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Phonons in 1D anharmonic chains

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With Hong Zhao, Jiao Wang, and Weicheng Fu

Outline

- Theoretical predictions about phonons in 1D lattices
- Simulation results
- Conclusions

What is a phonon?

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

$$V(x) = \frac{1}{2}x^2$$

- Phonons as quasiparticles

$$E_n = (n + \frac{1}{2})\hbar\omega$$

$$\frac{1}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$

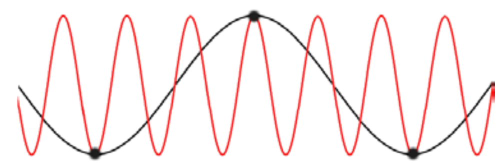
- Phonons as normal modes

$$Q_k = (\frac{2}{N})^{1/2} \sum_{i=1}^{N} x_i S_i^k$$

$$P_k = \dot{Q}_k$$

$$\omega_k = 2\sqrt{\frac{K}{m}} \sin(\frac{k\pi}{2N})$$

$$E_k = \frac{1}{2}\omega_k{}^2 Q_k{}^2 + \frac{1}{2}P_k{}^2$$

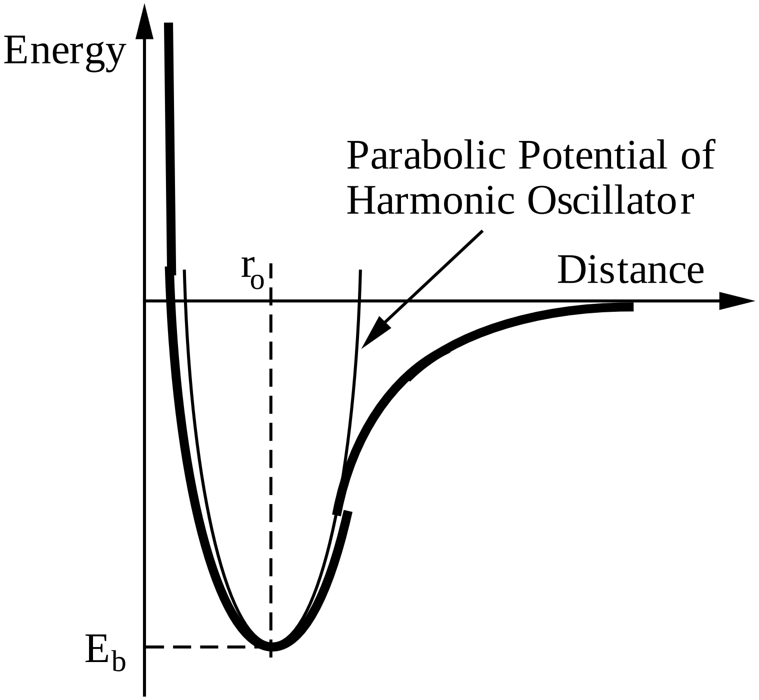


$$\frac{A}{2}e^{i\omega_h t}$$

No interaction among phonons in harmonic chains.

Anharmonic potential

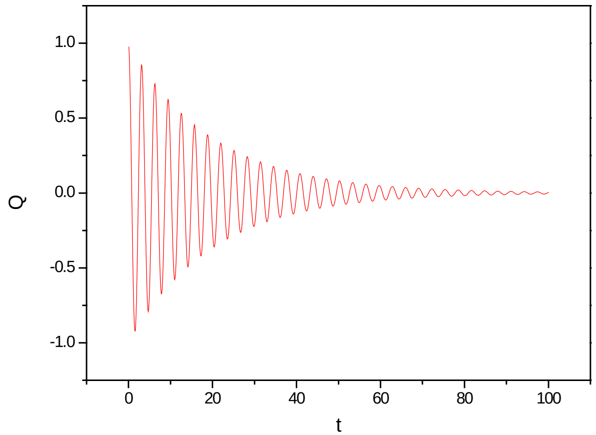
$$H = \sum_i \frac{p_i^2}{2} + V(x_i - x_{i-1})$$



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

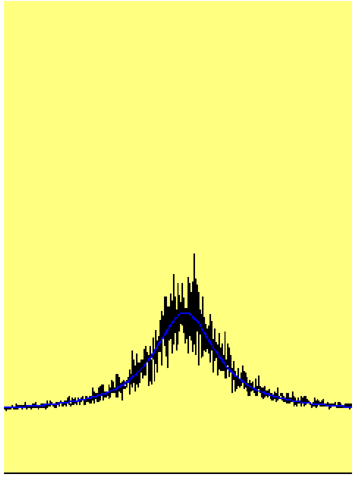
Phonons under anharmonicity (weak)

Kinetic theory for phonon gas: phonon Boltzmann equation.



$$\frac{A}{2}e^{-\Gamma t}e^{i\omega_m t}$$

Fourier transform



$$A\frac{\Gamma}{(\omega-\omega_m)^2+\Gamma^2}$$

Frequency shift: $\eta = \omega_m / \omega_h$

Linewidth: Γ

Lifetime: $\tau = 1/2\Gamma$

Phonons under anharmonicity (strong)

- Minimum heat conduction problem
  - mean free path ~ lattice constant

    C. Kittel, Phys.Rev. 75, 972 (1948)
  - a random walk for a phonon

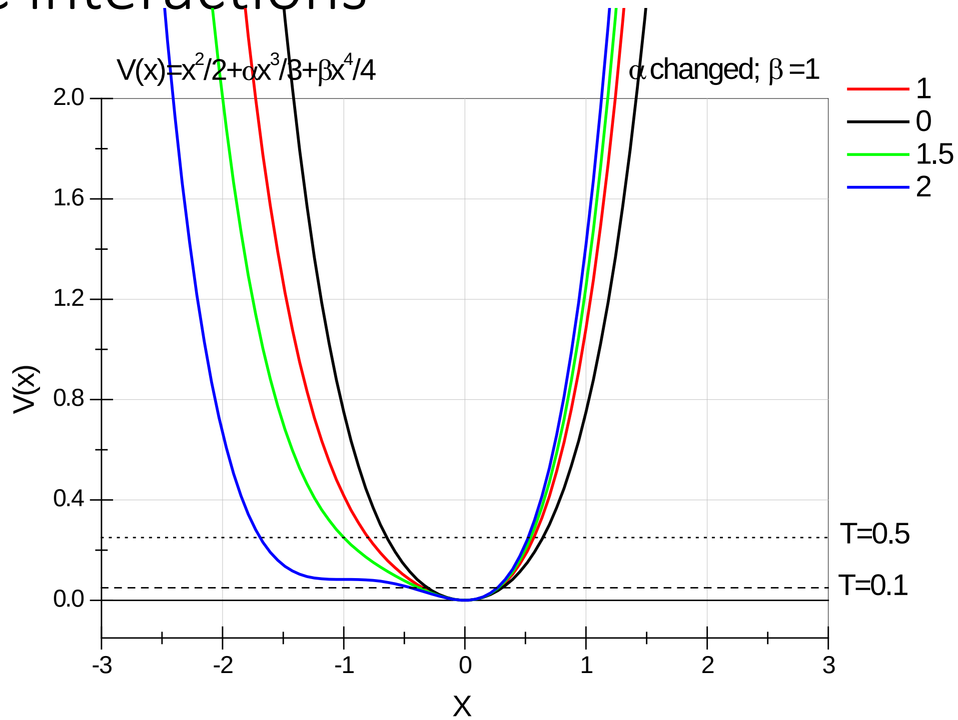
    D. G. Cahill, etc., Phys. Rev. B 46, 6131–6140 (1992)

- Solitons and breathers

1D model with asymmetric interactions

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

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



symmetric: $V(x) = V(-x)$ $\alpha = 0, FPU - \beta$

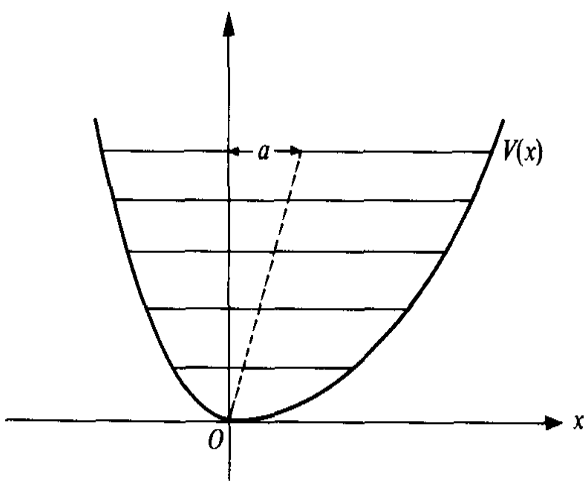
asymmetric: $V(x) \neq V(-x)$ $\alpha \neq 0, FPU - \alpha\beta$

High temperature limit (PFPU): $V(x) = \frac{\beta}{4}x^4$

low temperature limit(harmonic chain): $V(x) = \frac{1}{2}x^2$

Symmetry of a interaction potential is relevant

- Thermal expansion (contraction) in asymmetric cases, not in symmetric cases.



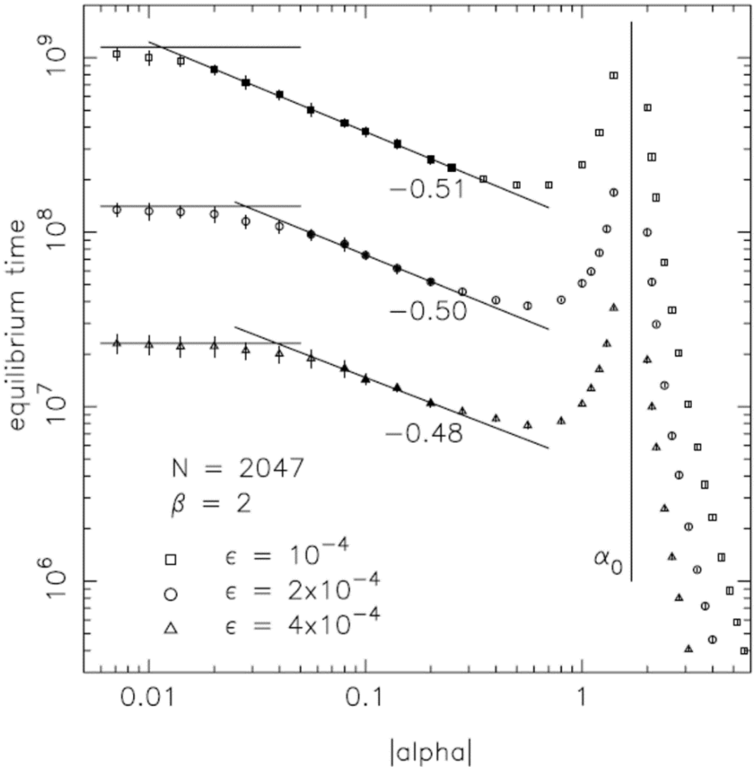
$$V(x) = cx^2 - gx^3 - fx^4 \qquad \langle x \rangle = \boxed{\frac{3g}{4c^2}} k_B T$$

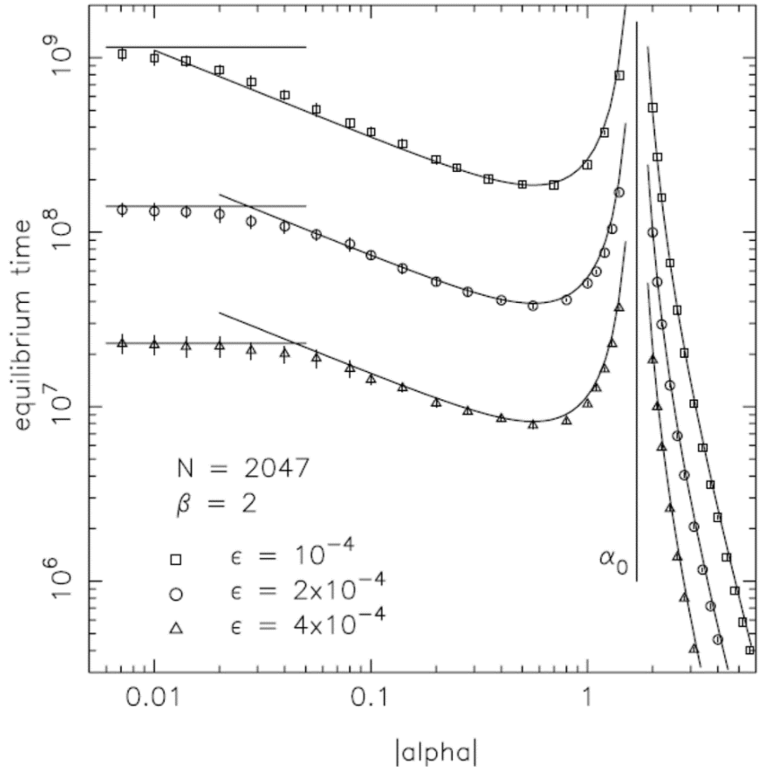
$$V(x) = \frac{1}{2}x^2 + \frac{\alpha}{3}x^3 + \frac{\beta}{4}x^4 \qquad -\alpha$$

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

Symmetry of a interaction potential is relevant

- shorter time to **energy equipartition among normal modes** in asymmetric cases than symmetric ones





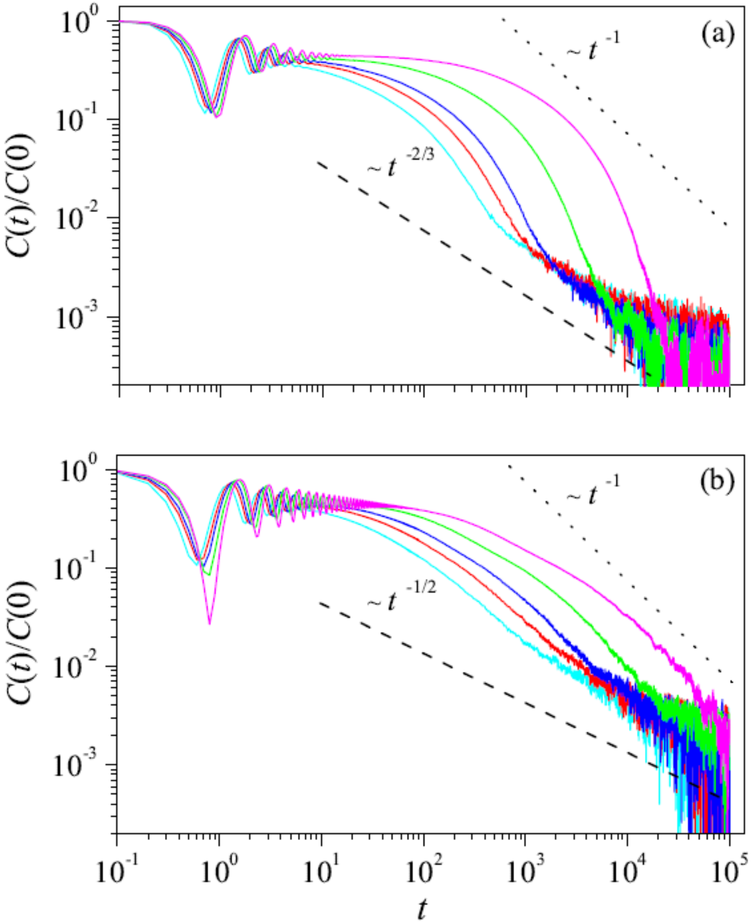
G. Benettin, A. Ponno, J. Stat. Phys. 144, 793(2011).

Symmetry of a interaction potential is relevant

- Is the heat conduction normal in 1D momentum-conserved lattices with asymmetric potentials ?

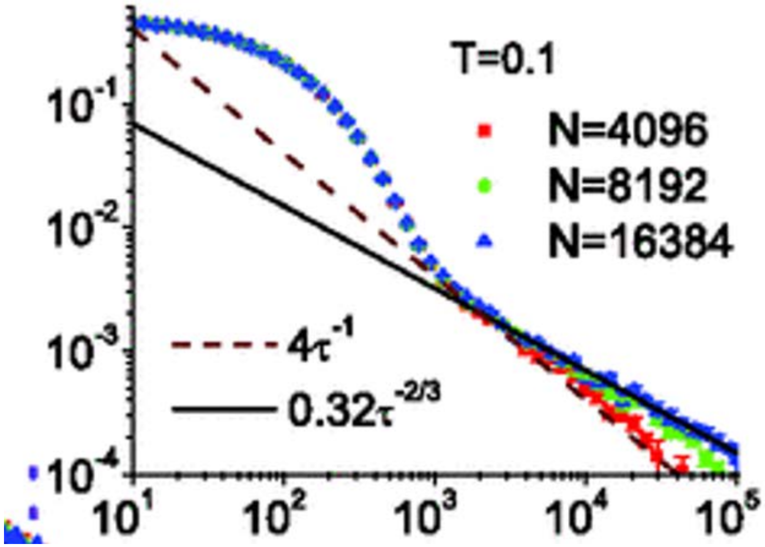
Anomalous heat conduction:

$$\langle J(t)J(0)\rangle \sim t^{-\lambda} (\lambda < 1)$$



arXiv: 1511.00292

Is the heat conduction normal in 1D momentum-conserved lattices with asymmetric potentials ?



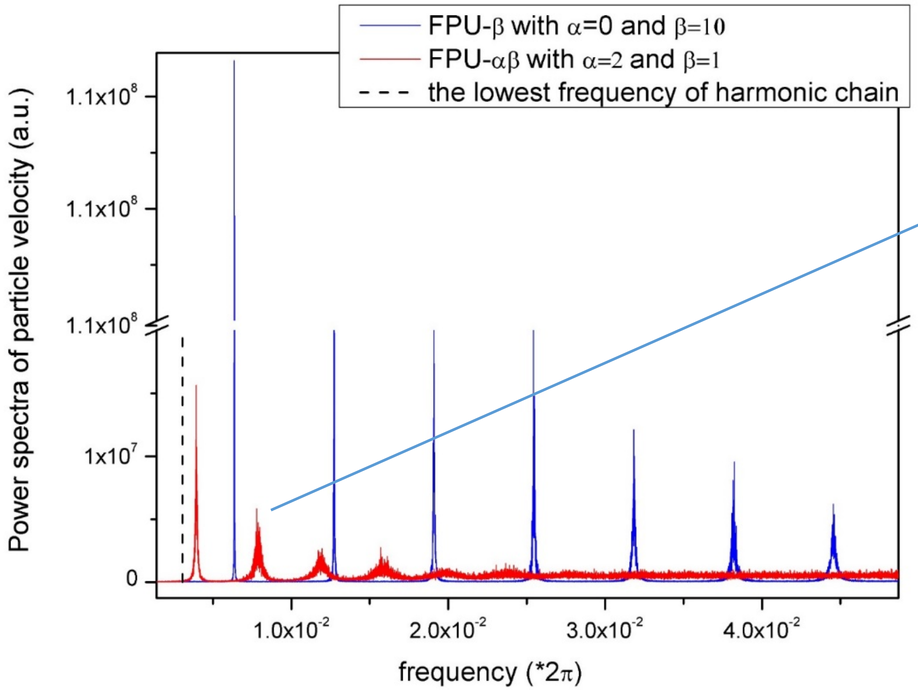
Fast decay of the flux correlation functions is more easily observed at the small alpha and low temperature !

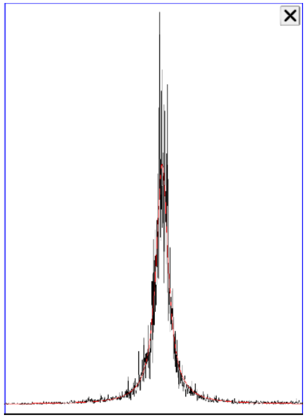
L. Wang, B. Hu, B. Li, Phys. Rev. E **88**, 052,112 (2013)
S. Das, A. Dhar, O. Narayan, J. Stat. Phys. **154**, 204 (2014)

Simulations

- periodic boundary conditions
- Equilibrium MD simulations at constant energy
- system size=2048
- Principles： the motion of any particle of a chain at equilibrium is superposition of phonons (normal modes)
- Methods: calculate the velocity power spectra of a particle

The phonon peaks with lowest frequencies





$$A\frac{\Gamma}{(\omega-\omega_m)^2+\Gamma^2}$$

$$\eta=\frac{\omega_m}{\omega_h}$$

arXiv:1301.2838
arXiv:1511.00551

Γ（τ=1/2Γ）

Phonon lifetime and heat conductivity

Phonon energy: $E_k = \frac{1}{2}\omega_k{}^2 Q_k{}^2 + \frac{1}{2} P_k{}^2$

Phonon heat current: $J_k = E_k v_k$

$$< J(t)J(0) > \sim < (\sum_k E_k(t))(\sum_k E_k(0)) > = < \sum_k E_k(t)E_k(0) > + < \sum_{k \neq k'} E_k(t)E_{k'}(0) >$$

$$\kappa \sim \int < J(t)J(0) > dt \sim \sum_k \int < E_k(t)E_k(0) > dt + \sum_{k \neq k'} \int < E_k(t)E_{k'}(0) > dt$$

Single mode relaxation approximation

Phonon lifetime and heat conductivity

$$< E_k(t)E_k(0) > \to < \delta E_k(t)\delta E_k(0) >$$

$$< \delta E_k(t)\delta E_k(0) > \sim e^{-\frac{t}{\tau_k}}, \ \ \tau \sim k^{-\gamma} \ \text{ or } \ \Gamma \sim k^{\gamma}$$

$$< J(t)J(0) > \sim < \sum_k \delta E_k(t)\delta E_k(0) > \sim t^{-\frac{1}{\gamma}}$$

$$\kappa \sim \sum_k \int_0^{N/v} < \delta E_k(t)\delta E_k(0) > dt \sim N^{1-\frac{1}{\gamma}}$$

A.J.C.Ladd, etc., Phys. Rev. B 34, 5058 (1986)

Theoretical predictions for phonon lifetimes

$$\tau_k \sim k^{-\gamma}$$

Phonon theories:

FPU-alpha-beta $\gamma = 3/2 \rightarrow t^{-2/3} \rightarrow N^{1/3}$

FPU-beta $\gamma = 5/3 \rightarrow t^{-3/5} \rightarrow N^{2/5}$

Pereverzev, Phys. Rev. E 68, 056124 (2003)
J. Lukkarimen and H. Spohn, Comm. Pure Appl. Math. 61, 1753(2008)
Santhosh G. and Deepak Kumar, Phys. Rev. E 76, 021105 (2007)
Santhosh G. and Deepak Kumar, Phys. Rev. E 77, 011113 (2008)

Mode-Coupling & Hydrodynamics

FPU-alpha-beta $\gamma = 3/2 \rightarrow t^{-2/3} \rightarrow N^{1/3}$

FPU-beta $\gamma = 2 \rightarrow t^{-1/2} \rightarrow N^{1/2}$

L. Delfini, S.Lepri, R. Livi, & A. Politi, J. Stat. Mech. 2007, P02007(2007).
O. Narayan and S. Ramaswamy, Phys. Rev. Lett. 89, 200601(2002)
H. Van Beijeren, Phys. Rev. Lett. 108, 180601 (2012)
C. B. Mendl, H. Spohn, Phys. Rev. Lett. 111, 230601 (2013).

The underlying hypothesizes of these theories

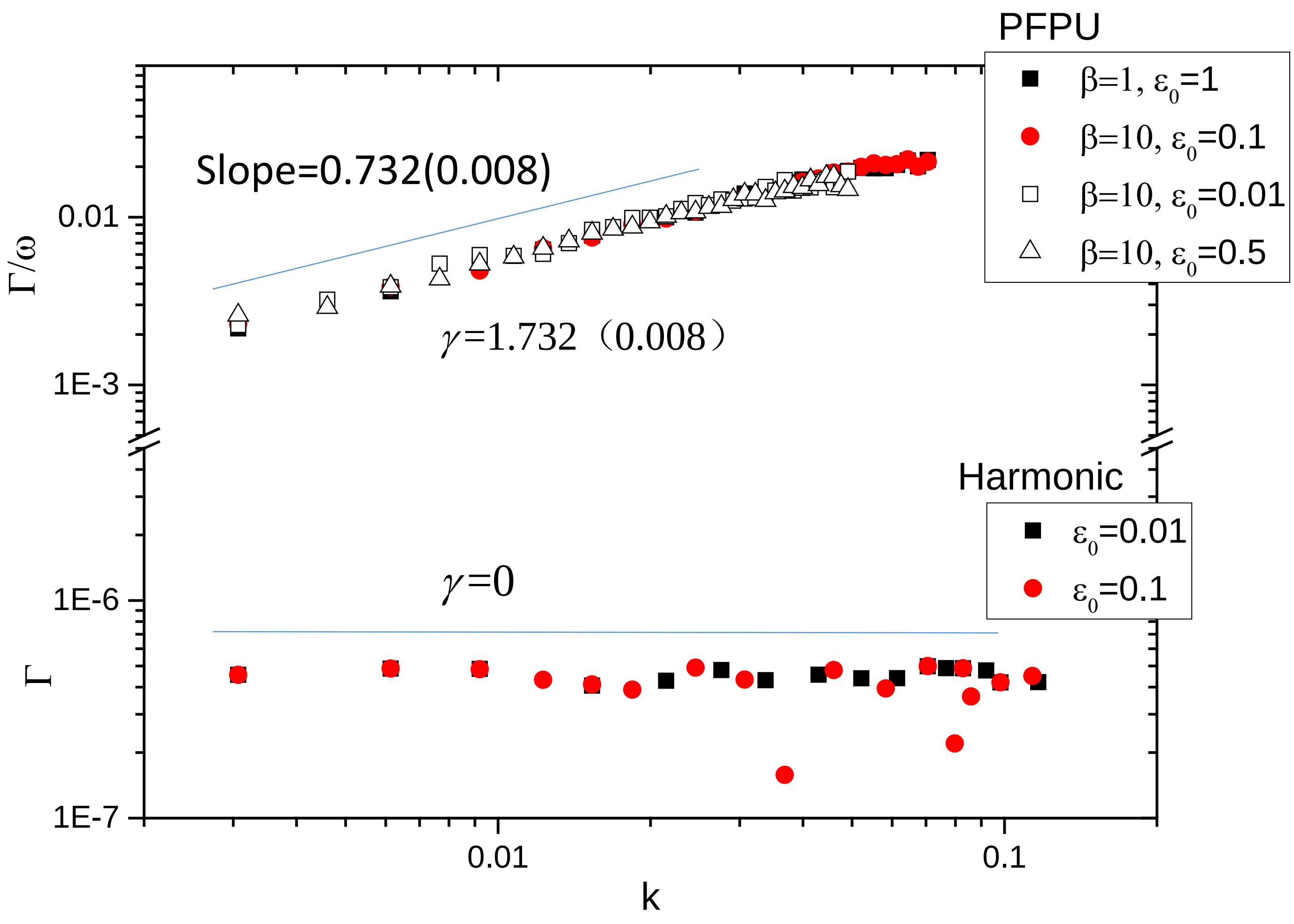
- Long-wavelength approximation,

$$k \rightarrow 0$$

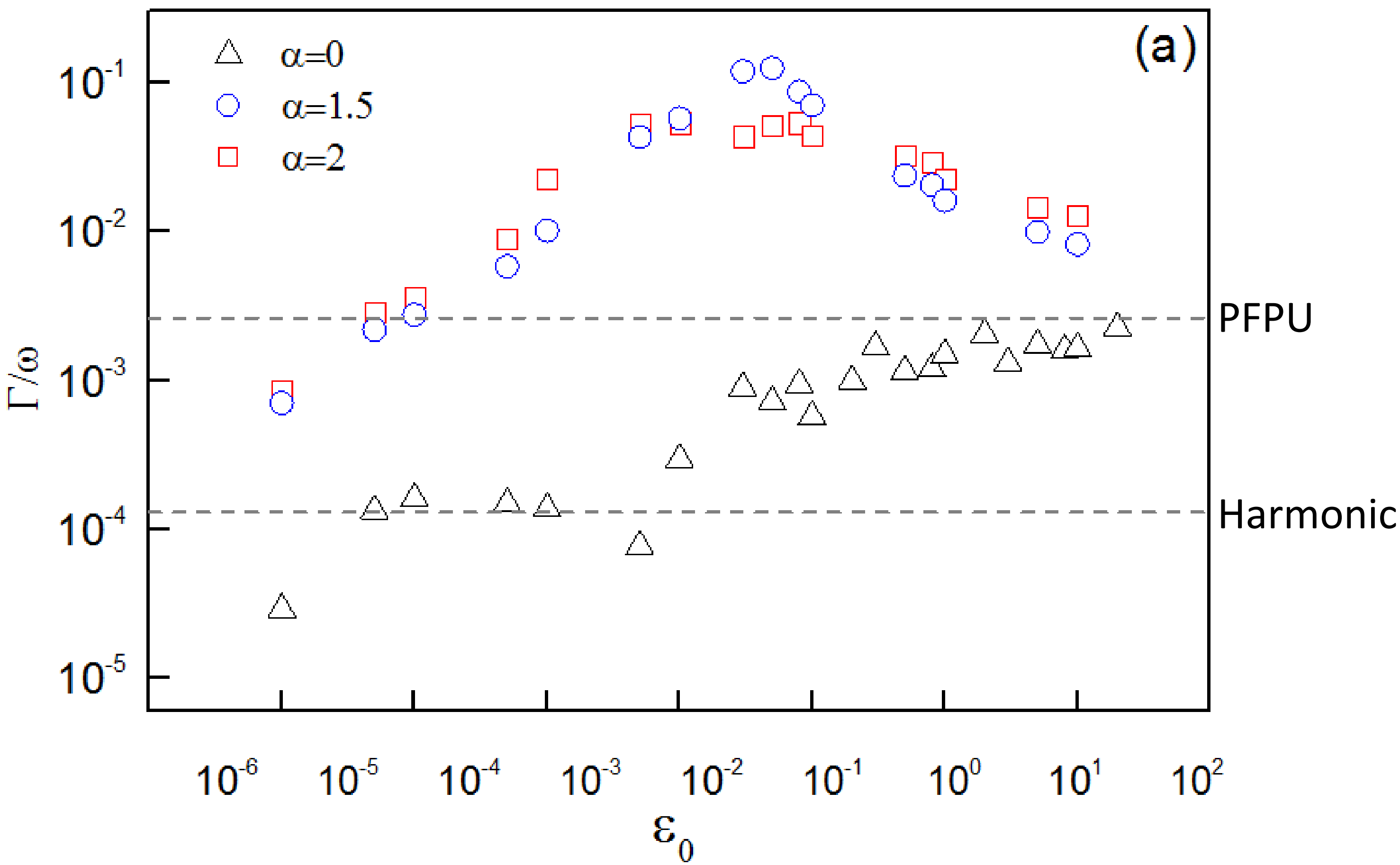
- Propagating phonons dominate the heat conduction processes, that mean:

lifetime >> period

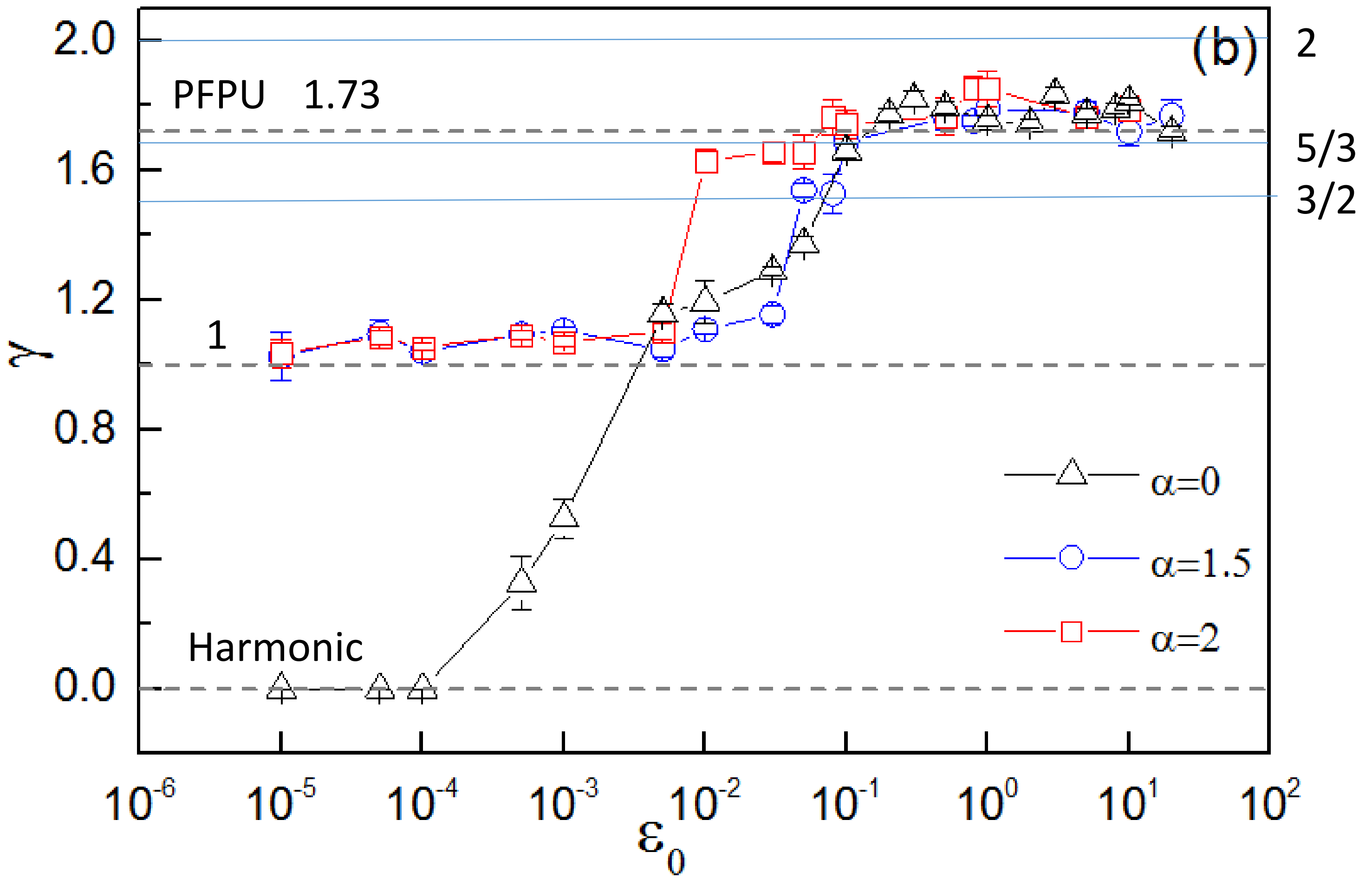
Harmonic limit & PFPU limit



The linewidth of the first mode vs energy density

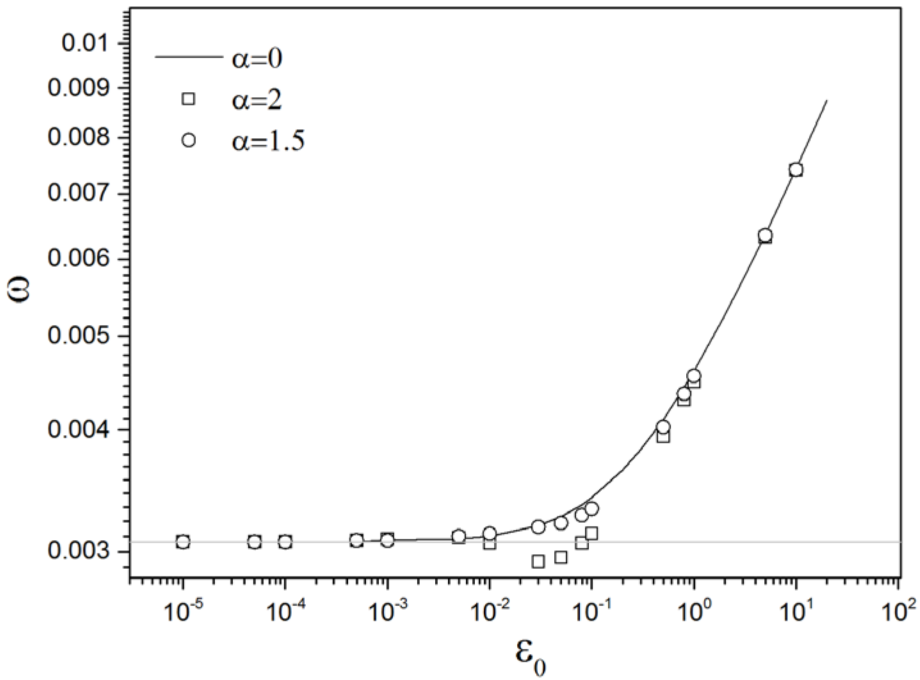


$$\tau_k \sim k^{-\gamma}$$



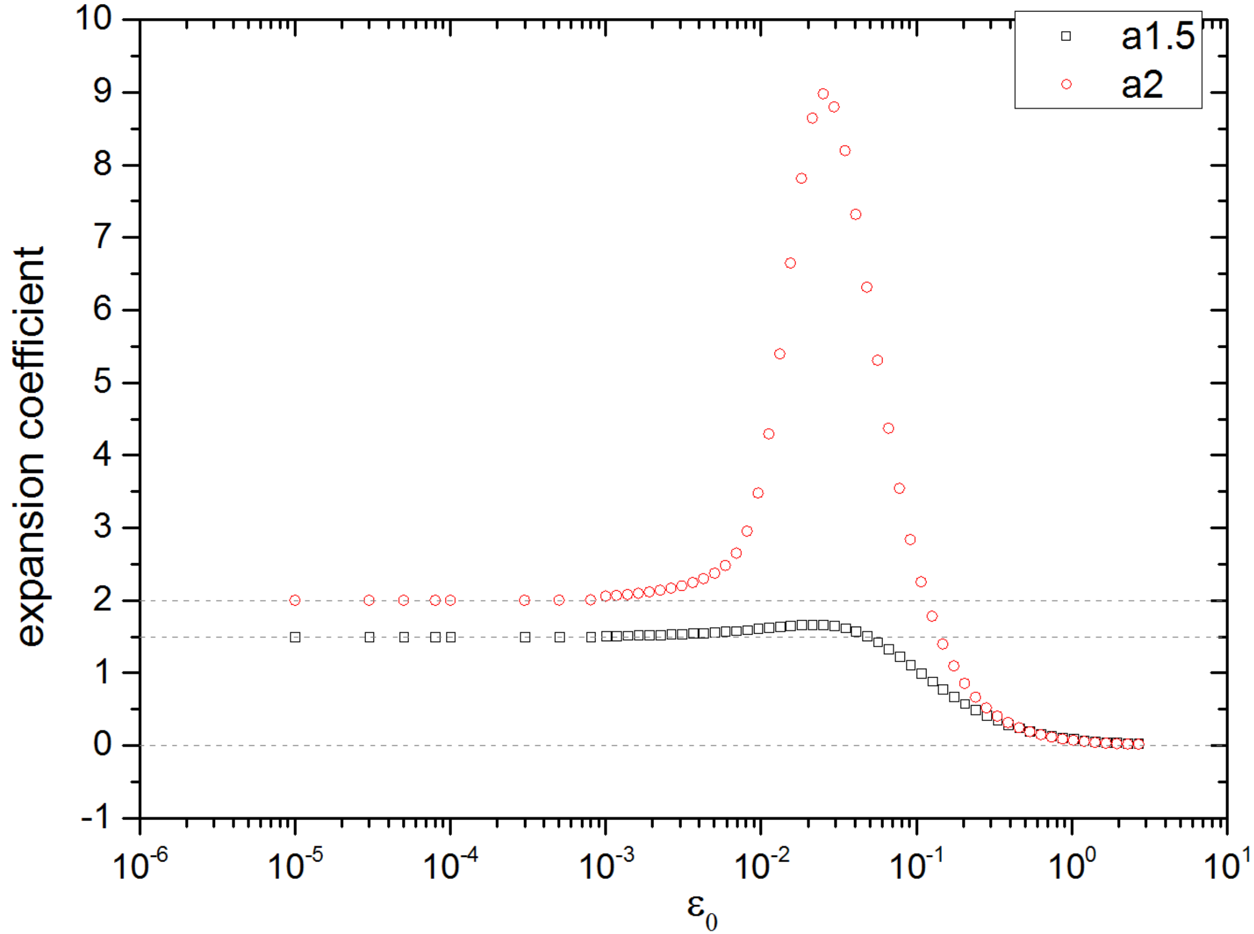
What happened in low temperature regime?

- The effect of Nonlinear potential energy tend to zero.



- But the lifetimes of phonons dramatically smaller than harmonic ones. It means there really exists anharmonic effect.

Expansion coefficient vs energy density



Anharmonicity from two sources in FPU-alpha-beta model

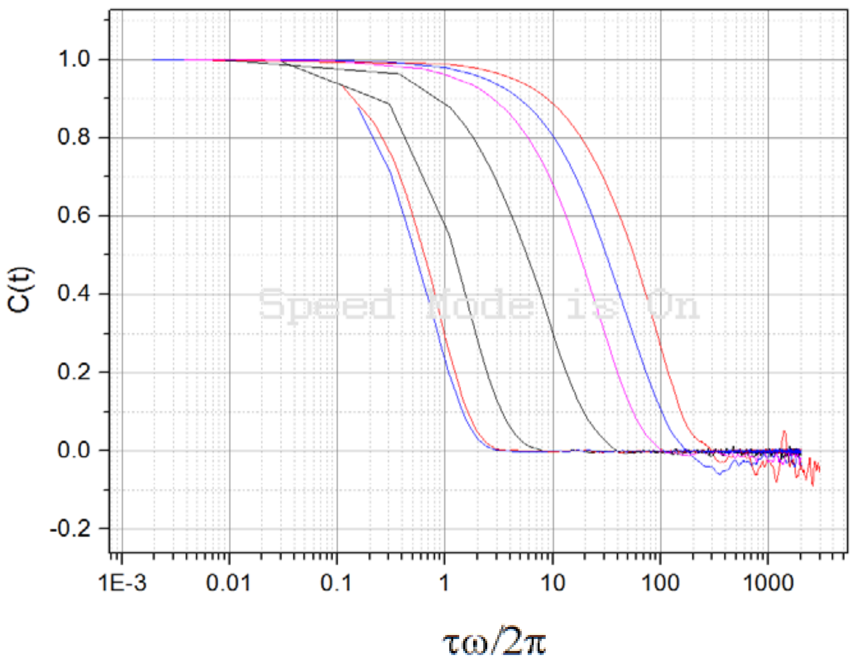
- Asymmetry dominate the phonon decay in the low temperature region.

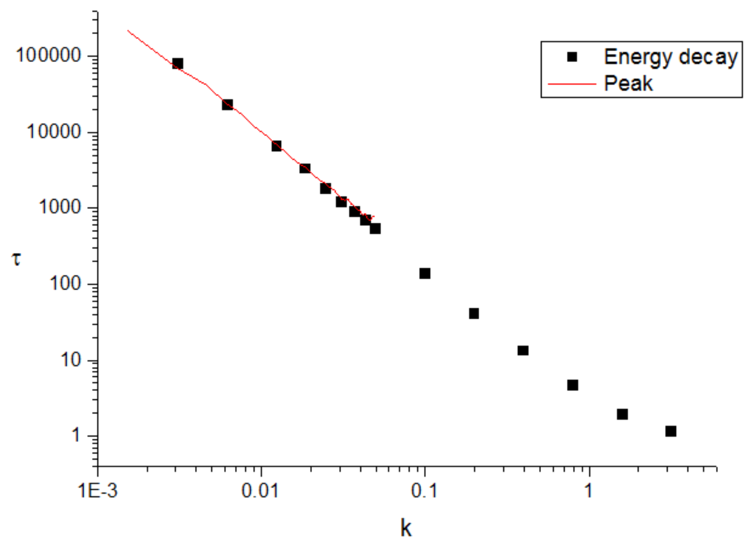
- (symmetric) Nonlinearity dominate the phonon decay in high temperature region.
  - Nonlinearity means that the force between neighboring particles as the function of relative displacement is not linear.
- In the middle region of temperature, there is mixing effect of bath asymmetry and nonlinearity on phonons.

Energy fluctuation relaxation of phonons

$$E_k = \frac{1}{2}\omega_k^{\ 2} Q_k^{\ 2} + \frac{1}{2} P_k^{\ 2} \qquad k = \frac{2\pi n}{N}, N = 2048, n = 2^m, m = 0,1,2,\cdots,10$$

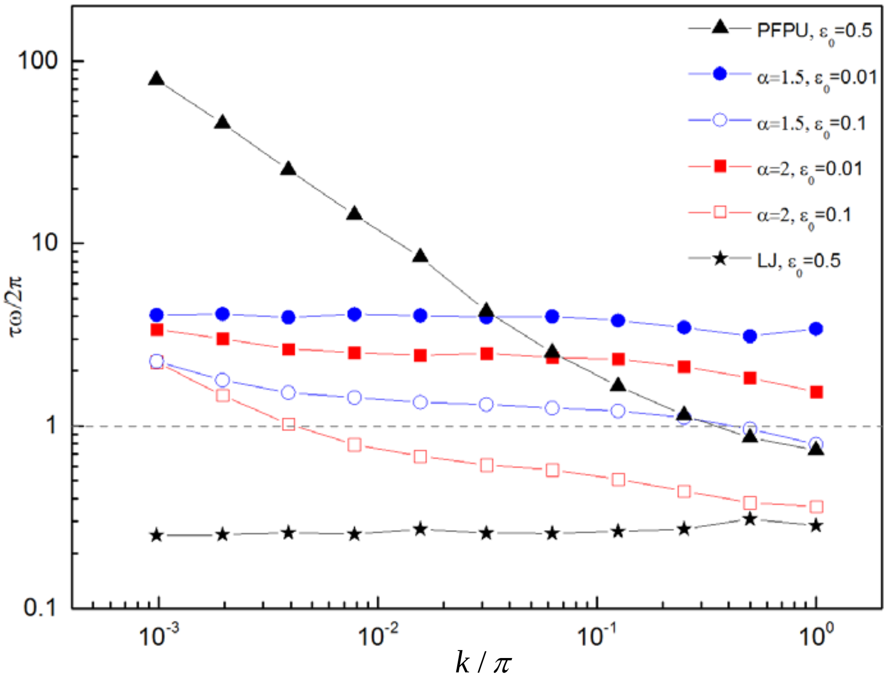
$$C_k(t) = <\delta E_k(t)\cdot \delta E_k(0)> \sim e^{-(\frac{t}{\tau_k})^{\sigma}}, 1 < \sigma < 2$$

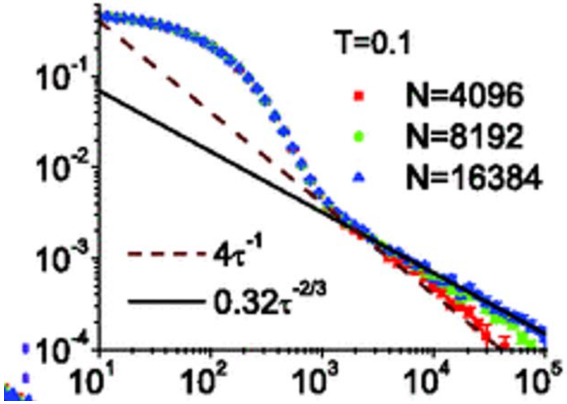




A.J.C.Ladd, etc., Phys. Rev. B 34, 5058 (1986)

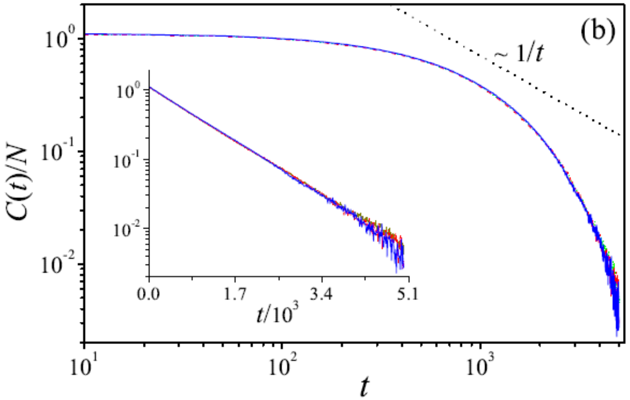
Lifetime overview of phonons covering full Brillouin zone





Ioffe-Regel crossover

$$V(x) = [(\frac{1}{x+1})^m - 2(\frac{1}{x+1})^n + 1], \mathrm{m} = 2, \mathrm{n} = 1$$



Conclusions

- Asymmetry dramatically reduce phonon lifetimes and lead to violate the hypotheses “*lifetime >> period*”.
- Small Asymmetry alone lead to the behavior $\gamma \sim 1$
- large asymmetry facilitates the hydrodynamic behaviors
- Strong symmetric nonlinearity lead to hydrodynamic behavior $\gamma \sim (1.5, 2)$ and *lifetime >> period*