Thermal transport in low-dimensional lattices:

negative temperature jump and impacts of thermal expansion

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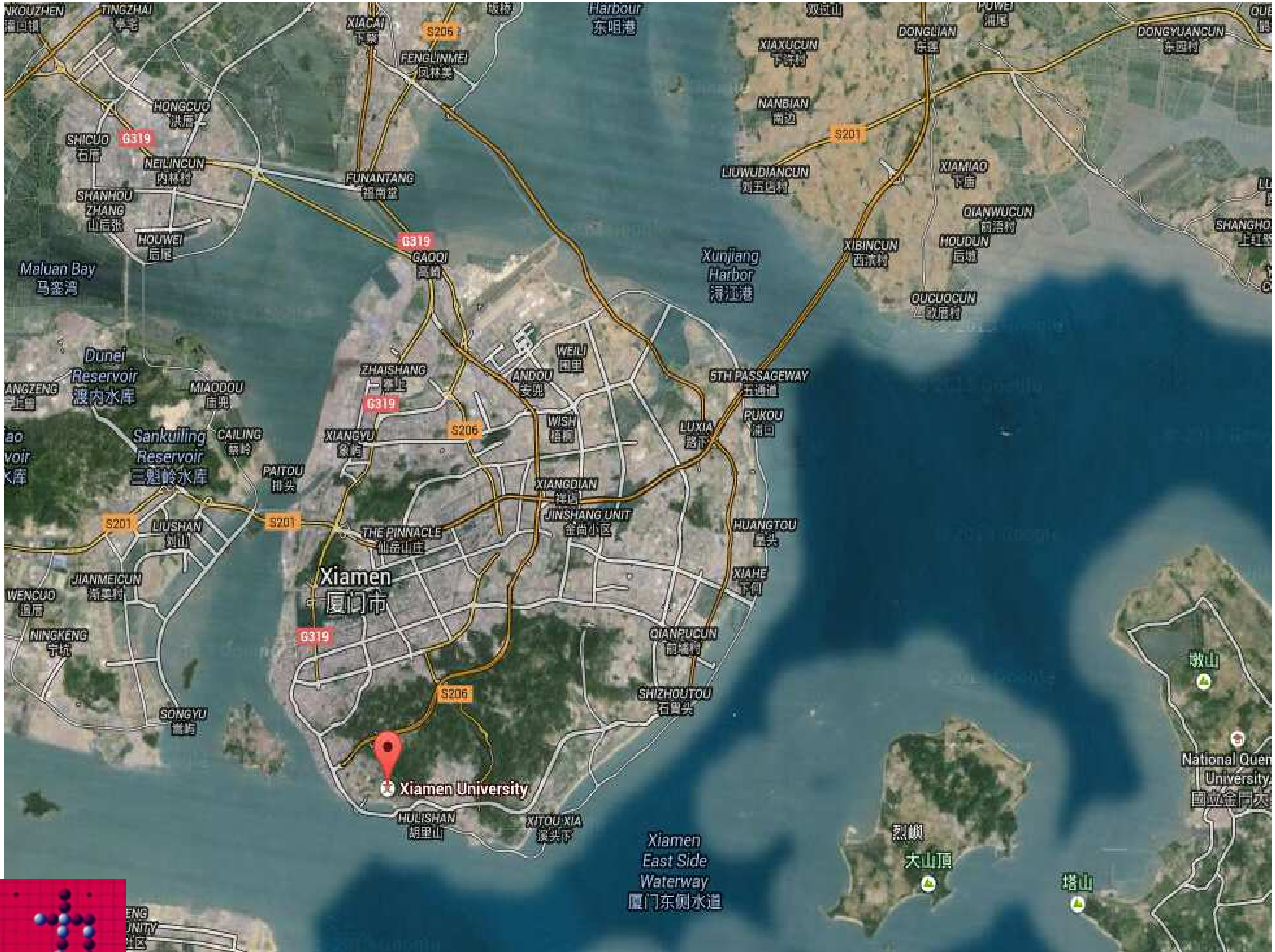
November, 2015



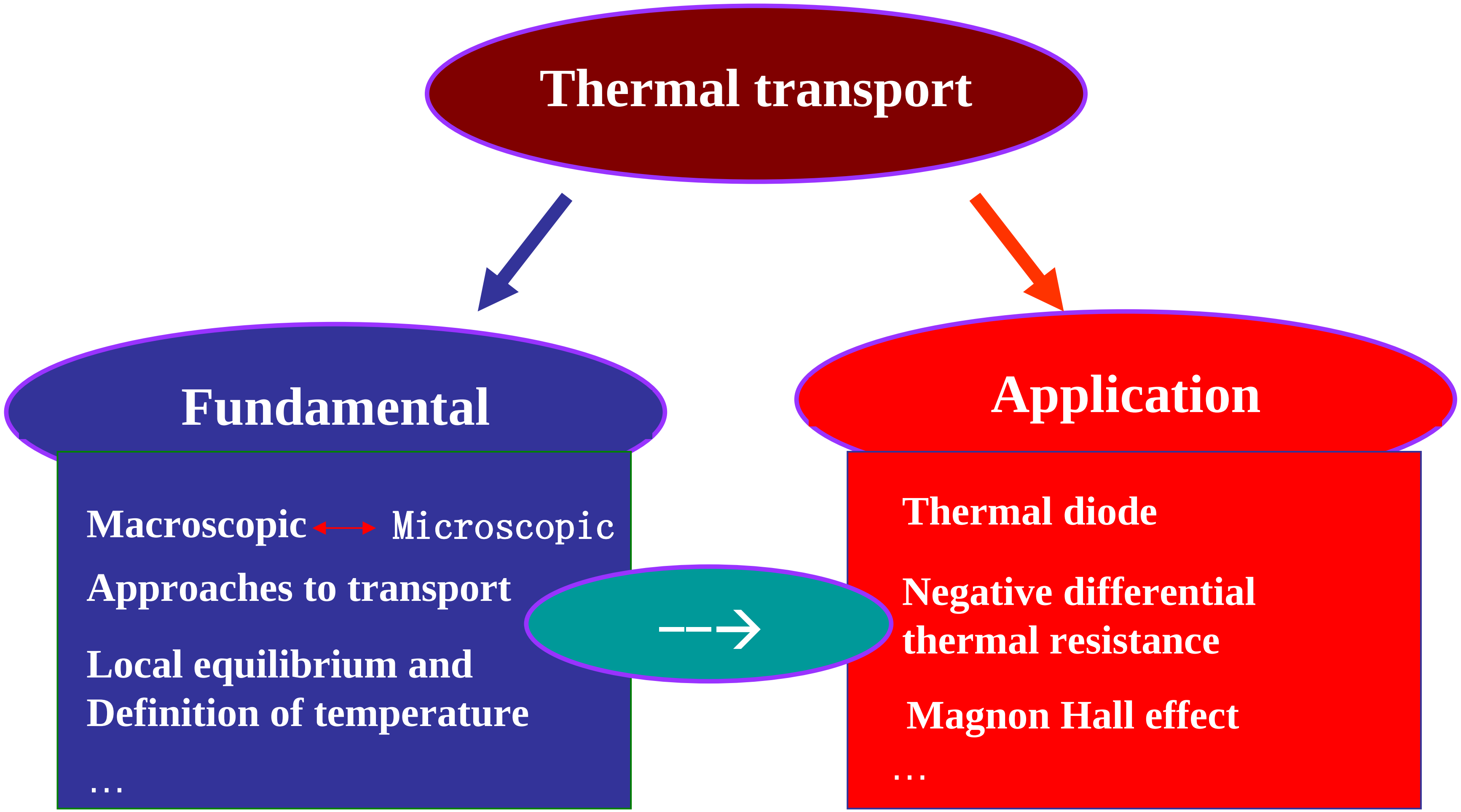
STATPHYS 19
The 19th IUPAP International Conference on Statistical Physics

The 19th IUPAP International Conference on Statistical Physics (1995)

Outline

1. Introduction
2. Interfacial thermal conduction and negative temperature jump
3. Thermal expansion and its impacts on thermal transport
4. Conclusion and remarks

Introduction



DH, S. Buyukdagli, and B. Hu, Phys. Rev. E (2008).

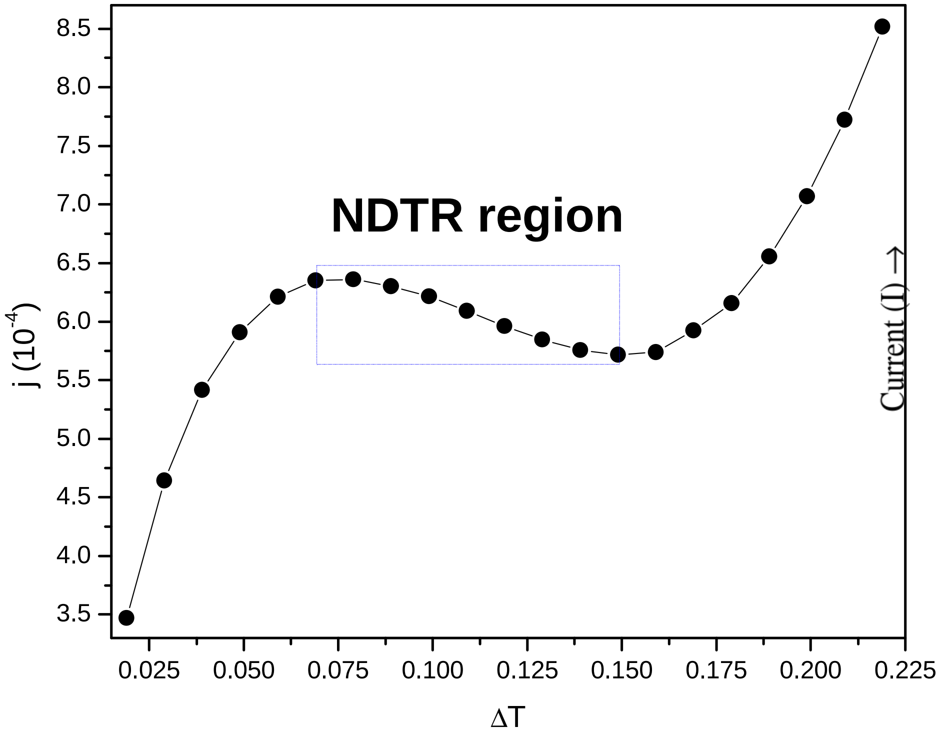
L. Wang, **DH**, and B. Hu, Phys. Rev. Lett. (2010).

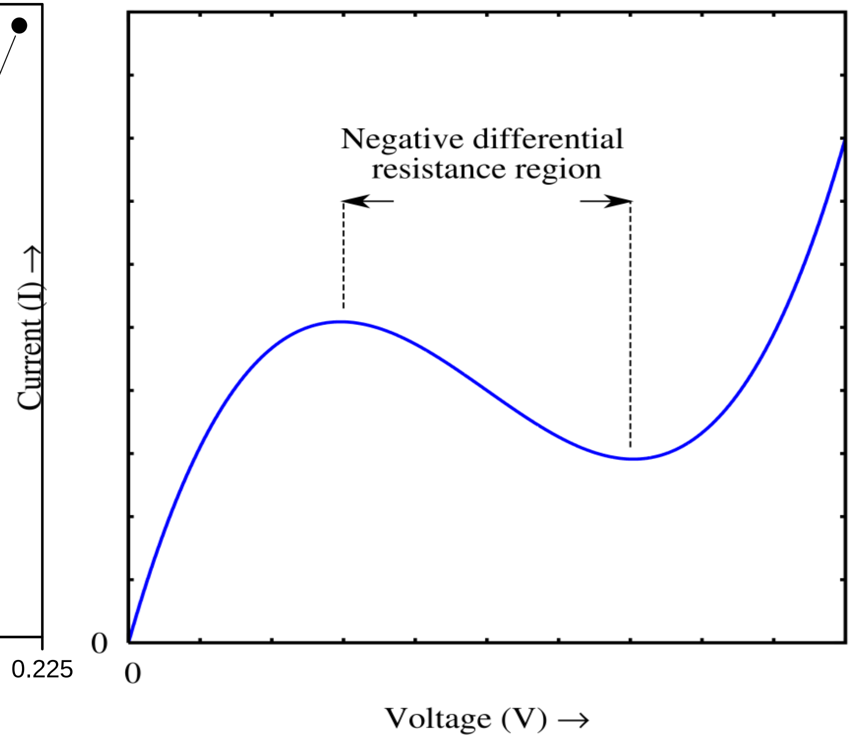
J. Wang, **DH,** Y. Zhang, J. Wang and H. Zhao, Phys. Rev. E (2015).

DH, S. Buyukdagli, and B. Hu, Phys. Rev. B (2009).

DH, B. Ai, H. Chan, and B. Hu, Phys. Rev. E (2010).

Negative differential thermal resistance





Negetive differential thermal resistance in the Frenkel- Kontorova (FK) model

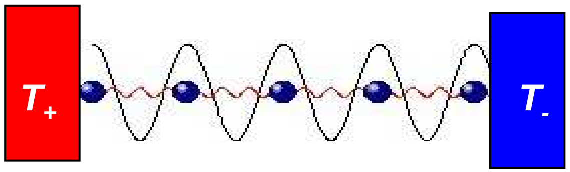
DH, B. Ai, H. Chan, and B. Hu, *Phys. Rev.* **E 81**, 041131 (2010)

Negetive differential electrical resistance in tunneling diode

Illustrative figure for the work by L. Esaki, *Phys. Rev*. **109**, 603 (1958)

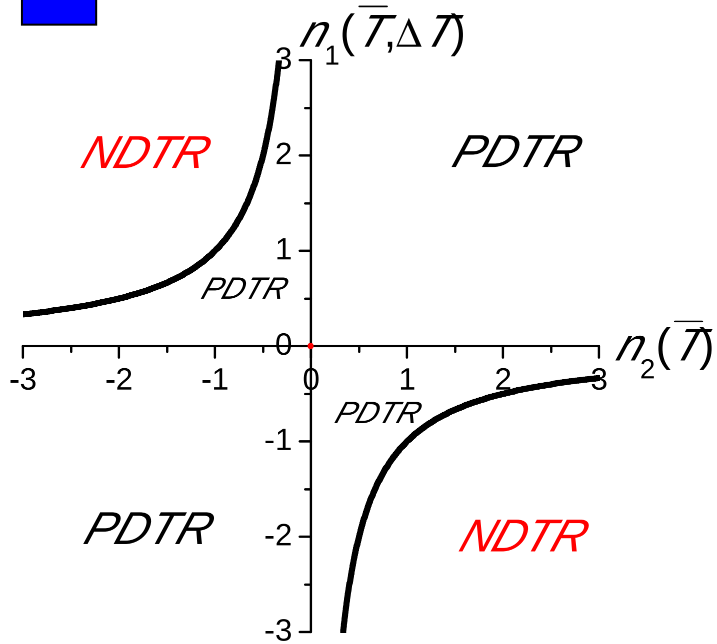
http://en.wikipedia.org/wiki/File:Negative_differential_resistance.png

A general theoretical analysis for NDTR



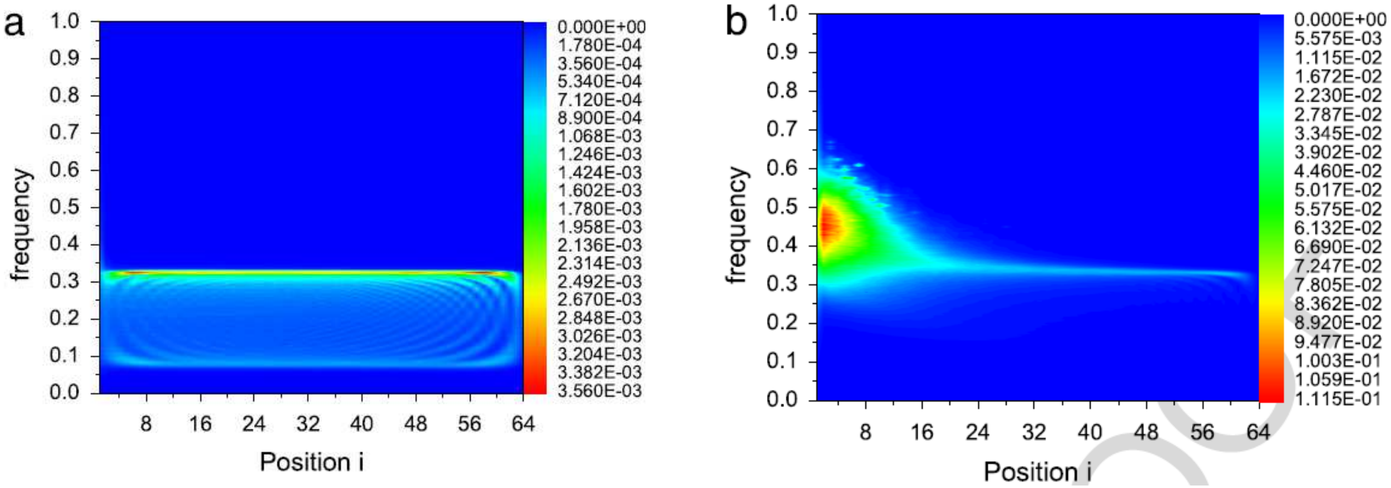
Conditions for NDTR：

$$n_1(\bar{T},\Delta T)n_2(\bar{T}) < -1$$



H.-K. Chan, **DH**, B.Hu, *Phys. Rev.* **E** 89, 052126 (2014).

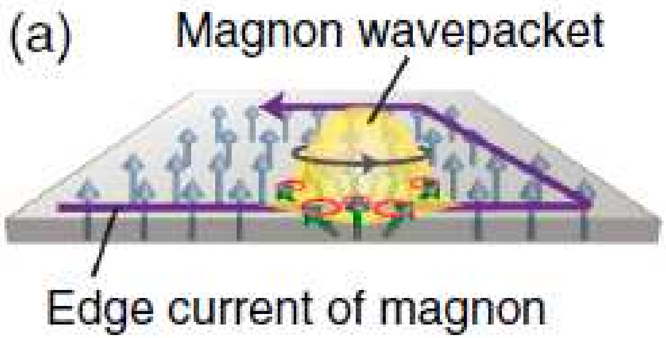
Effect of dynamical localization on NDTR

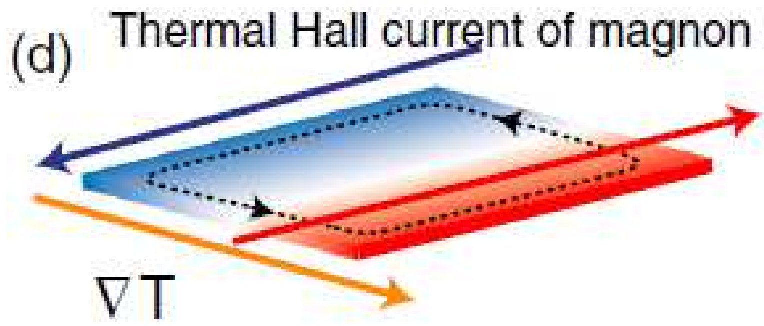


The mechanism for the presence of NDTR is understood based on dynamical localization of oscillation modes.

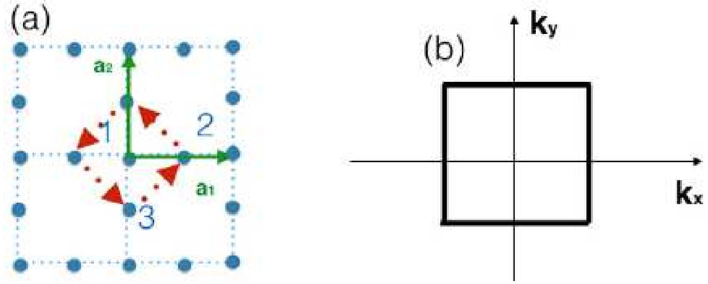
W. Fu, T. Jin, **DH**, S. Qu, *Physica* A 433, 211 (2015).

Magnon Hall effect on the Lieb lattice





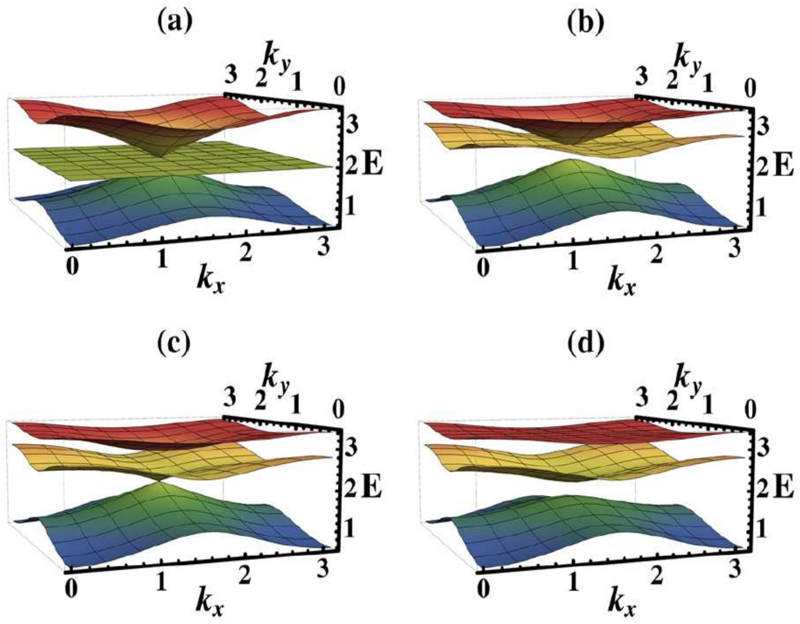
Question: Can magnon Hall effect occur on a lattice with inversion symmetry?



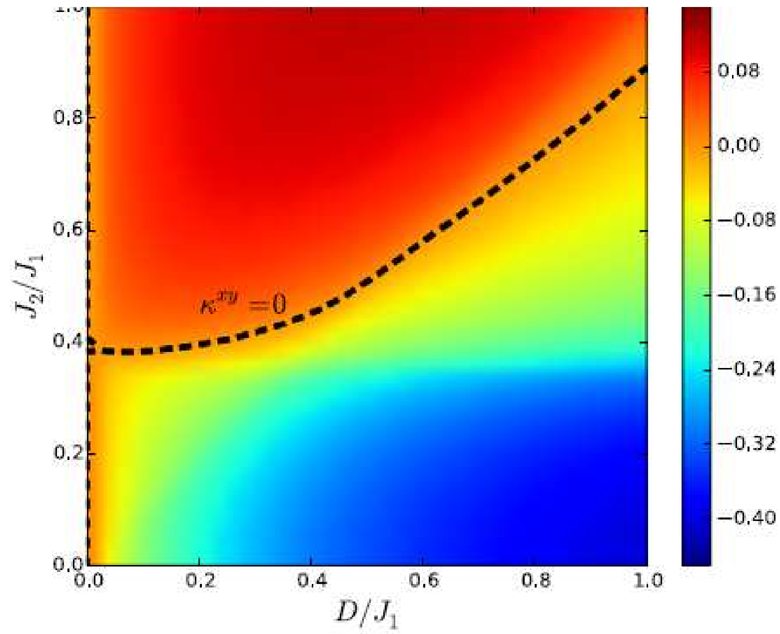
Lieb lattice

X. Cao, K. Chen and **DH**, *J. Phys.: Condens. Matter* 27, 166003 (2015).

Magnon Hall effect on the Lieb lattice



Magnon band structure



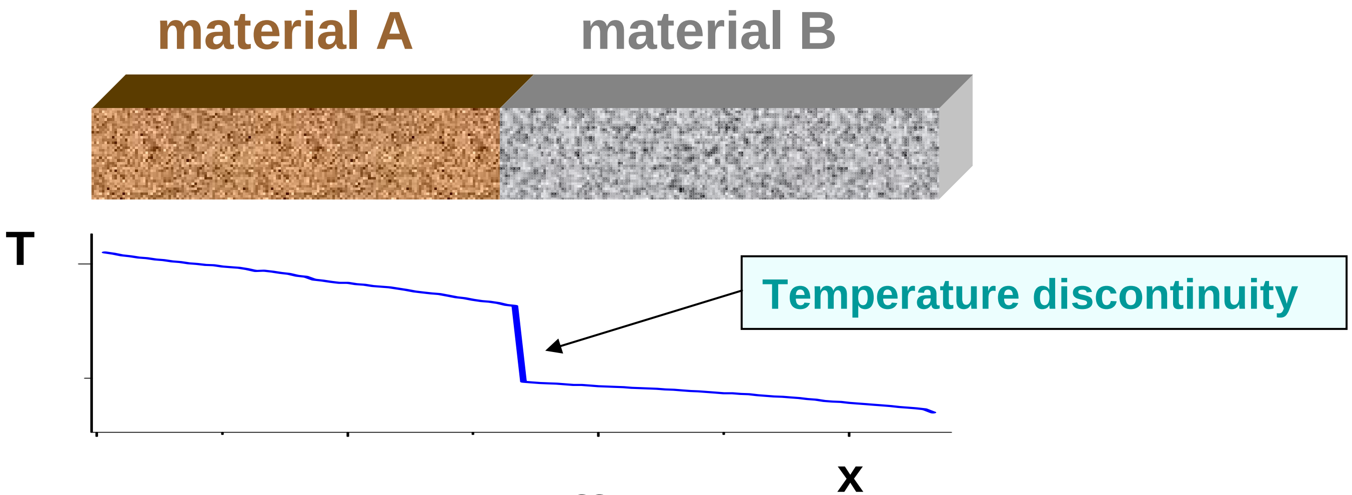
Transverse thermal conductivity

X. Cao, K. Chen and **DH**, *J. Phys.: Condens. Matter* 27, 166003 (2015).

Part I

Interfacial thermal conduction and negative temperature jump

Interfacial thermal conduction: Kapitza Resistance



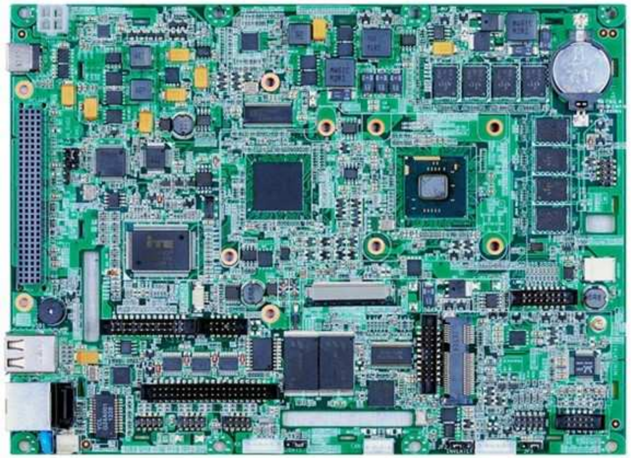
Kapitza Effect

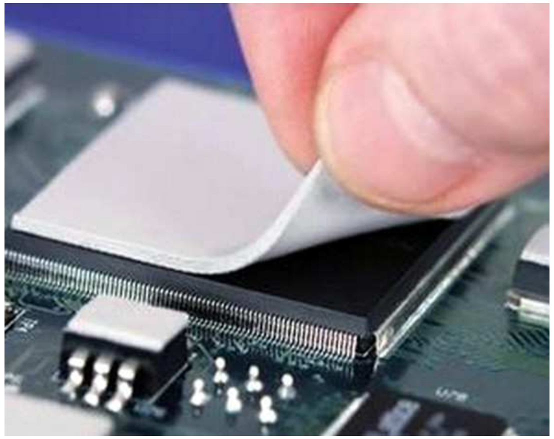
$$R_b = \frac{\Delta T_b}{J}$$

- 1941, **Kapitza** reported his measurements of the **temperature drop** near the boundary between helium and a solid when heat flows across the boundary.
- 1952, **Khalatnikov** presented the **acoustic mismatch model**.
- 1959, **Little** extended the acoustic mismatch model to **solid- solid boundaries**.
- 1987, **Swartz** developed the so called **diffuse mismatch model**.

[1] Swartz and Pohl, *Rev. Mod. Phys.* 61, 605 (1989).

Interfacial thermal conduction at atomic scale





Molecular dynamics simulation

B. Li, J. Lan, L. Wang, *Phys. Rev. Lett.* 95, 104302 (2005).

Scattering boundary method

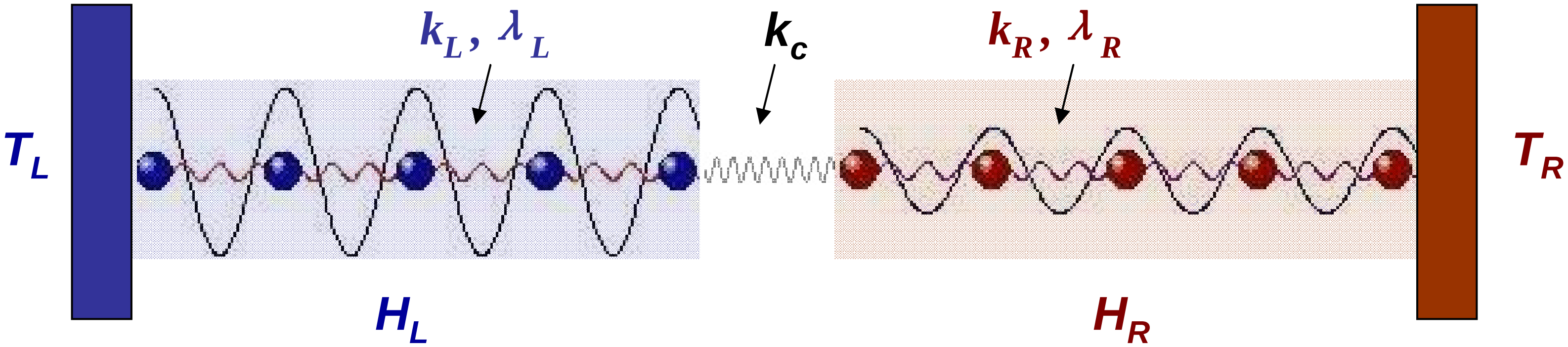
Lumpkin, Saslow and Visscher, Phys. Rev. ***B*** 17, 4295 (1978).

L. Zhang, P. Keblinski, J.-S. Wang, and B. Li, Phys. Rev. ***B*** 83, 064303 (2011).

Self-consistent phonon theory

DH, S. Buyukdagli, B.Hu, Phys. Rev. ***B*** 80, 104302 (2009).

Model



$$H = H_L + \frac{k_c}{2}(x_{N/2} - x_{N/2+1})^2 + H_R$$

whre $$H_L = \sum_{i=1}^{N/2}\left(\frac{p_i^2}{2m} + \frac{f_L}{2}x_i^2 + \frac{\lambda_L}{4}x_i^4\right) + \sum_{i=0}^{N/2-1}\frac{k_L}{2}(x_{i+1} - x_i)^2,$$

$$H_R = \sum_{i=N/2+1}^{N}\left(\frac{p_i^2}{2m} + \frac{f_R}{2}x_i^2 + \frac{\lambda_R}{4}x_i^4\right) + \sum_{i=N/2}^{N-1}\frac{k_R}{2}(x_{i+1} - x_i)^2,$$

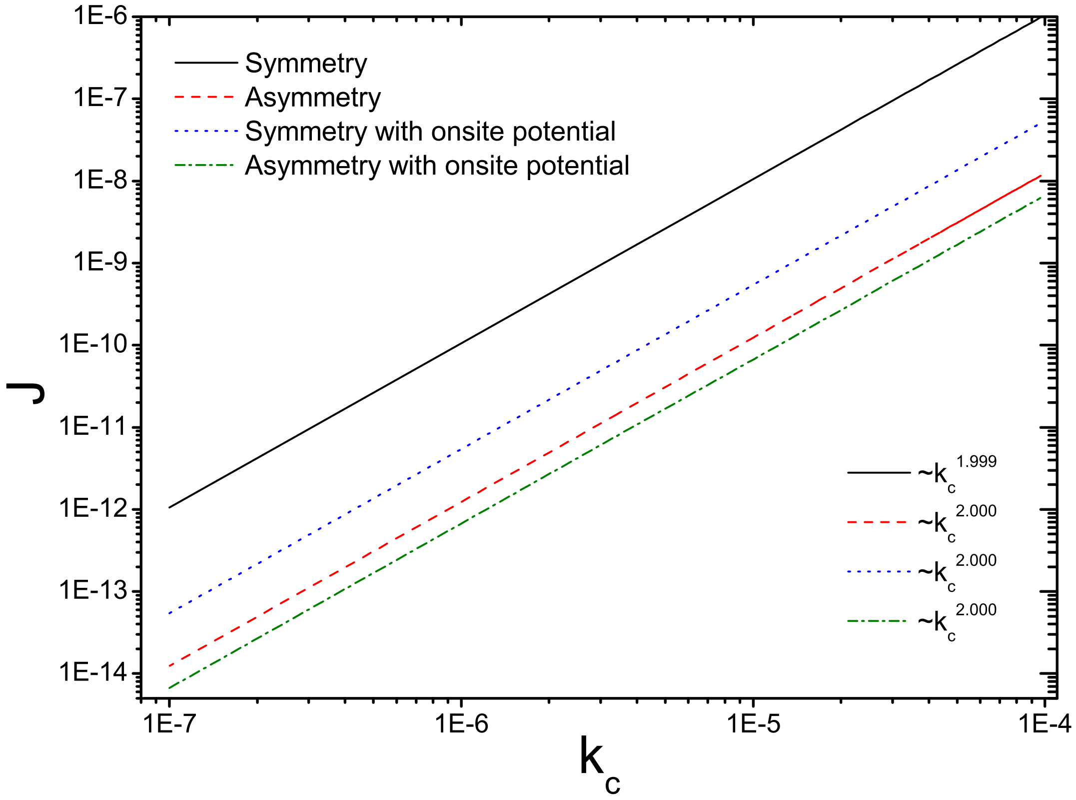
X. Cao and **DH**, Phys. Rev. E 92, 032135 (2015).

Harmonic system: weak coupling

Harmonic system: $\lambda_{L,R} = 0$

Langevin equations and Green function method:

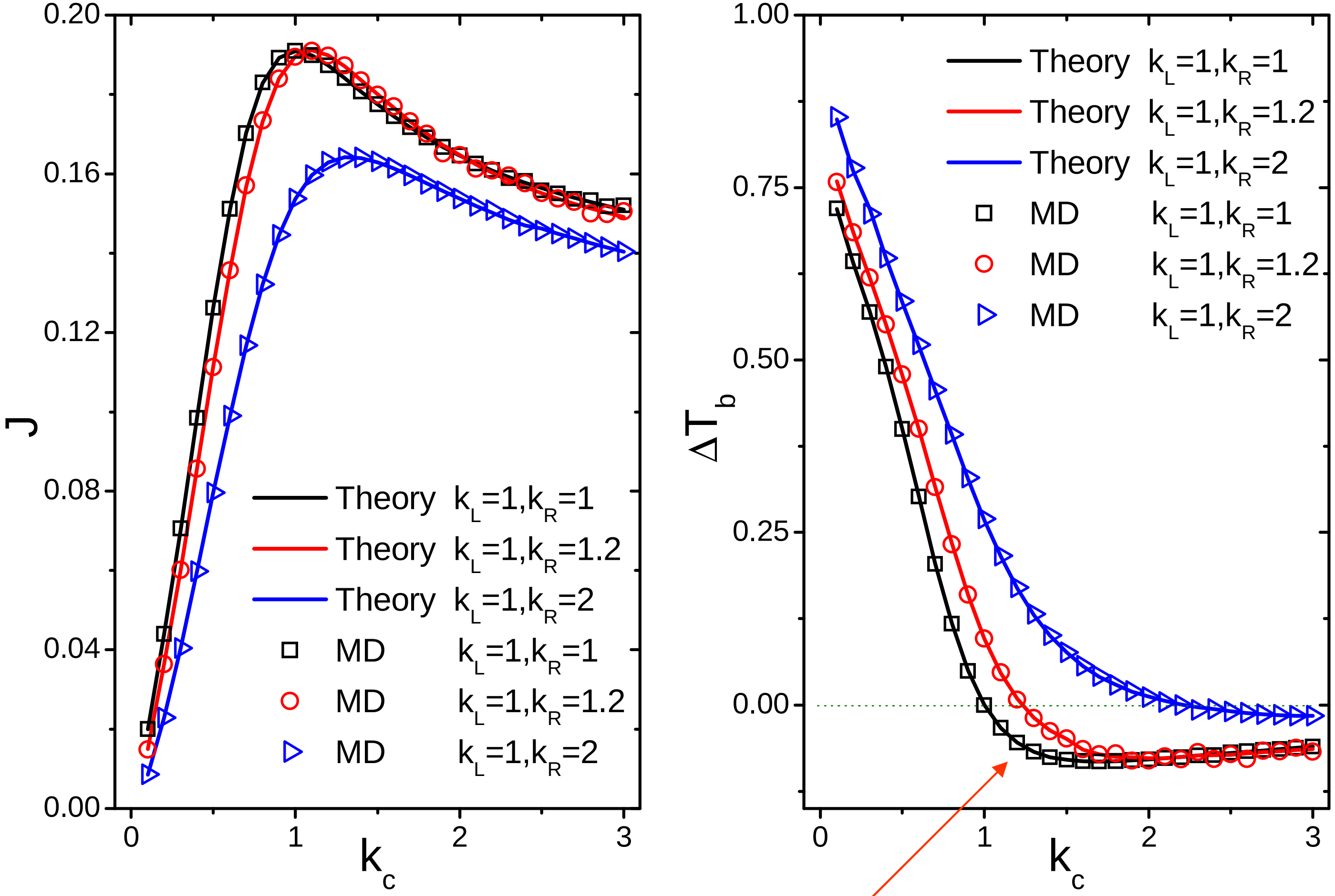
$$J = \frac{k_B(T_L - T_R)}{\pi}\int_{-\infty}^{+\infty} d\omega \, \mathrm{Tr}\left[G_S^+(\omega)\Gamma_L(\omega)G_S^-(\omega)\Gamma_R(\omega)\right]$$



$J \sim k_c^2$

Harmonic system: strong coupling

$$\Delta T_b = T_{N/2} - T_{N/2+1}$$



Negative temperature jump !

Contribution of phonon modes to local temperature

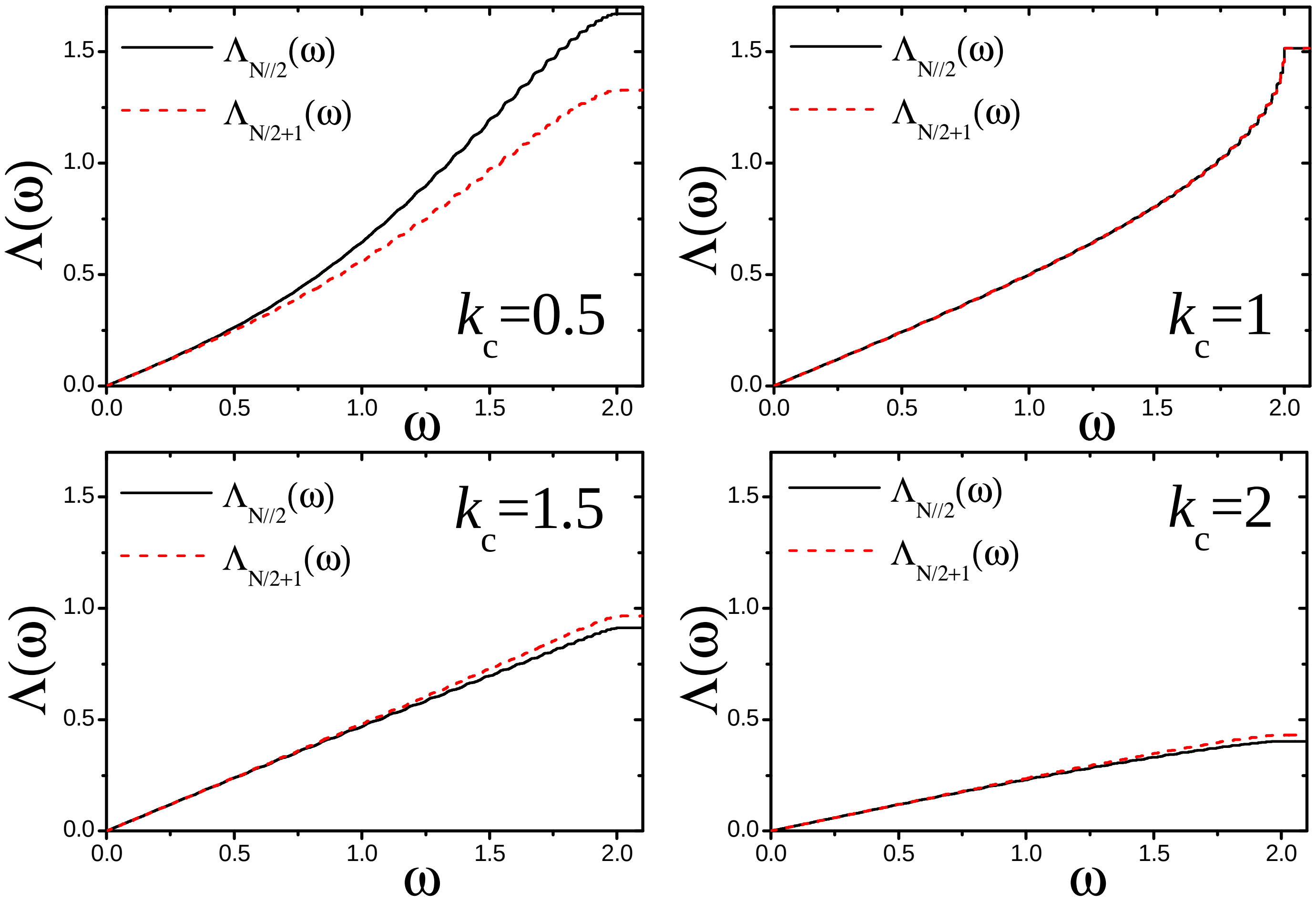
$$\mathrm{K} = \left\langle \dot{\tilde{X}}_S \dot{\tilde{X}}_S^T \right\rangle = \frac{k_B T_L}{\pi} \int_{-\infty}^{+\infty} d\omega\, \omega G_S^+(\omega) \Gamma_L(\omega) G_S^-(\omega)$$
$$+ \frac{k_B T_R}{\pi} \int_{-\infty}^{+\infty} d\omega\, \omega G_S^+(\omega) \Gamma_R(\omega) G_S^-(\omega)$$

Local temperature $T_i = m K_{ii}$

Let $T_i = \Lambda_i(\omega_{\max})$

$$\Lambda_i(\omega) = \frac{2 m k_B}{\pi} \int_0^{\omega} d\omega' \omega' \begin{bmatrix} T_L G_S^+(\omega') \Gamma_L(\omega') G_S^-(\omega') \\ + T_R G_S^+(\omega') \Gamma_R(\omega') G_S^-(\omega') \end{bmatrix}$$

Contribution of phonon modes to local temperature



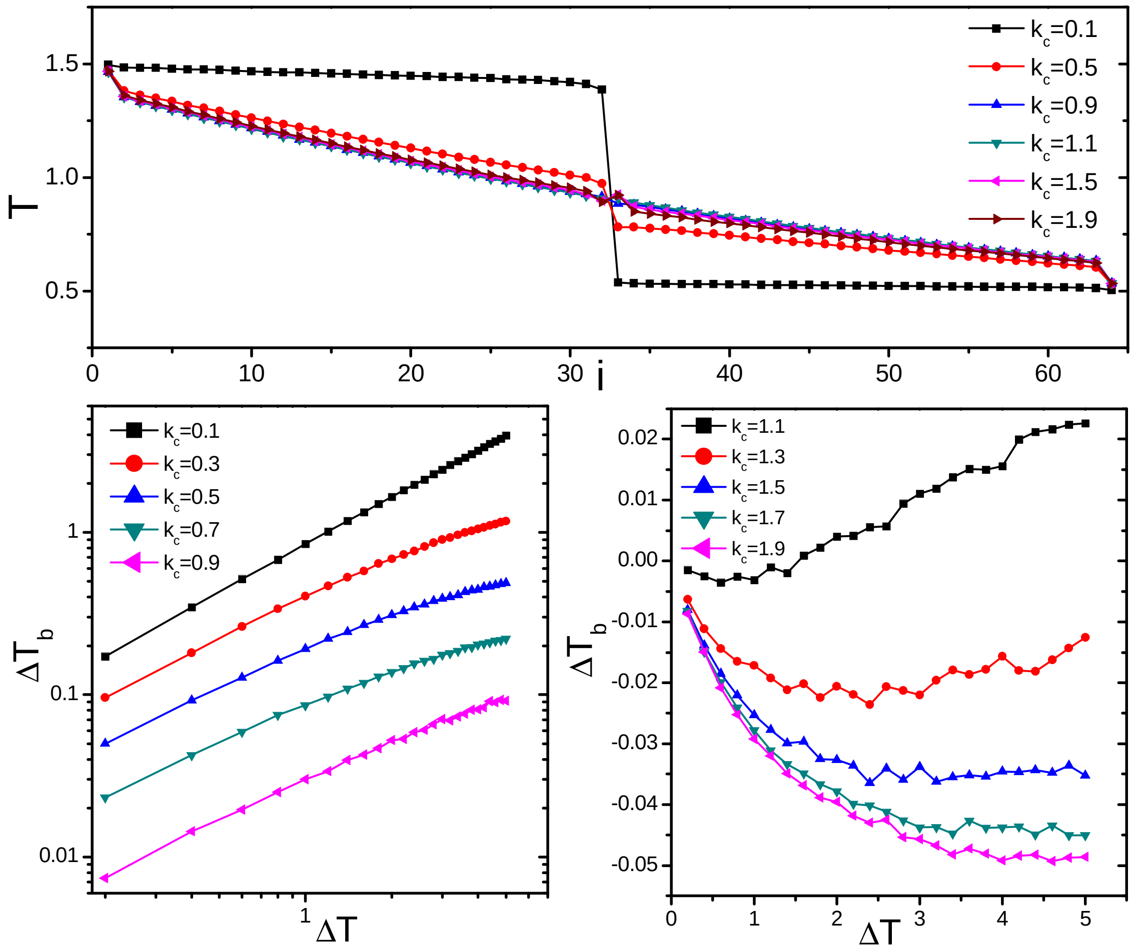
- Question 1:

  Is the negative temperature jump an artificial effect due to the integrability of the system?

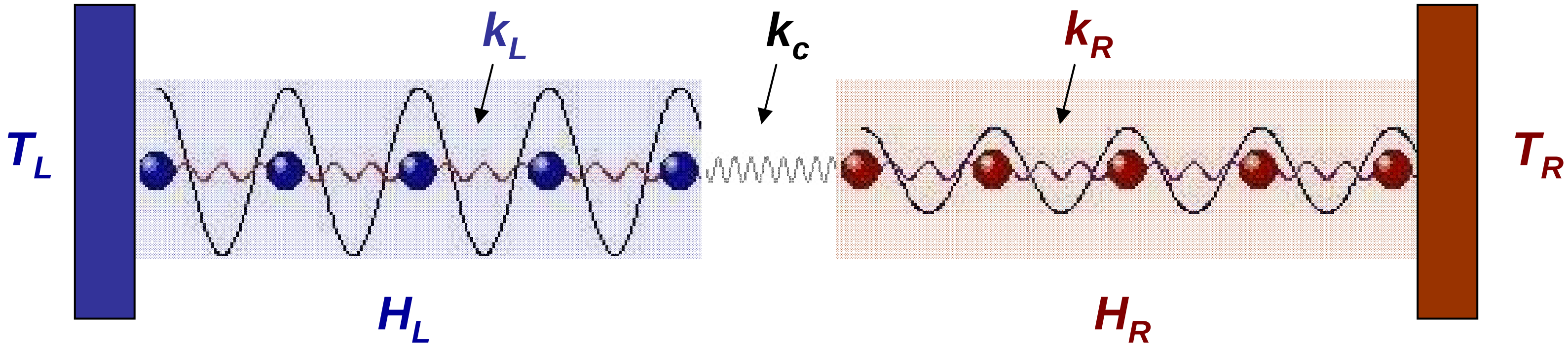
- Question 2:

  Does the negative temperature jump come from the ill-defined interface with a sharp discontinuity of the interfacial coupling?

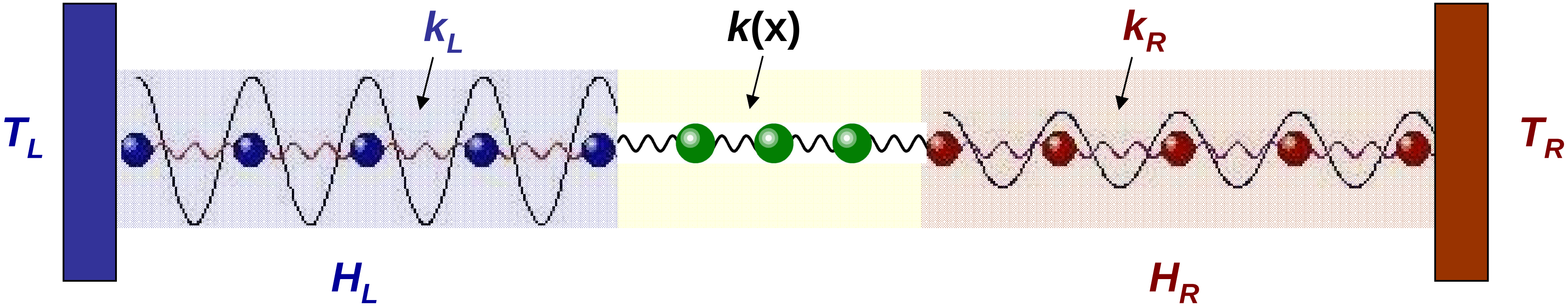
Negative temperature jump: the ϕ^4 model



Extended model with an intermediate junction



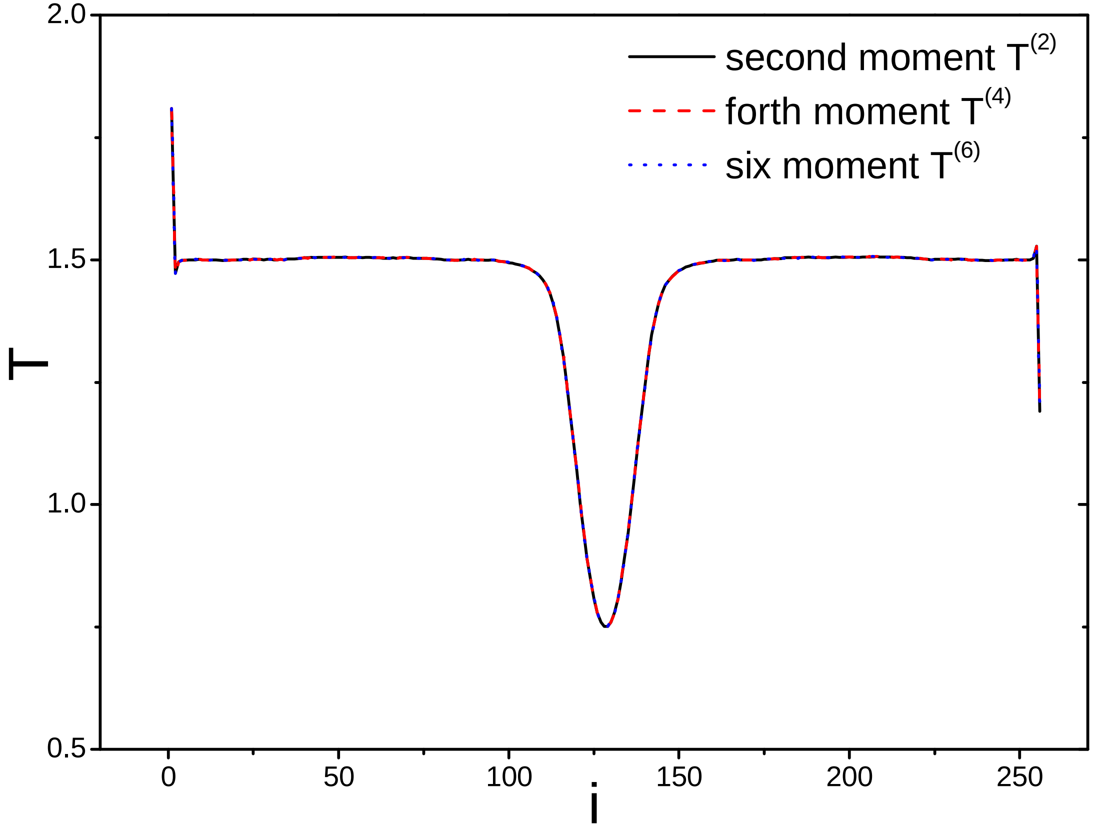
Extended model with an intermediate junction



Smooth variation of spring constants inside the interfacial region

$$k_i = \exp(-(i - N/2)^2/50) + 1$$

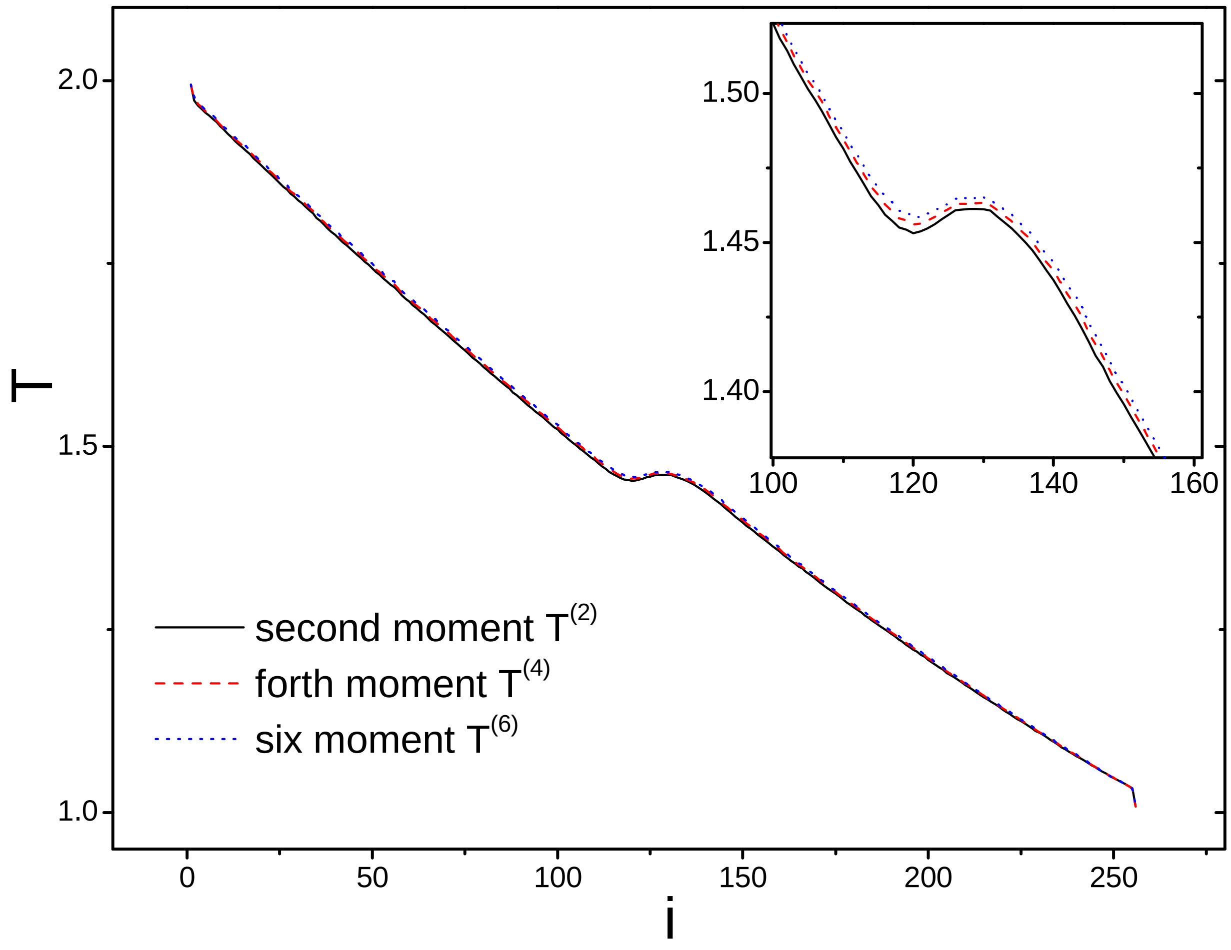
Temperature profile: the harmonic model



$$T_i^{(2)} = m\left\langle \dot{x}_i^2 \right\rangle,\quad T_i^{(4)} = m\left((\dot{x}_i^4)/3 \right)^{1/2},\quad T_i^{(6)} = m\left((\dot{x}_i^6)/15 \right)^{1/3}$$

T. Mai, A. Dhar, and O. Narayan, PRL 98, 184301 (2007)

Temperature profile: the ϕ^4 model



Part II

Thermal expansion and its impacts on thermal transport in the FPU-α-β model

X. Cao, **DH**, H. Zhao, and B. Hu, AIP Advances 5, 053203 (2015)

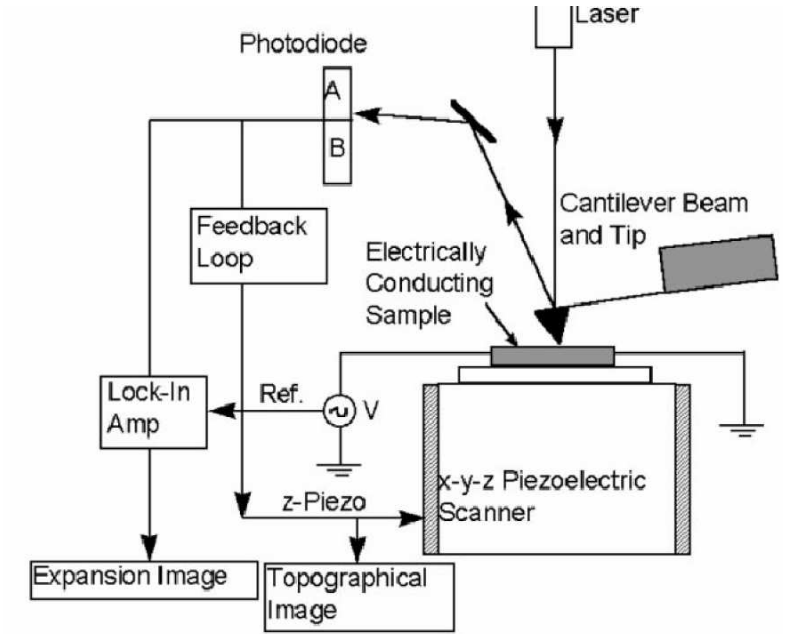
Motivation I

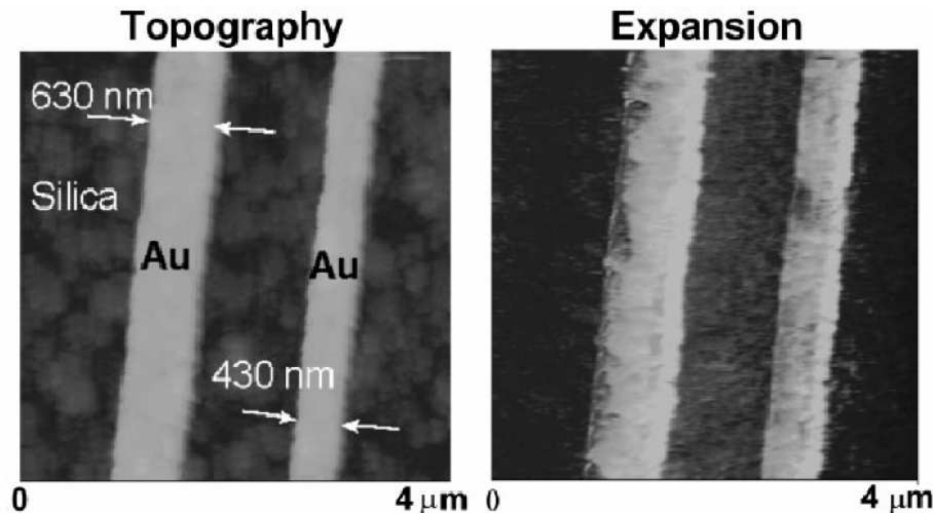
- Recent controversy on the effect of asymmetric interaction potential on normal thermal conduction.

  (Hong Zhao's and Yong Zhang's talk)

Motivation II: application aspects

With the rapid development of nanotechnique, thermal expansion plays an important role for thermal measurement, designing nanodevices with intriguing electronic, mechanical and thermal properties. .





Appl. Phys. Lett. 66, 694

Motivation III: theoretical aspects

Most of previous analytical studies used the perturbation approach, such as lattice-dynamics calculations, and Nonequilibrium Green's function theory, which is incapable of dealing with strong anharmonicity for which some concerned intriguing properties occur. .

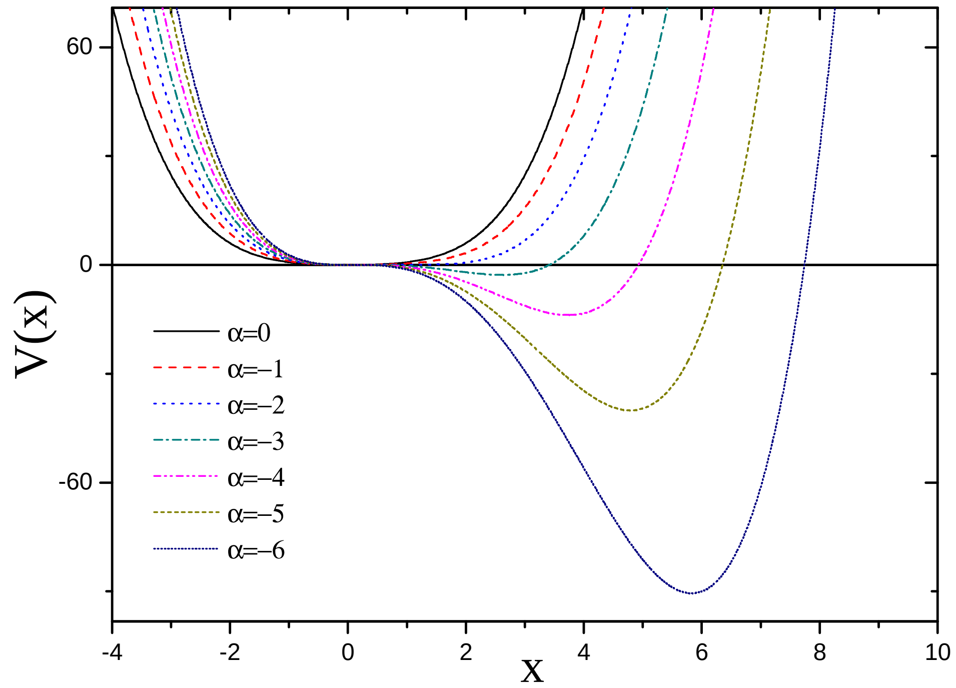
J. Fabian, and P. B. Allen, *Phys. Rev. Lett*. 79, 1885 (1997).

D. A. Broido, A. Ward, and N. Mingo, *Phys. Rev. B* 72, 014308 (2005).

J.-W. Jiang, J.-S. Wang, and B.Li, *Phys. Rev. B* 80, 205429 (2009).

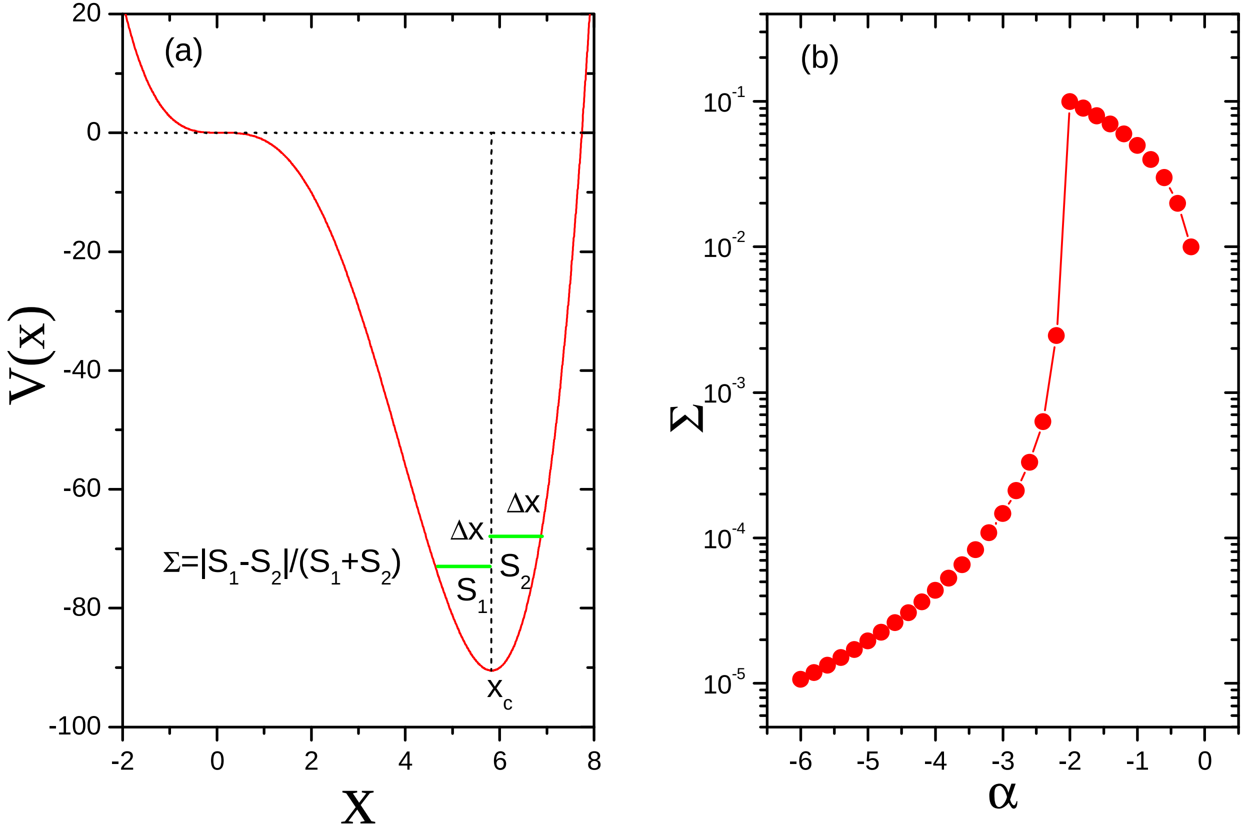
Potential Profile of FPU-α-β model

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i=1}^{N-1} V(q_{i+1} - q_i) \qquad V(x) = \frac{k}{2}x^2 + \frac{\alpha}{3}x^3 + \frac{\beta}{4}x^4$$

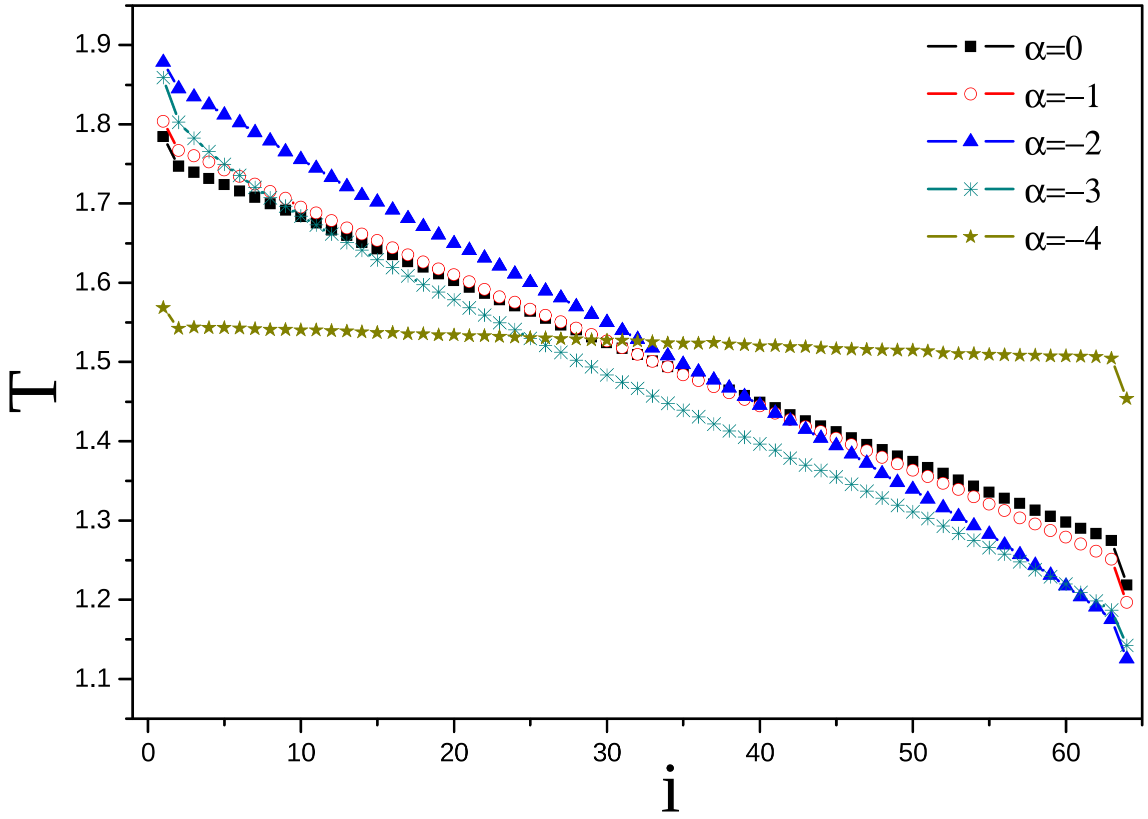


Quantify the asymmetry

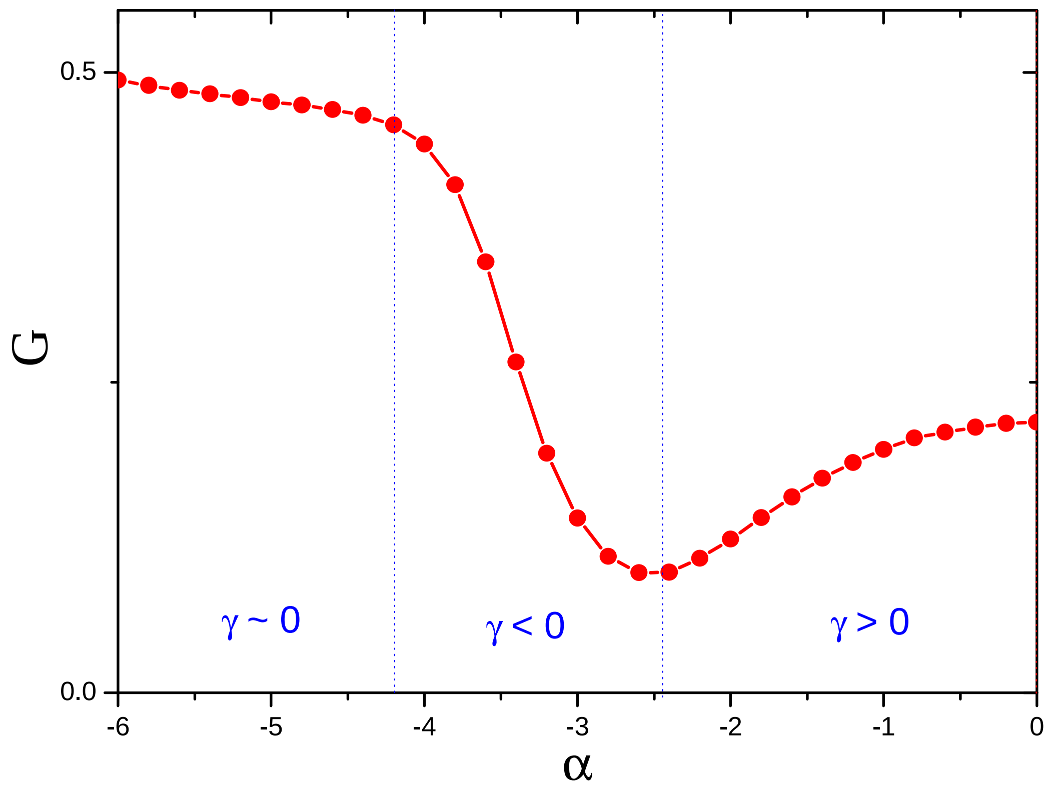
$$\Sigma = |S_1 - S_2|/(S_1 + S_2)$$



Temperature profile



Thermal conductance



The nonmonotonic behavior of G can be divided by three domains, corresponding to negative, positive and vanishing coefficient of thermal expansion γ , respectively.

X. Cao, **DH**, H. Zhao, and B. Hu, AIP Advances 5, 053203 (2015)

Self-consistent phonon theory (SCPT)

Incorporating the nonlinearity into normal modes by renormalizing the harmonic frequency spectrum, which is realized by performing thermal average with respect to a trial Hamiltonian

$$H^{eff} = \sum \frac{p_i^2}{2m} + \frac{f}{2}(u_{i+1} - u_i)^2$$

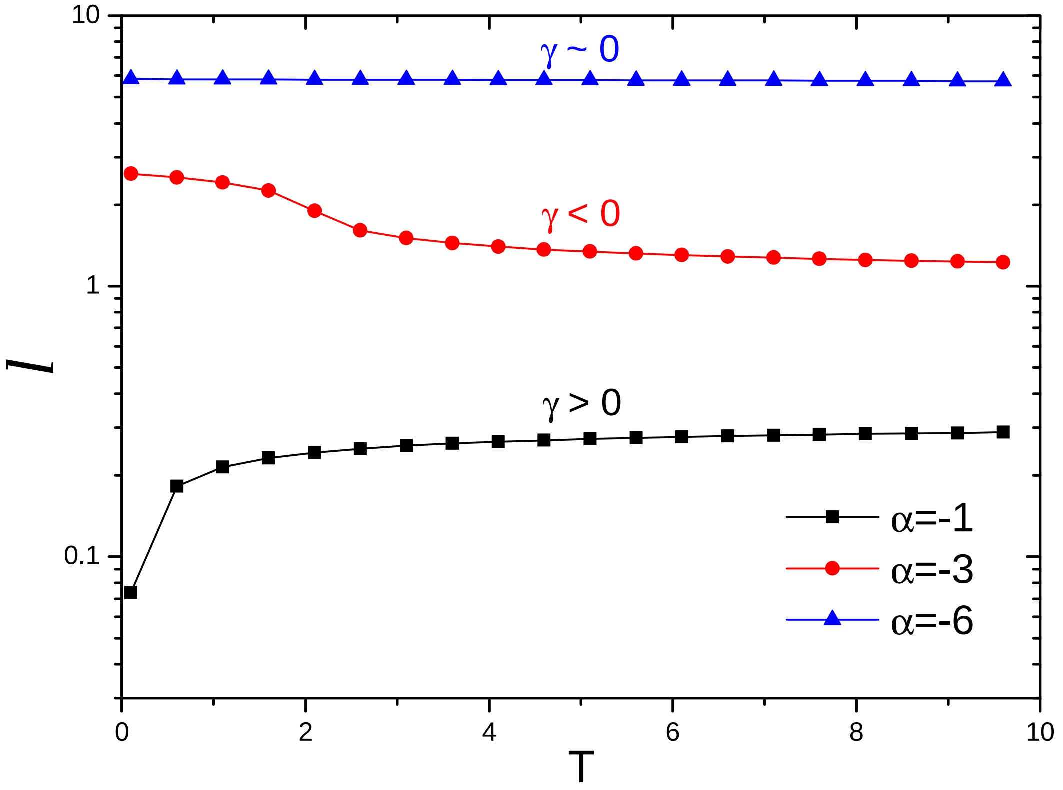
Where the effective harmonic potential coefficient f(T) can be obtained from the self-consistent equations:

$$\left\langle \frac{\partial V(x)}{\partial x} \right\rangle_0 = 0, \qquad \left\langle \frac{\partial^2 V(x)}{\partial x^2} \right\rangle_0 = f$$

T. Dauxois, et al, *Phys. Rev.* **E** 47, 684(1993)

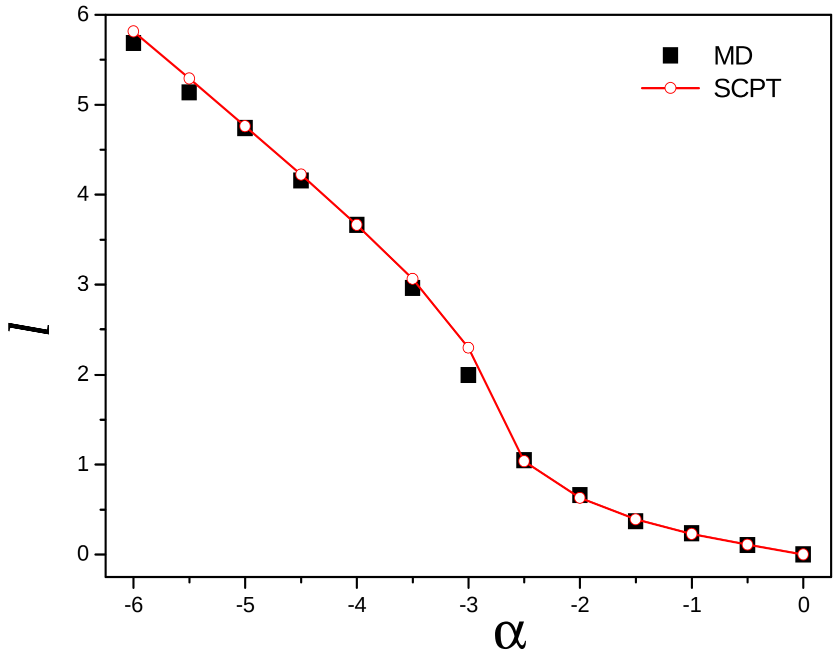
DH, S. Buyukdagli, and B. Hu, *Phys. Rev.* **E 78**, 061103 (2008)

Coefficient of thermal expansion



notes

Effect of nonlinearity on thermal expansion



Thermal expansion as a function of anharmonicity

Scaling relation for thermal conductance:

$$G(sT_{L,R}, s^{-\frac{1}{2}}\alpha, s^{-1}\beta) = G(T_{L,R}, \alpha, \beta)$$

X. Cao, **DH**, H. Zhao, and B. Hu, *AIP Advances* 5, 053203 (2015).

Conclusion and remarks

- The occurrence of the negative temperature jump is not trivially artificial due to the integrability or sharp discontinuity of the interfacial coupling.

- One should reexamine the concept of **temperature**
  - Definition of local temperature in microscopic models.
  - Do we need a "nonequilibrium temperature"?

- The second law is not violated, although we might need a good way to manifest it.

X. Cao and **DH**, Phys. Rev. E 92, 032135 (2015).

Conclusion and remarks

- Three domains of thermal conductance with respect to α are identified, which is related to thermal expansion effect.

- Self-consistent phonon theory is developed to study the effect of thermal expansion, which agrees well with the numerical simulations.

X. Cao, **DH**, H. Zhao, and B. Hu, AIP Advances 5, 053203 (2015)

Thank You !