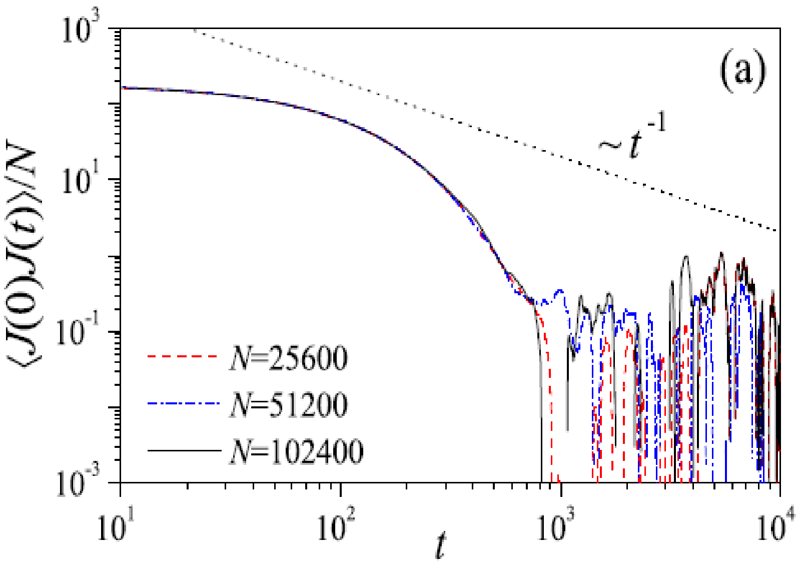
(g) Diatomic lattice with approached mass rate

(g1)



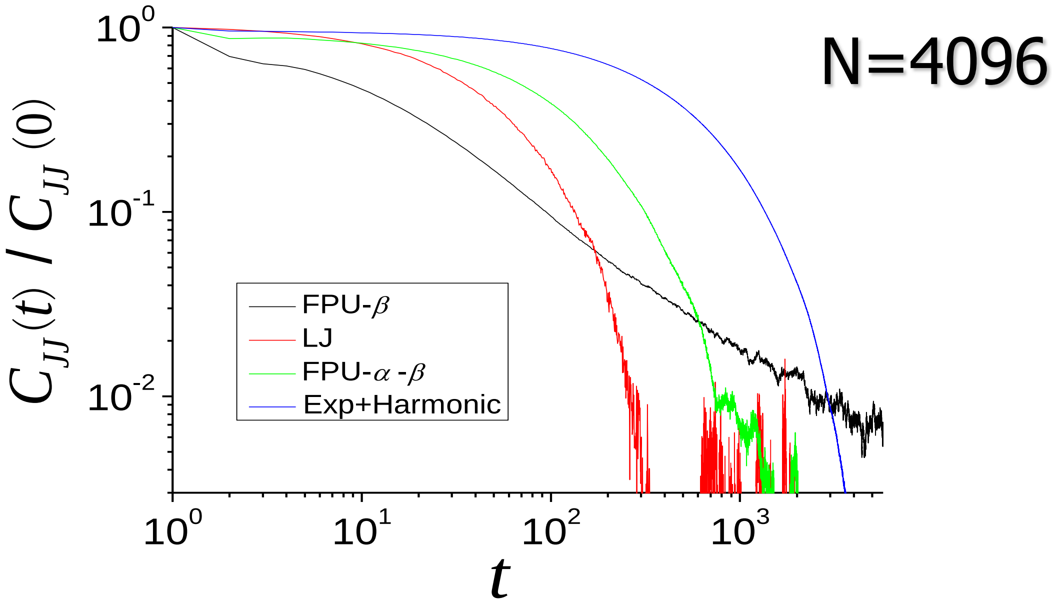
(g2) Diatomic Toda Chain





Chen, S., Wang, J., Casati, G. & Benenti, G. *Phys. Rev. E* **90**, (2014).

So, asymmetry may induce the faster decay of the current autocorrelation function and result a normal thermal conduct behavior



S. Chen Y. Zhang, J. Wang and H. Zhao , arXiv:1204.5933 (2012)

Asymmetry can make difference

(a) Thermal expansion

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

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

$$g=0: \quad < x >= 0$$

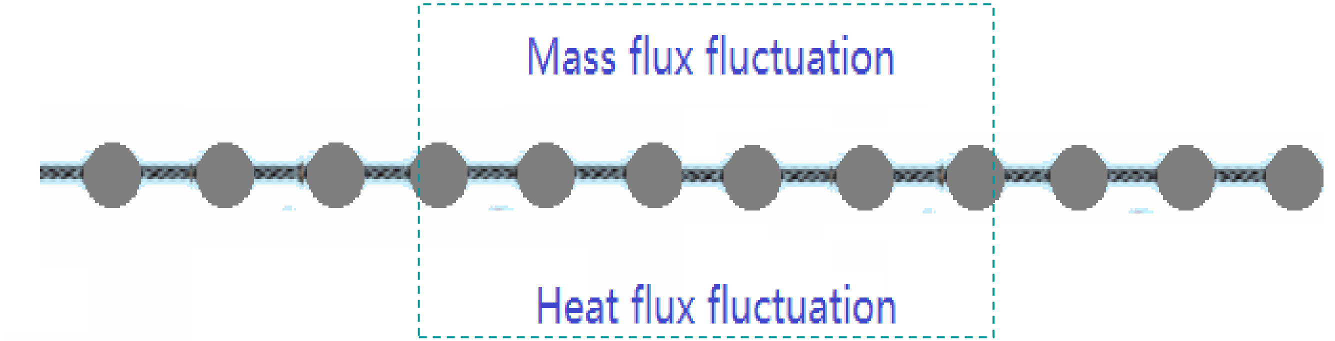
Asymmetric potential: $c_p \neq c_v, P_{in} \neq 0,$ Thermal expansion

Symmetric potential: $c_p = c_v, P_{in} = 0,$ No thermal expansion

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

Asymmetry can make difference

(b) coupling between local energy current and local mass current

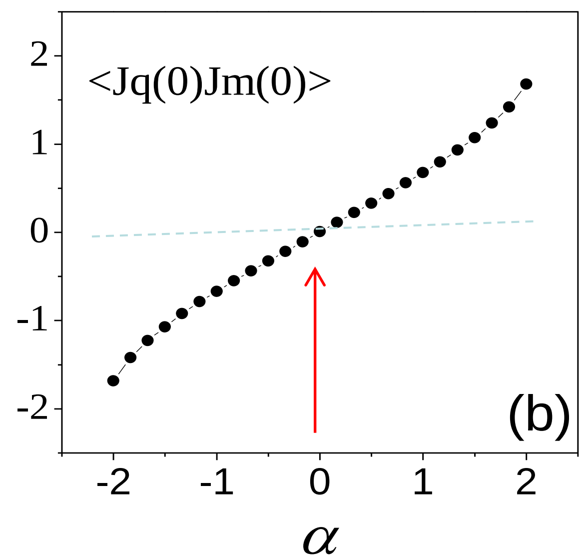


$$C_{em}(t) = < J_e(t) J_m(0) >$$

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

$$J_e(t) = \sum j_i^e(t)$$

$FPU - \alpha\beta$ model:



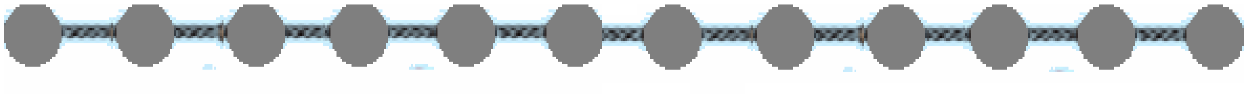
S. Chen Y. Zhang, J. Wang and H. Zhao , arXiv:1204.5933 (2012)

So, the asymmetry can make difference!

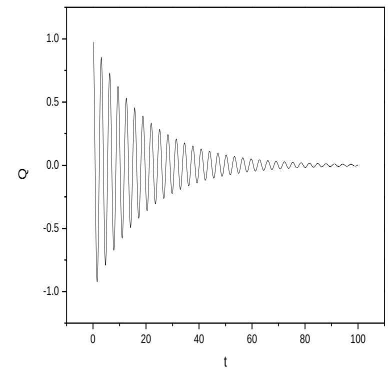
But why it violates the theoretical predictions?

----- our answer is that it may violate the “single model relax assumption”

Single mode relaxation approximation



N particles, N normal modes



$$J_e = \sum_i n_i \omega_i v_i$$

$$\kappa_e = \frac{1}{3Vk_B T^2} \sum_{i,j} \omega_i \omega_j v_i v_j \int_0^\infty < n_i(t) n_j(0) > dt$$

$$\approx \frac{1}{3Vk_B T^2} \sum_i \omega_i^2 v_i^2 \int_0^\infty < n_i(t) n_i(0) > dt$$

$$= \frac{k_B}{3V} \sum_i v_i^2 \tau_i$$

$$n_j = m\omega_j Q_j^* Q_j$$

$$Q_j(t) = A_j e^{-\Gamma_j t} e^{-i\omega_j t}$$

$$\tau = (2\Gamma)^{-1}$$

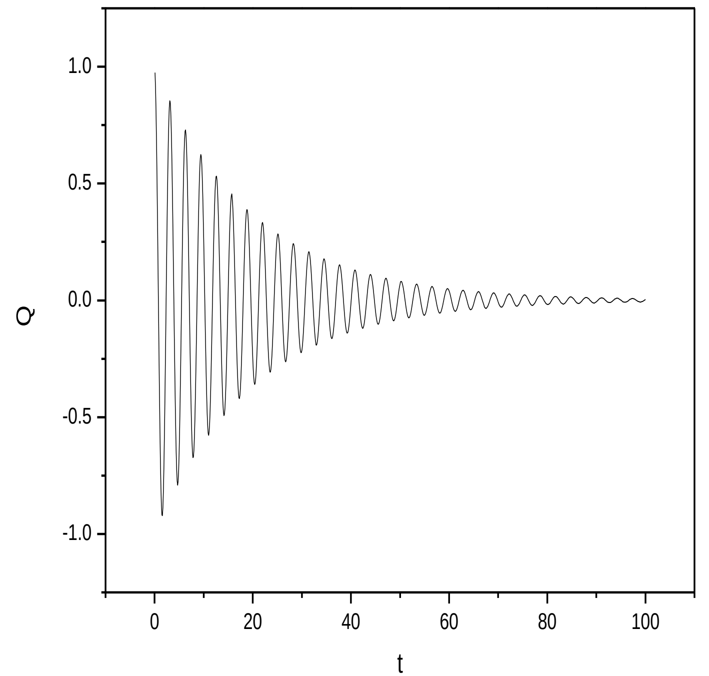
$$\tau = \frac{\int_0^\infty \langle \delta n(t) \delta n(0) \rangle dt}{\langle (\delta n)^2 \rangle},$$

A. J. C. Ladd, B. Moran, W. G. Hoover, *Phys. Rev. B* **34**, 5058–5064 (1986).

$$n_j = m\omega_j Q_j^* Q_j$$

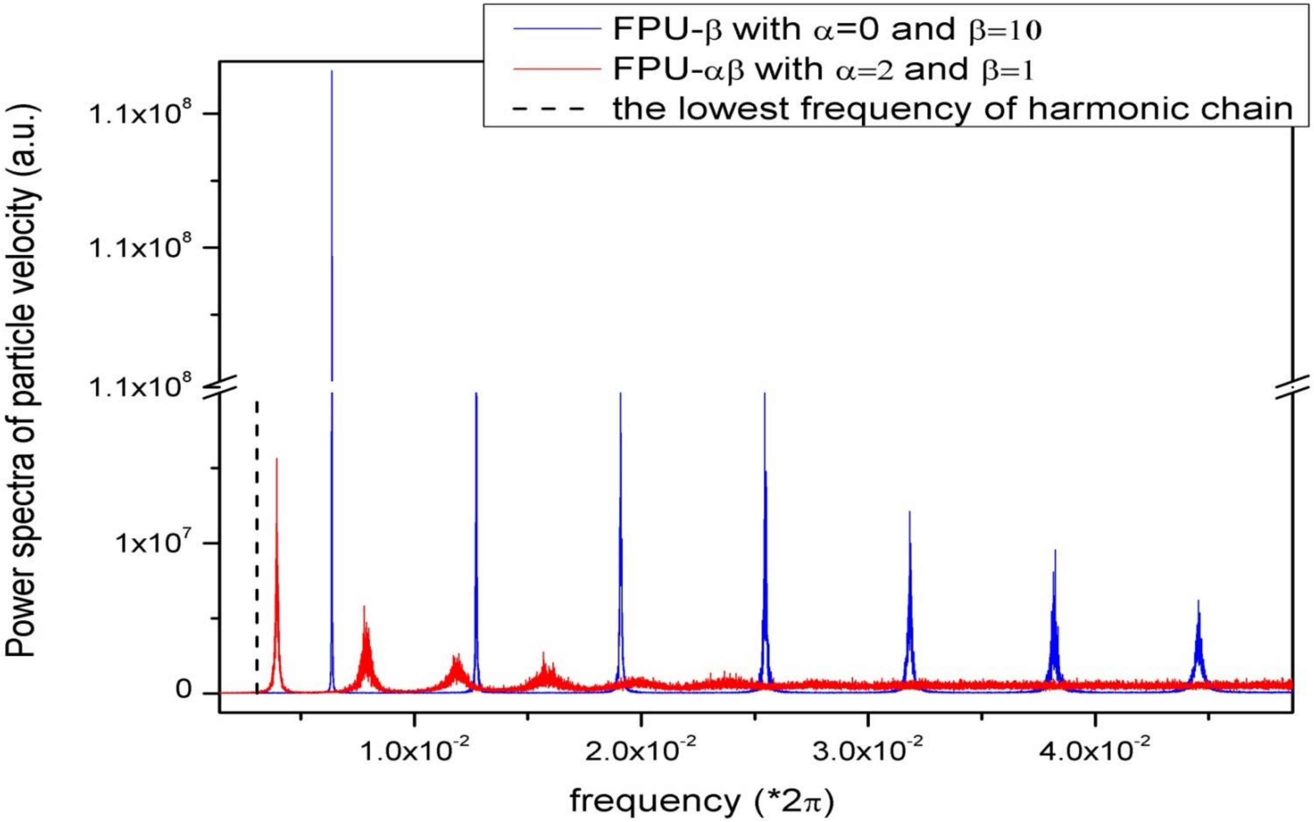
$$Q_j(t) = A_j e^{-\Gamma_j t} e^{-i\omega_j t}$$

$$\tau = (2\Gamma)^{-1}$$



$$\Gamma(\mathrm{q}) \sim q^{\delta} \Rightarrow < J(t)J(0) > \sim \int e^{-q^{\delta} t} dk \sim t^{-\frac{1}{\delta}} \quad \Rightarrow \kappa \sim L^{1-\frac{1}{\delta}} (1D)$$

Breakdown of single mode relaxation approximation

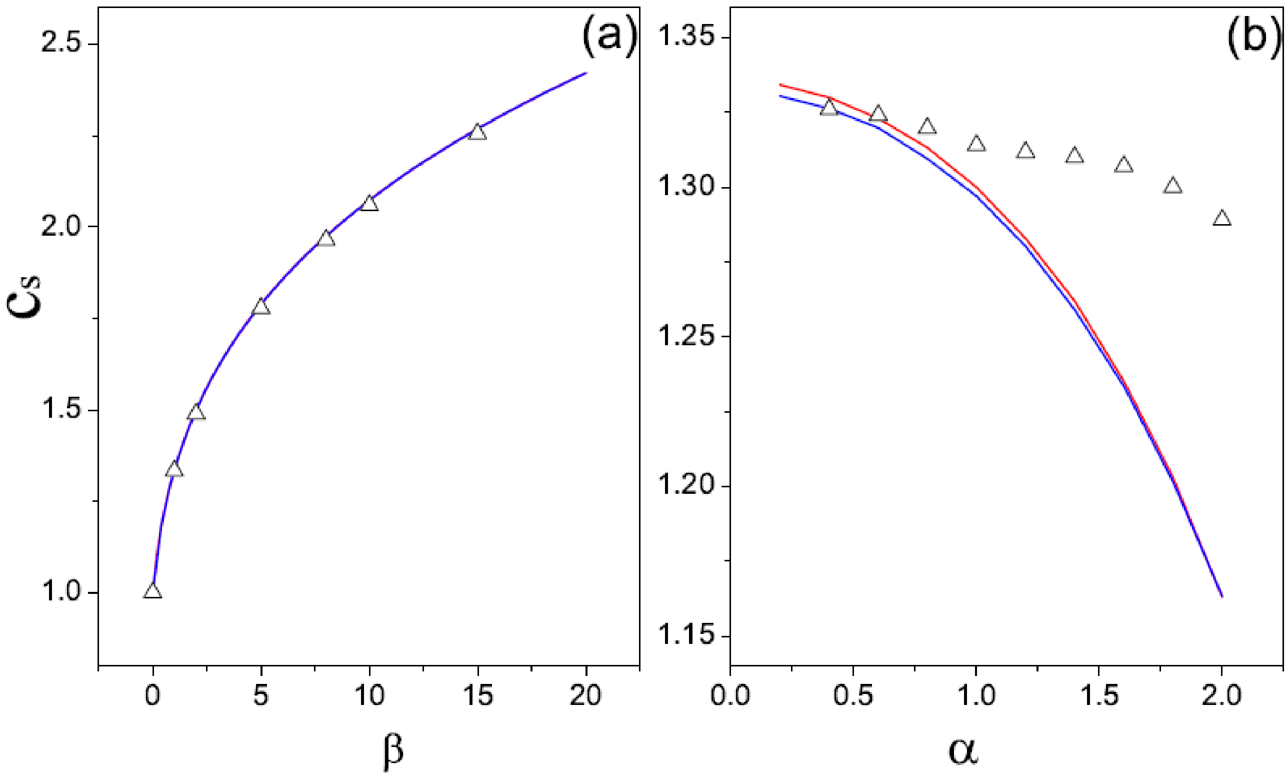


Y. Zhang et. al, arXiv:1301.2838 (2013)

Breakdown of single mode relaxation approximation

The violation of sound-velocity prediction for asymmetry models

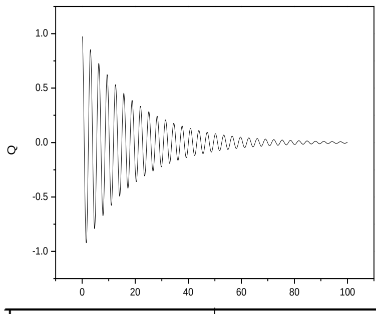
FPU-β model　　　FPU-$\alpha\beta$ model



Y. Zhang et. al, arXiv:1301.2838 (2013)

Breakdown of single mode relaxation approximation

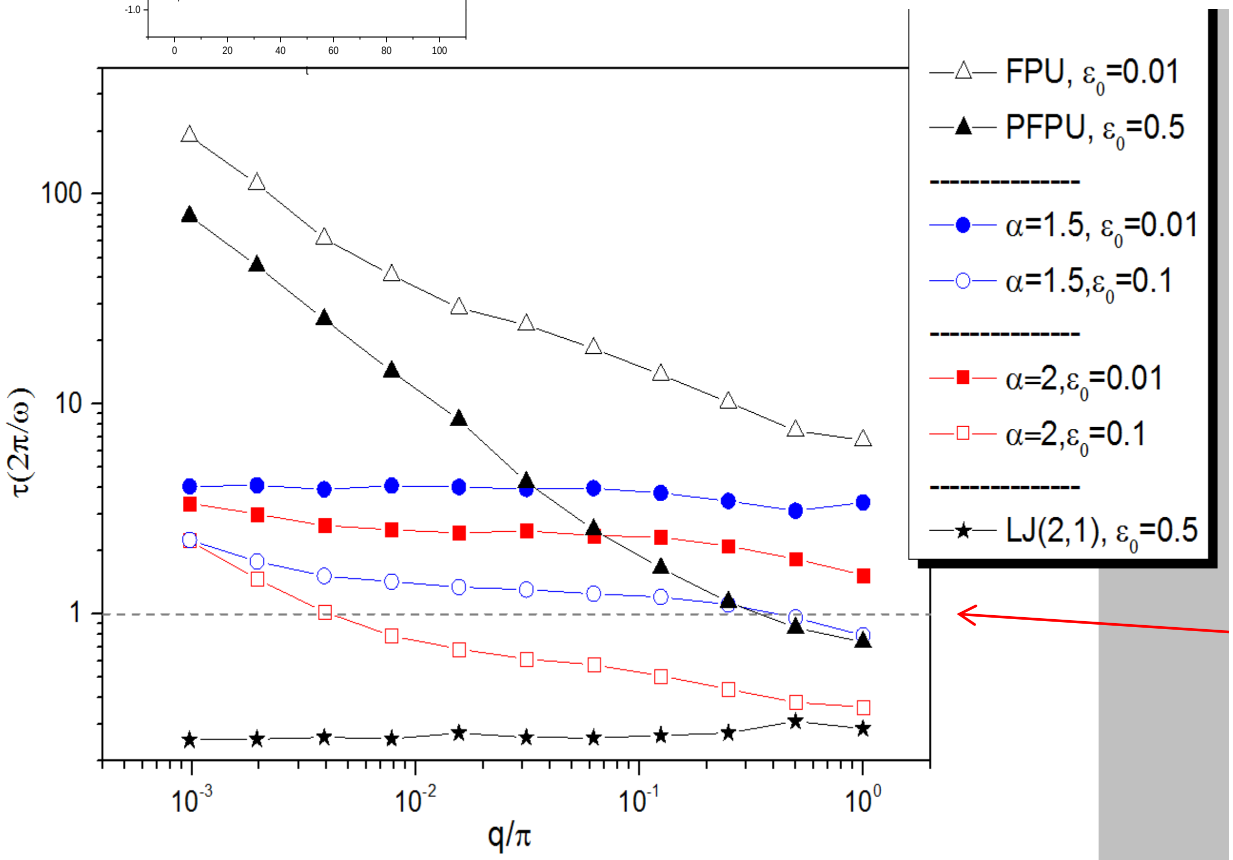
The lifetime of normal modes



$$< E_q(t)E_q(0) > \sim e^{-\frac{t}{\tau_q}}$$

$$V(x) = [(\frac{x_c}{x+x_c})^2 - 2(\frac{x_c}{x+x_c})^1 + 1]$$

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



Ioffe-Regel crossover

$$q = \omega_0 2^n$$

Y. Zhang et. Al.

Summary

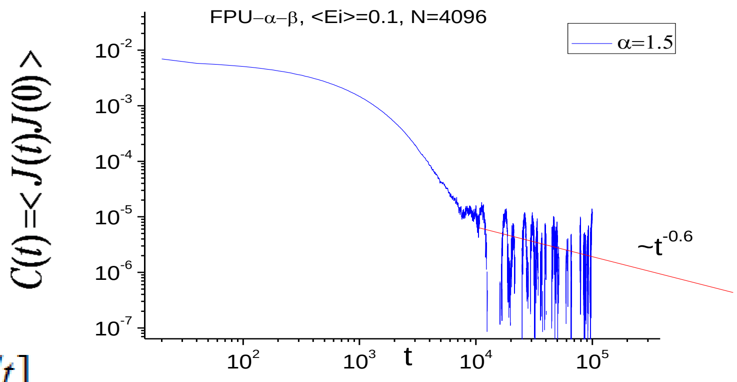
- **Proper asymmetry interactions may induce faster decay which results a normal heat conductivity.**
- **Asymmetry interactions may remarkably decrease the survival time of phonons**

The theories may not applicable in this case

----- Open problem!

Discussion

If only the rapid decay extend a sufficient long time, a size-independent thermal conductivity may observed practically, even the long time tail may appears in the thermodynamical limit



$$\kappa = \frac{1}{k_B T^2}\left[\int_0^{\tau_e} \frac{1}{N} C(t)\,dt + \int_{\tau_e}^{\tau_{tr}(N)} \frac{1}{N} C(t)\,dt\right].$$

$$\kappa \sim \frac{1}{k_B T^2}\left[4 + 2.6\text{x}10^{-3} \mathrm{t}^{\frac{1}{3}}\Big|_{t_\tau}^{t_{tr}}\ \right],\ \ \text{suppose } \mathrm{C(t)} \sim \mathrm{t}^{-\frac{2}{3}}, t_{tr} \sim \frac{N}{v_s}$$

The contribution of the tail part is comparable to that of the faster decaying part until the system size reaches up to $10^9 \sim 10cm$

A guess

- L-J model: there is no long-time tail
- FPU-$\alpha\beta$ model: the power-law tail may appear finally but physically a normal thermal conduct behavior can be observed in the sufficient long 1D lattice.