Scaling analysis of negative differential thermal resistance

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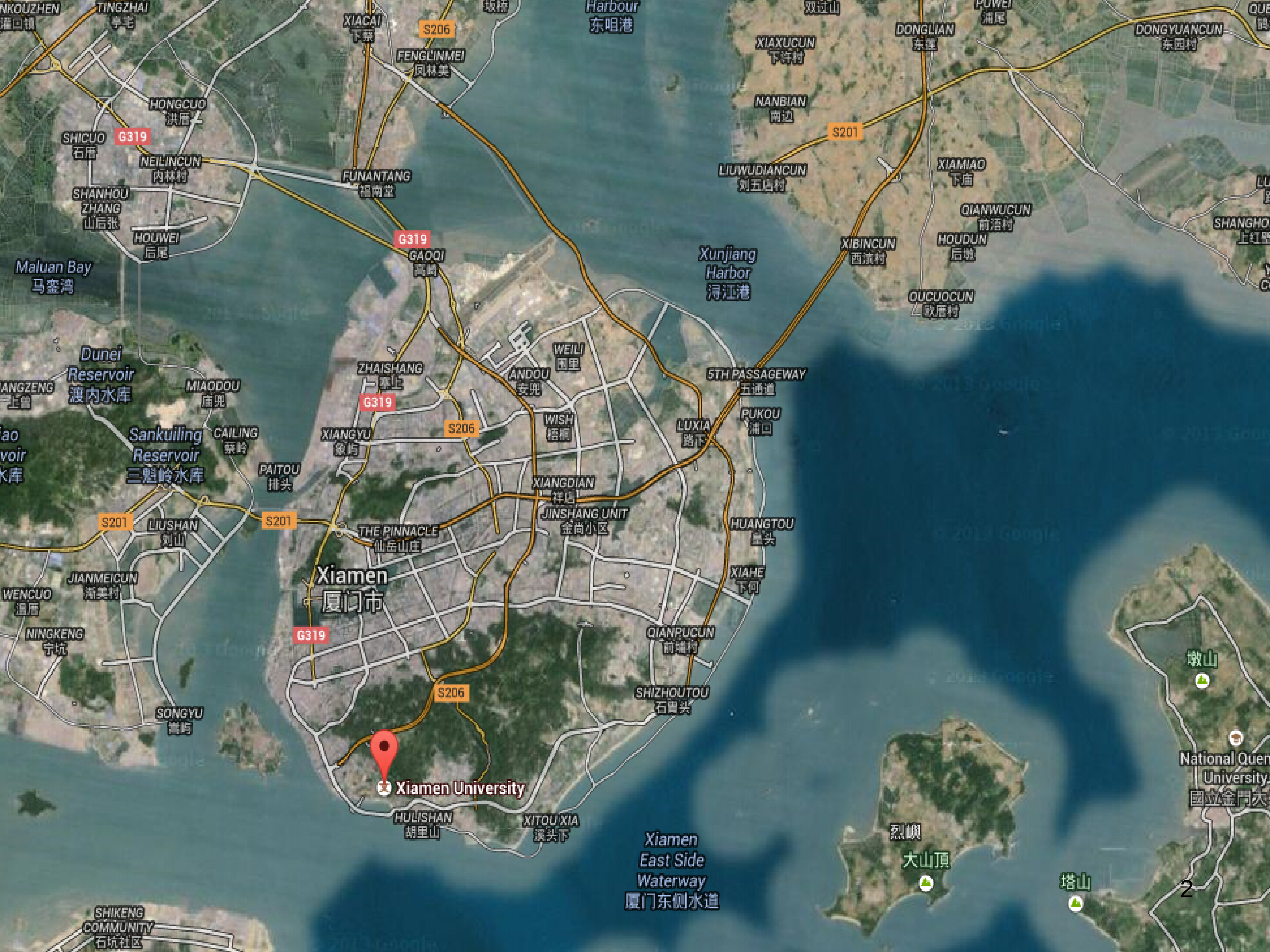
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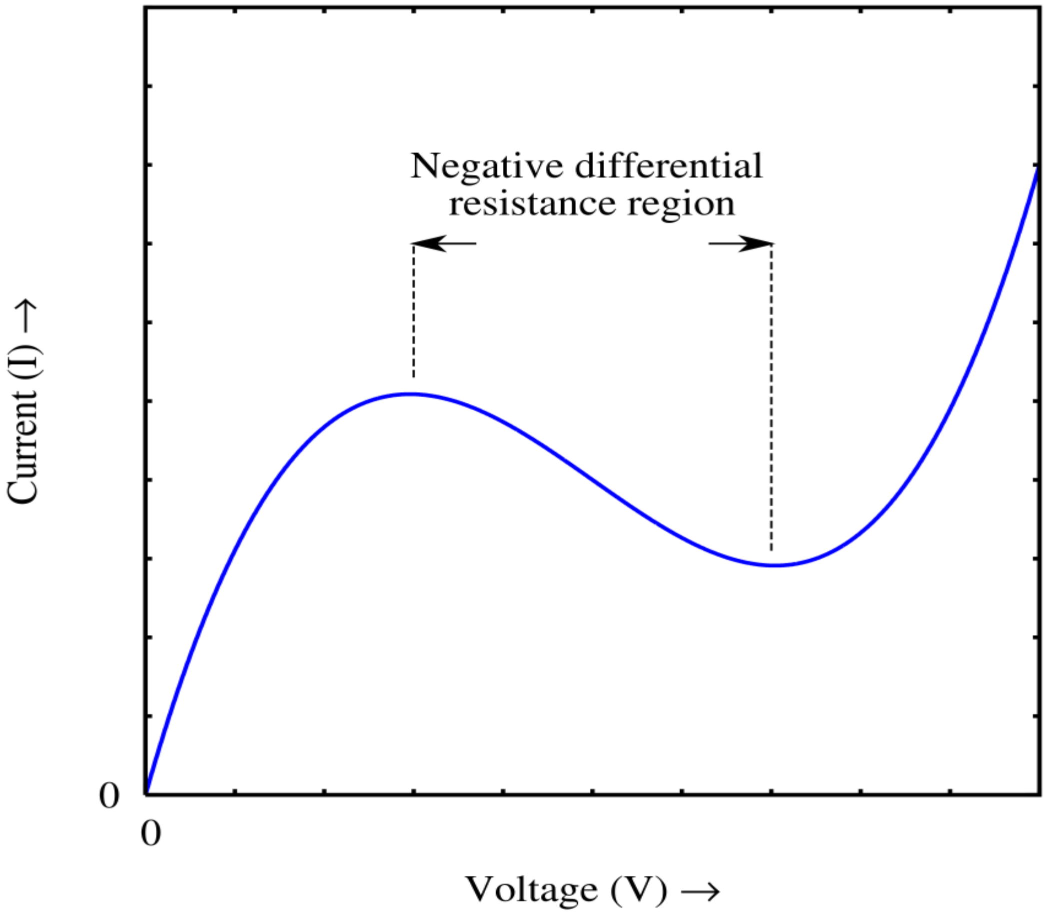
Part I

Outline

1. Introduction
2. Analysis
3. Examples
4. Conclusion

Negative differential electrical resistance in tunneling diode

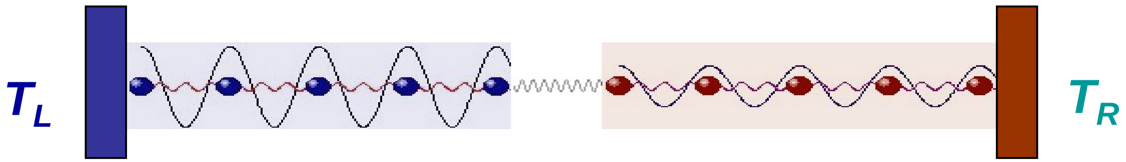


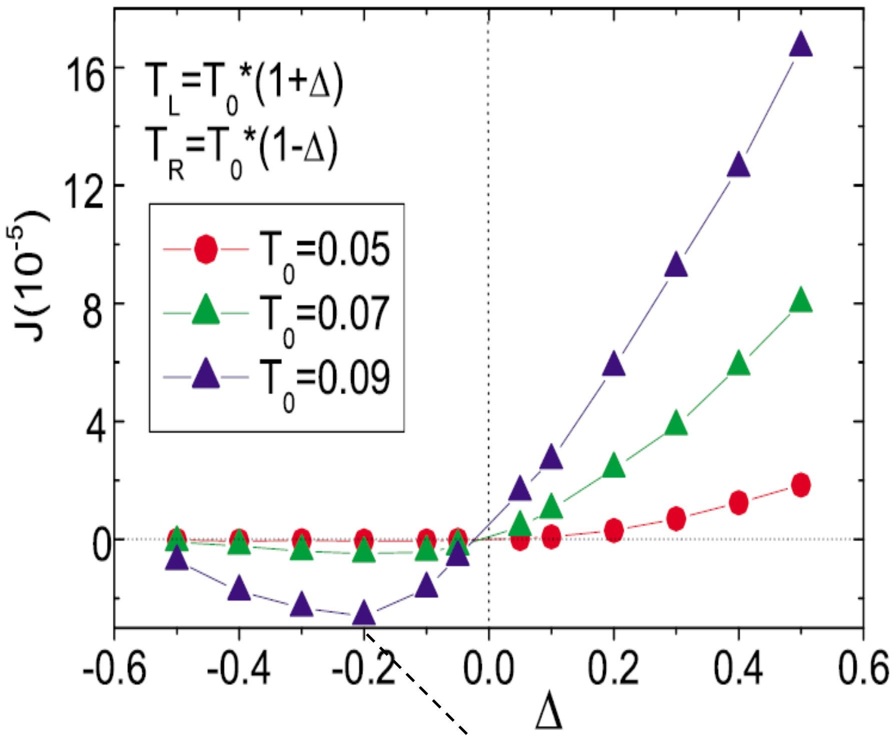
Leo Esaki (1925-)
Nobel Prize in Physics（1973）

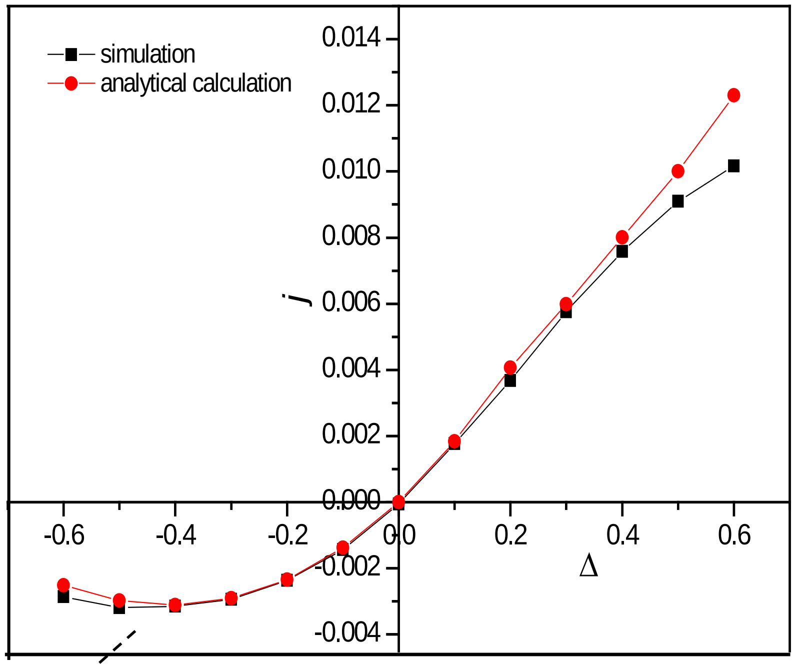
Illustrative figure for the work by L. Esaki, Phys. Rev. 109, 603 (1958)

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

NDTR in thermal diode







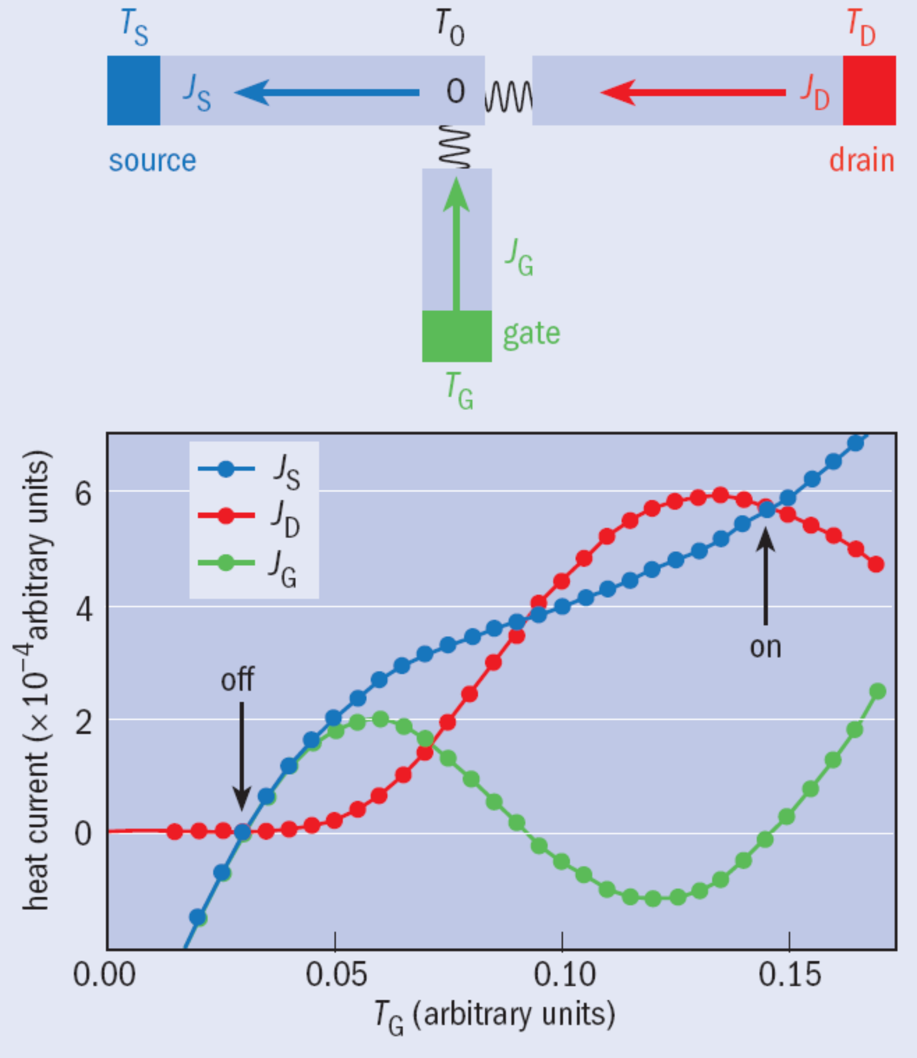
B. Li, L. Wang, G. Casati, PRL 93, 184301 (2004)

B. Hu, **DH**, L.Yang, Y. Zhang, PRE 74, 060101 (2006)

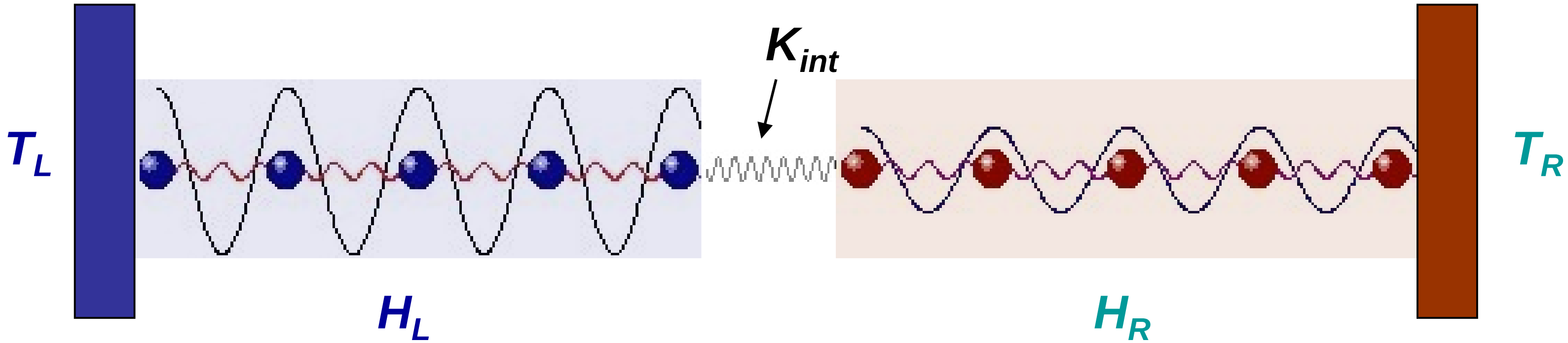
Negative differential thermal resistance (NDTR)

NDTR in thermal transistor

B. Li, L. Wang, G. Casati, APL 88, 143501 (2006)



Mechanism of NDTR



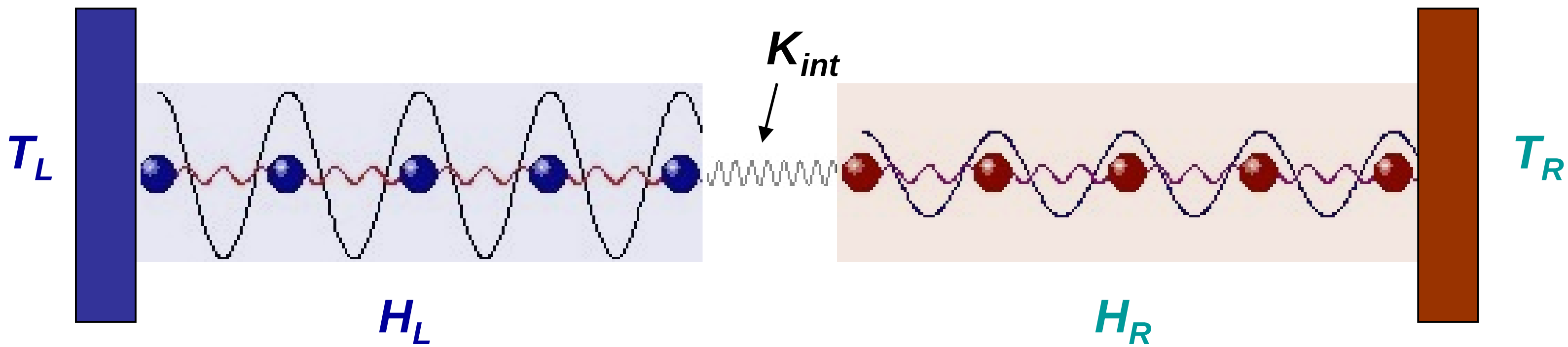
$$H = H_L + \frac{K_{\text{int}}}{2}(x_1 - x_0)^2 + H_R$$

$$\text{whre } H_{L,R} = \frac{p_i^2}{2} + \frac{1}{2}(x_{i+1} - x_i)^2 + U_{L,R}(x_i)$$

Difficulty of analysis :

I. Nonequilibrium stationary state
II. Nonlinearity
III. Qusi-particle entity of phonons

Mechanism of NDTR



$$H = H_L + \frac{K_{\text{int}}}{2}(x_1 - x_0)^2 + H_R$$

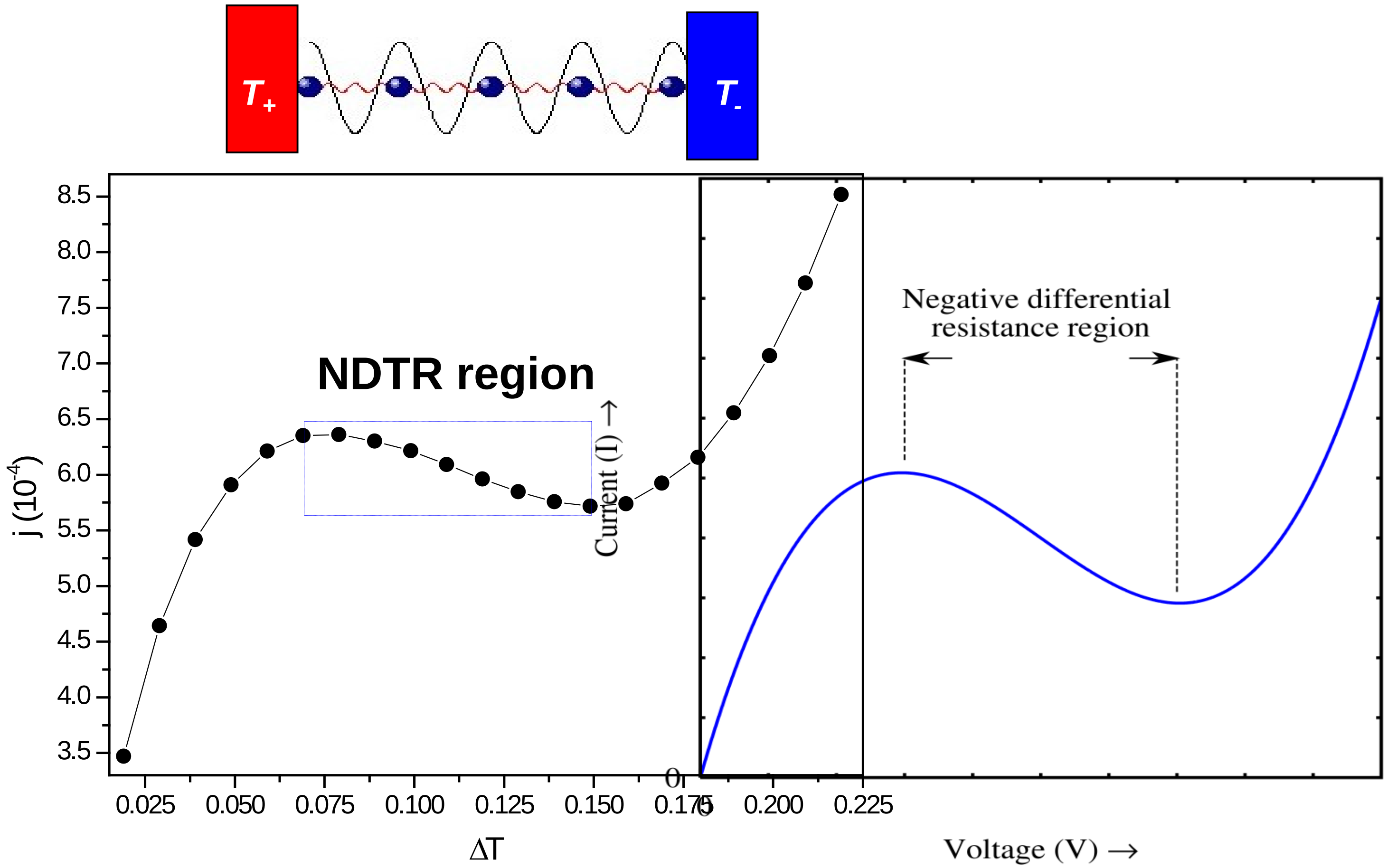
whre $H_{L,R} = \frac{p_i^2}{2} + \frac{1}{2}(x_{i+1} - x_i)^2 + U_{L,R}(x_i)$

$$j = \sigma \Delta T$$

where $\sigma = \frac{k_B}{2\pi}\int_{\omega_{\min}}^{\omega_{\max}} \alpha(\omega) d\omega$

Transport process in the nonlinear response regime

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



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

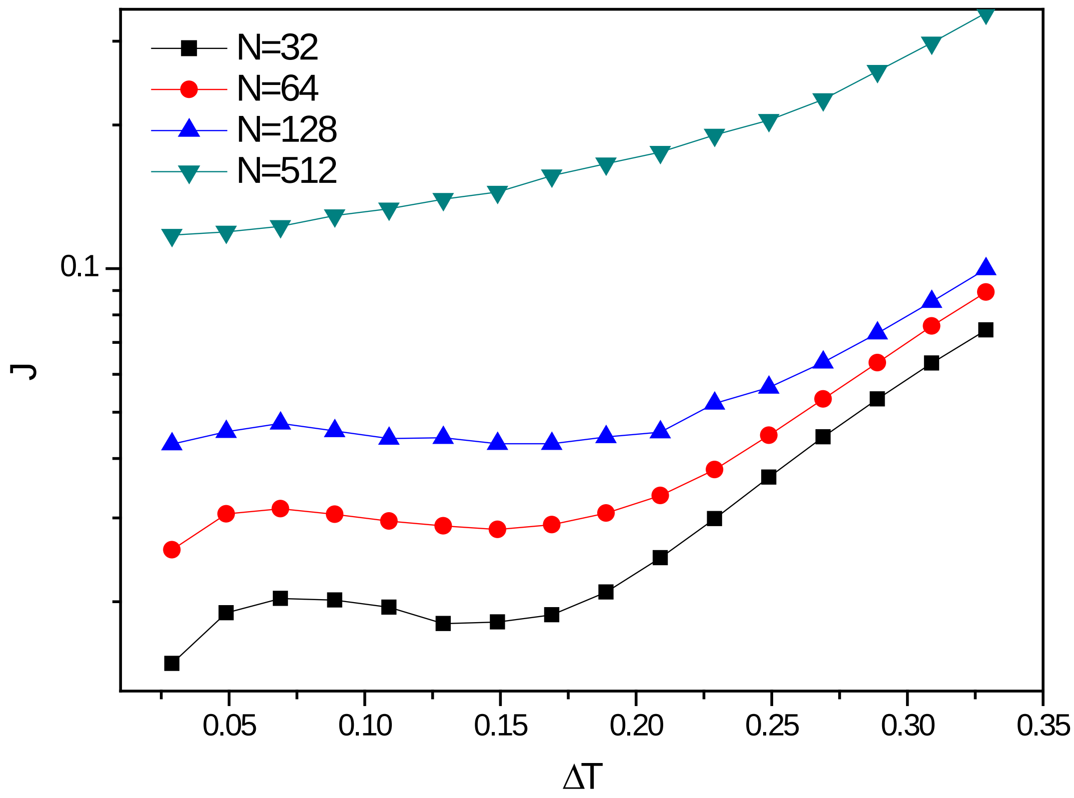
DH, B. Ai, H. Chan, and B. Hu, *Phys. Rev.* **E 81**, 041131 (2010)

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

Size effect of NDTR

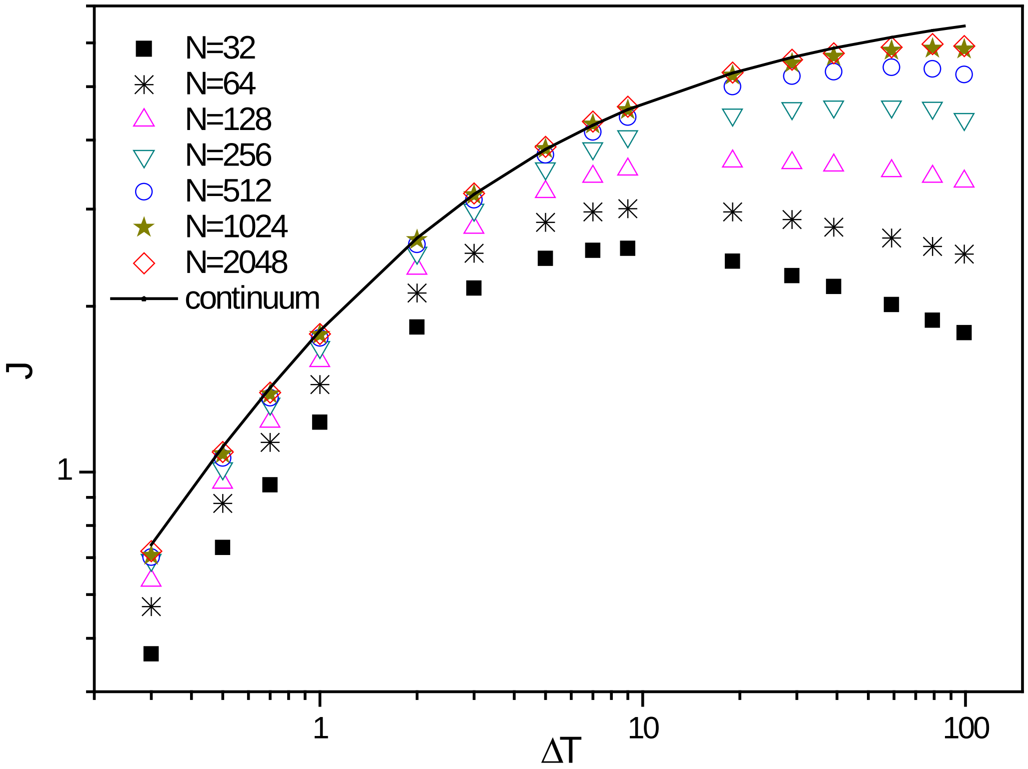


$J = Nj$

Shrinkage of the NDTR regime for increasing *N*: **FK model**

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

Size effect of NDTR



$J = Nj$

Heat current approaches to saturation as *N* increases: **ϕ^4 model**

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

Q1: what is the necessary conditions for the occurring of NDTR?

1. Spatially asymmetric structure? (×)
2. Nonlinearity? (√) (Φ^4 vs. FPU-β?)
3. Temperature?
4. System size?

Q2: Is it possible to give a prediction of the occurring of NDTR?

A general theoretical analysis for NDTR

$$j(T_+, T_-) = j(\overline{T}, \Delta T)$$

$$\overline{T} = \frac{T_+ + T_-}{2}$$

$$\Delta T \equiv T_+ - T_- \in [0, 2\overline{T}]$$

$$dj(\overline{T}, \Delta T) = \left.\frac{\partial j(\overline{T}, \Delta T)}{\partial \overline{T}}\right|_{\Delta T} d\overline{T} + \left.\frac{\partial j(\overline{T}, \Delta T)}{\partial \Delta T}\right|_{\overline{T}} d\Delta T$$

For *a* particular constraint $F(\overline{T}, \Delta T) = 0$

Along this curve, negative differential thermal resistance (*NDTR*) corresponds to

$$\left.\frac{\partial j(\overline{T}, \Delta T)}{\partial \Delta T}\right|_{F(\overline{T}, \Delta T)=0} < 0$$

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

A general theoretical analysis for NDTR

NDTR: $$n_1(\bar{T},\Delta T)n_2(\bar{T},\Delta T) < -[1+n_3(\bar{T},\Delta T)]$$

where

$$n_1(\bar{T},\Delta T) \equiv \left.\frac{d\ln\bar{T}}{d\ln\Delta T}\right|_{F(\bar{T},\Delta T)=0}$$

a particular way of varying the temperature difference

$$n_2(\bar{T},\Delta T) \equiv \left.\frac{\partial\ln\kappa_e(\bar{T},\Delta T)}{\partial\ln\bar{T}}\right|_{\Delta T}$$

Dependence of the effective thermal conductivity κ_e on $\bar{T}$

$$n_3(\bar{T},\Delta T) \equiv \left.\frac{\partial\ln\kappa_e(\bar{T},\Delta T)}{\partial\ln\Delta T}\right|_{\bar{T}}$$

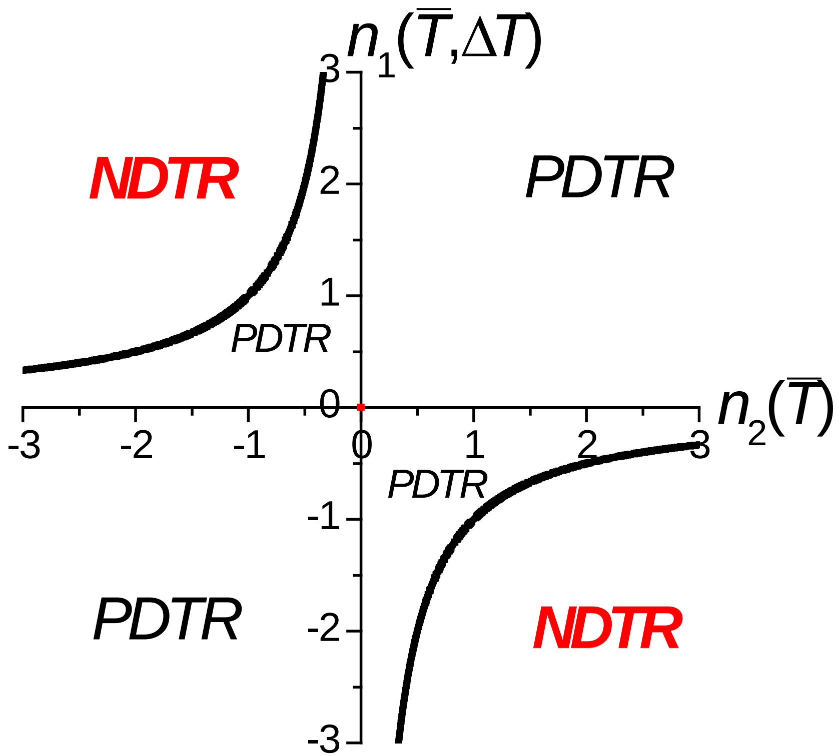
Dependence of the effective thermal conductivity κ_e on ΔT

$$\kappa_e(\bar{T},\Delta T) \equiv \frac{Nj}{\Delta T}$$

Example: $$dT_- = 0, \quad \bar{T} = \frac{\Delta T}{2} + const, \quad n_1(\bar{T},\Delta T) = \frac{\Delta T}{2\bar{T}} \in [0,1]$$

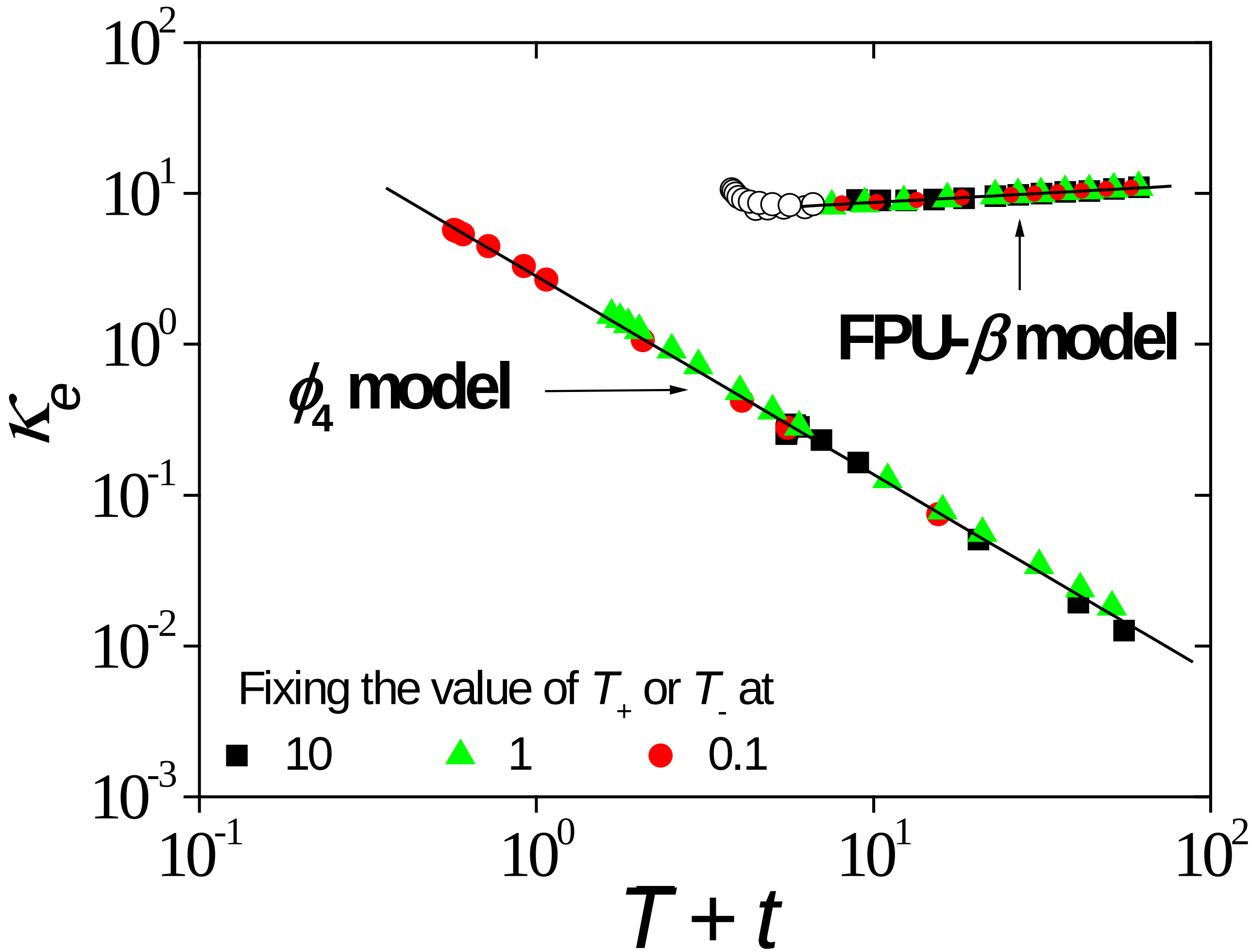
NDTR:

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



Note: one can always ensure the inequality is satisfied by choosing a suitable value of $n_1(\bar{T}, \Delta T) \in (-\infty, +\infty)$

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



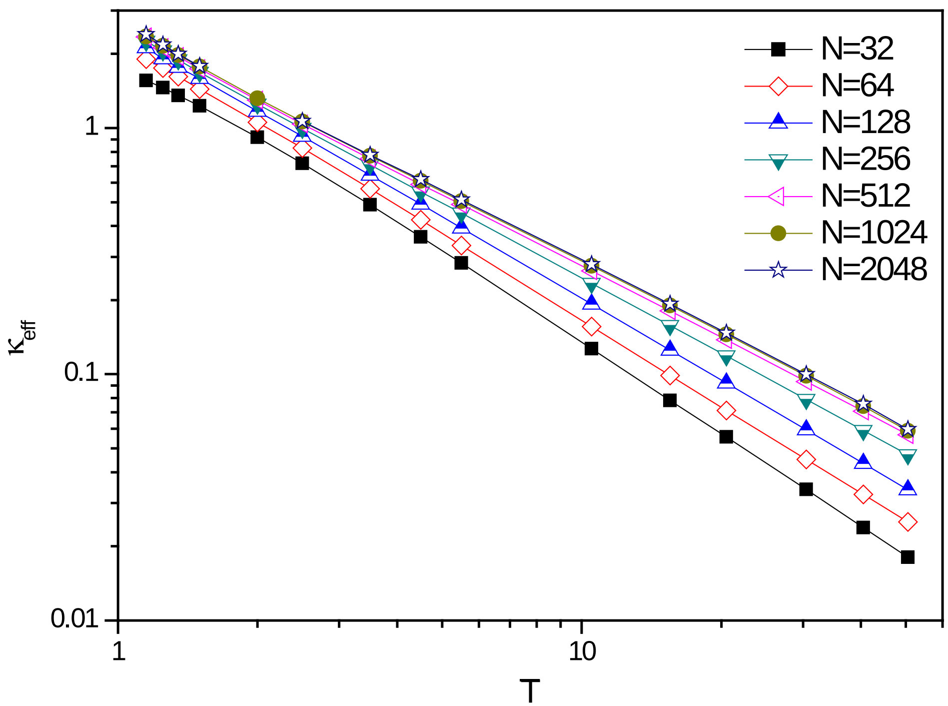
$$\kappa_e(\bar{T}) \equiv \frac{Nj}{\Delta T} \approx C(\bar{T}+t)^{-\gamma}$$

Example 1

Φ^4 model

$$H = \sum_i \frac{p_i^2}{2} + \frac{1}{2}(x_{i+1} - x_i)^2 + \frac{1}{4}x_i^4$$

Constraint: fix T_-



$$\kappa_{eff}(\bar{T}) = C(\bar{T} + t)^{-\gamma},$$

where $\gamma \in [0.95,\ 1.24], \quad t \square 0$

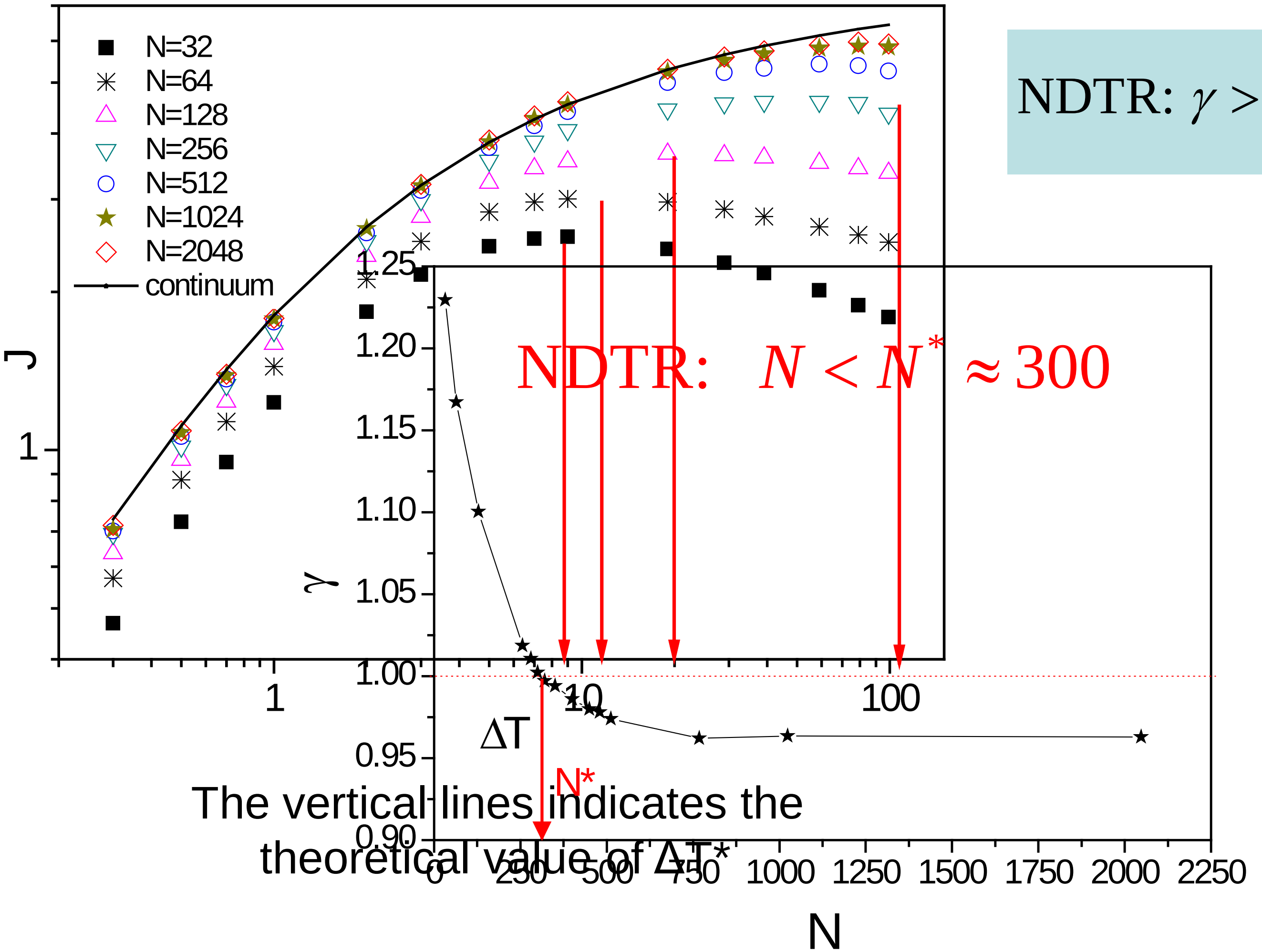
NDTR: $n_1 n_2 < -1$

⇓

$$\gamma > 1, \quad \Delta T > \Delta T^*$$

where: $\Delta T^* = \dfrac{2(T_- + t)}{\gamma - 1}$

$$\text{NDTR: } \gamma > 1, \quad \Delta T > \Delta T^* = \frac{2(T_- + t)}{\gamma - 1}$$



The vertical lines indicates the theoretical value of ΔT*

Example 2

Φ^4 model

$$H = \sum_i \frac{p_i^2}{2} + \frac{1}{2}(x_{i+1} - x_i)^2 + \frac{1}{4}x_i^4$$

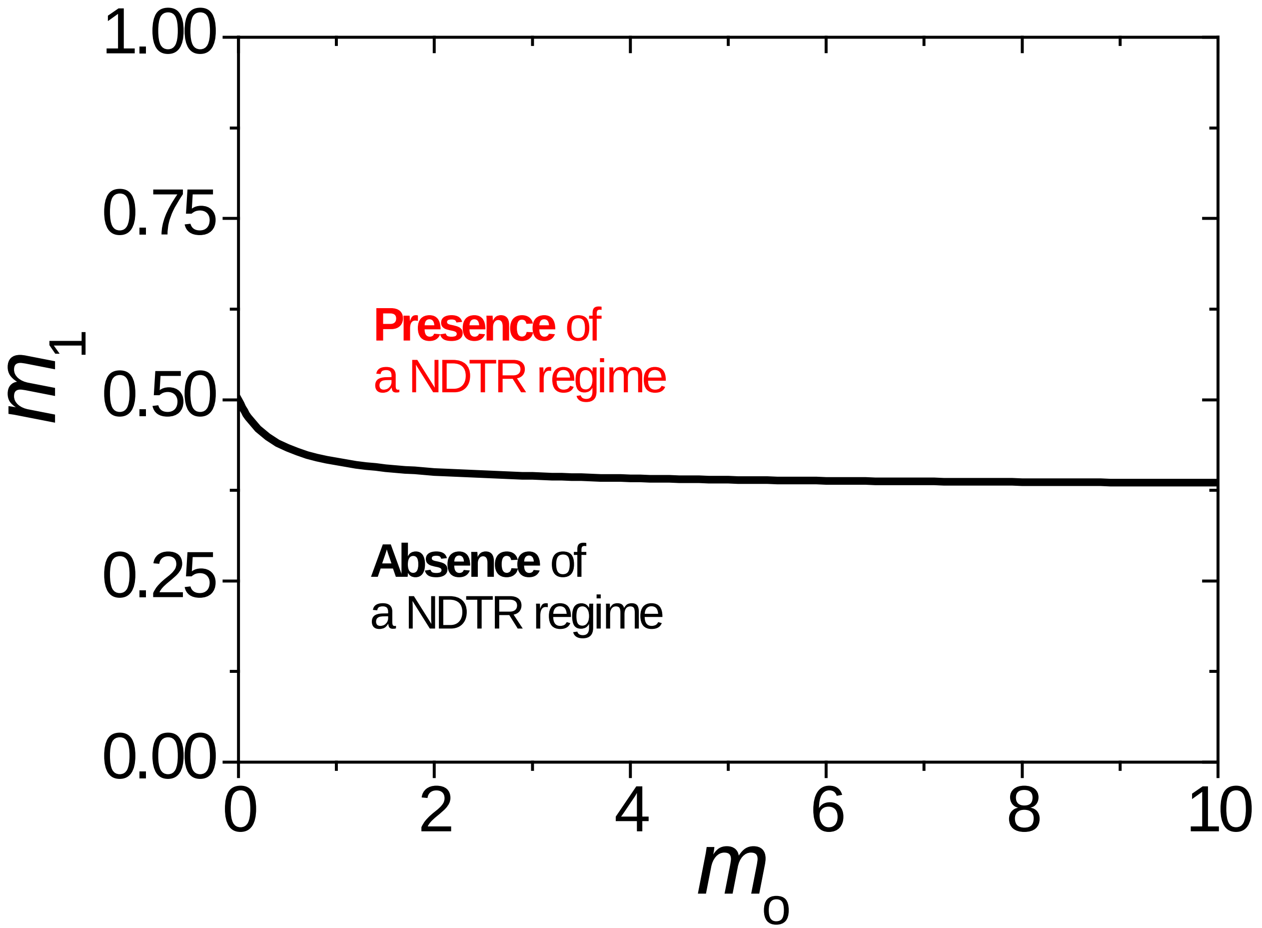
Constraint: $\bar{T} = \frac{T_+ + T_-}{2} = T_- + \frac{1}{2}\Delta T$, $\quad \bar{T} = m_0 + m_1 \Delta T$

$$\Delta T_{\max} = \frac{m_0}{1/2 - m_1}$$

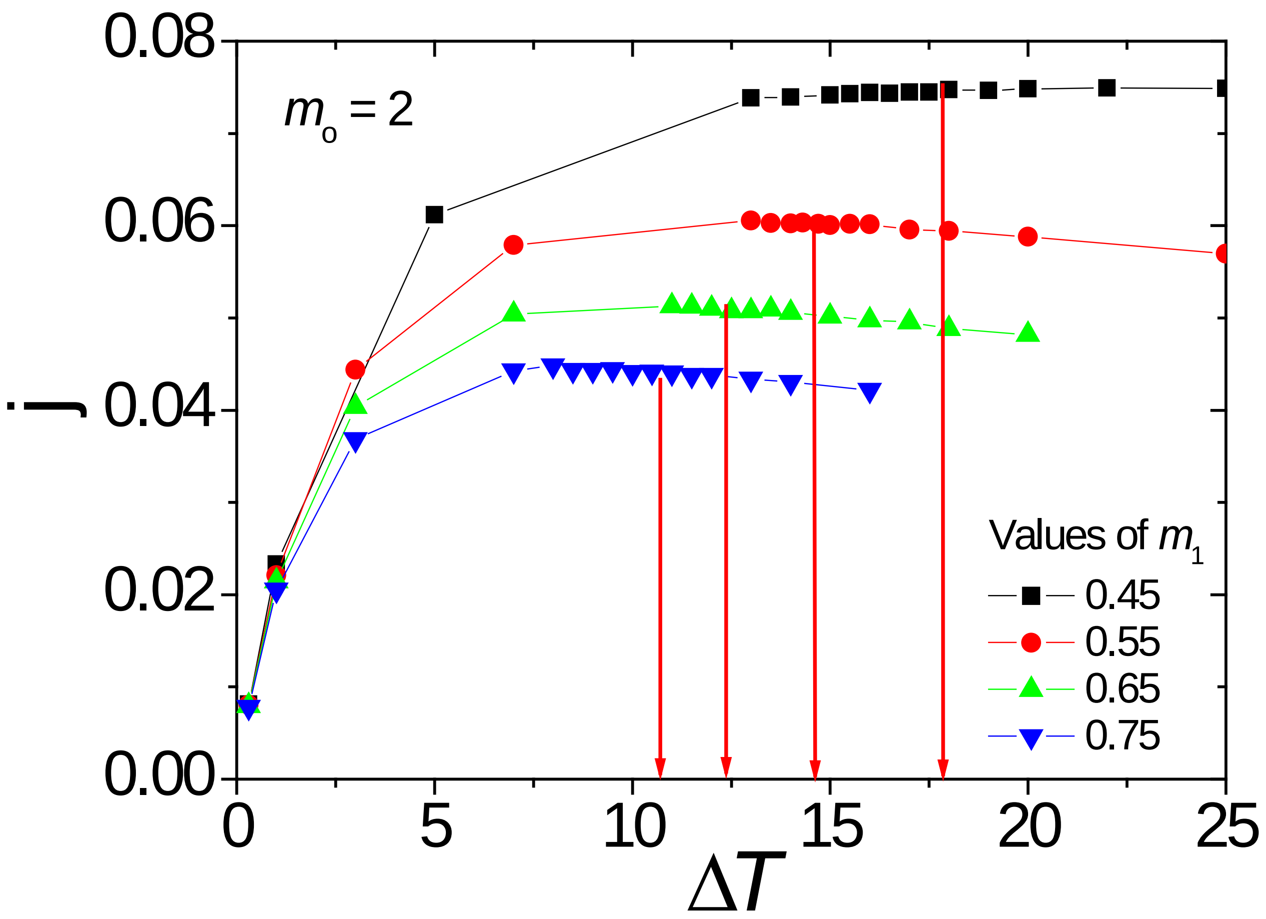
$$n_1 = \frac{m_1 \Delta T}{\bar{T}}, \qquad n_2 = -\frac{\gamma}{1 + t/\bar{T}}$$

NDTR: $(\gamma - 1)m_1 > 0, \;\; \Delta T > \Delta T^* = \dfrac{m_0 + t}{(\gamma - 1)m_1}$

$$\Rightarrow \qquad m_1 > \frac{1}{2}\left[\frac{1 + t/m_0}{\gamma + t/m_0}\right]$$



“Phase diagram” of m_1 and m_o for the ϕ^4 model



The vertical lines indicate the theoretical values of $\Delta T^* = \dfrac{m_0 + t}{(\gamma - 1)m_1}$

Example 3

FPU-β model

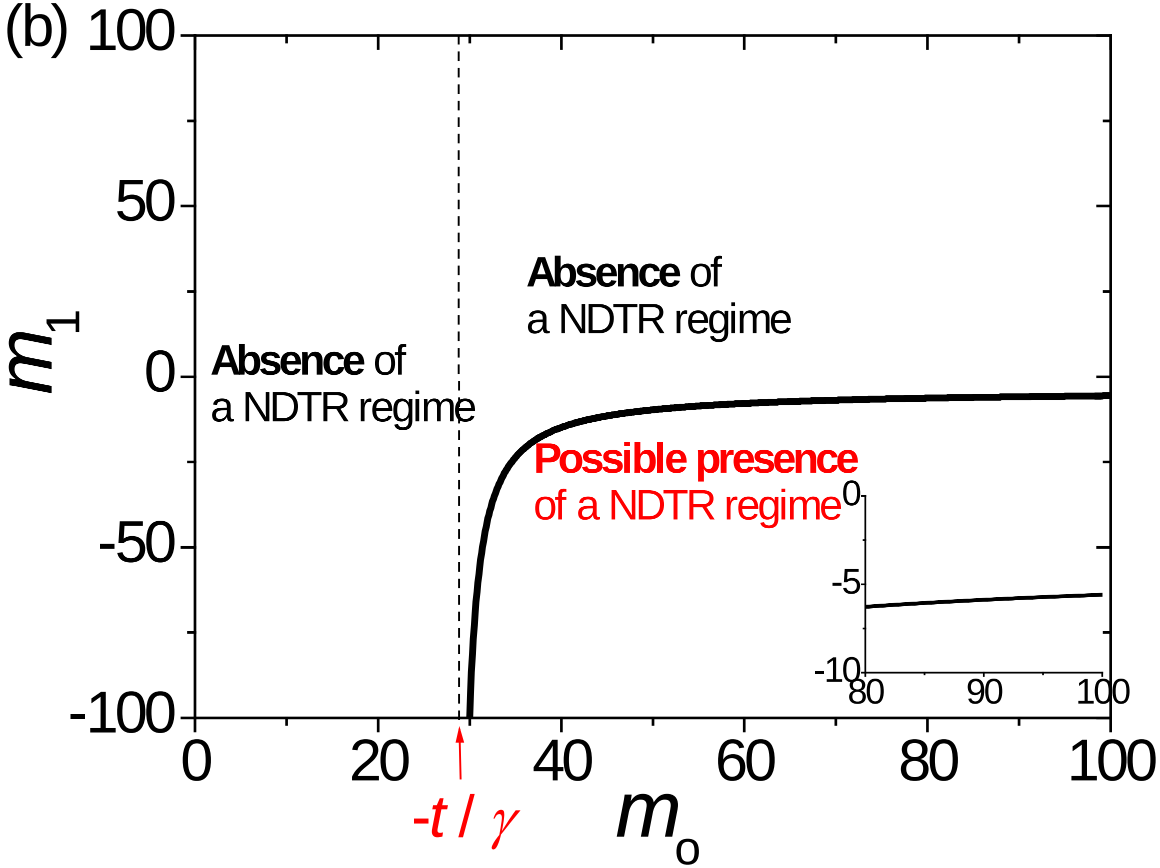
$$H=\sum_i \frac{p_i^{\,2}}{2}+\frac{1}{2}(x_{i+1}-x_i)^2+\frac{1}{4}(x_{i+1}-x_i)^4$$

Constraint: $\bar{\mathrm{T}}=m_0+m_1\Delta T$

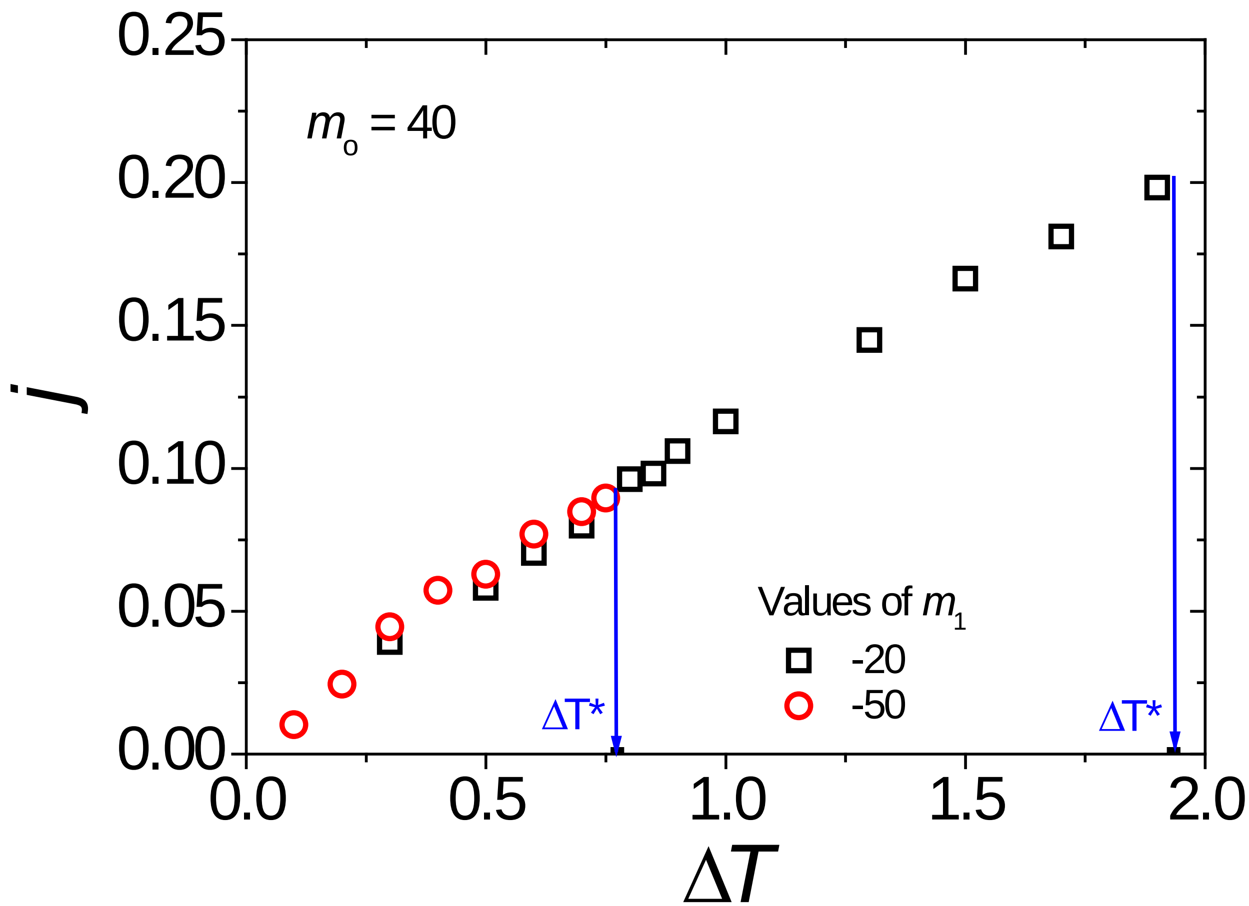
$$n_1=\frac{m_1\Delta T}{\bar{T}},\qquad n_2=-\frac{\gamma}{1+t/\bar{T}}$$

NDTR: $$(\gamma-1)m_1>0,\ \ \Delta T>\Delta T^*=\frac{m_0+t}{(\gamma-1)m_1}$$

$$\Rightarrow\ m_0>-\frac{t}{\gamma},\qquad m_1<\frac{1}{2}\left[\frac{1+t/m_0}{\gamma+t/m_0}\right]$$



“Phase diagram” of m_1 and m_o for the FPU-β model



Note that $\Delta T^* / \Delta T_{\max} \approx \frac{1}{1-\gamma} = 0.987$ $\qquad \Delta T_{\max} = \frac{m_0}{1/2 - m_1}$

NDTR regime is too narrow to be observed !

A very specific example

FPU-β model

Consider a change of temperatures of heat baths

$$(T_+, T_-) = (51,\ 49) \quad \rightarrow \quad (T_+, T_-) = (41.005,\ 38.995)$$

$$\Delta T = 2 \quad \rightarrow \quad \Delta T = 2.01$$

Theory: $$n_1 = \frac{\Delta T}{\overline{T}} \frac{d\overline{T}}{d\Delta T} \approx -44.56, \qquad n_1 n_2 \approx -5.35 < -1$$

Numerics: $$j = 0.2664 \quad \rightarrow \quad j = 0.2457$$

Conclusion

- We develop a system-independent scaling analysis, and obtain the general condition for the occurrence of NDTR.

- Based on the condition, one can judge whether NDTR exist; If NDTR exist, ΔT^* and N^* can be predicted.

- The occurrence of NDTR can be manipulated for any nonlinear model by suitably choosing the way of varying T_+ and T_-.

Thank You !

Part II

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

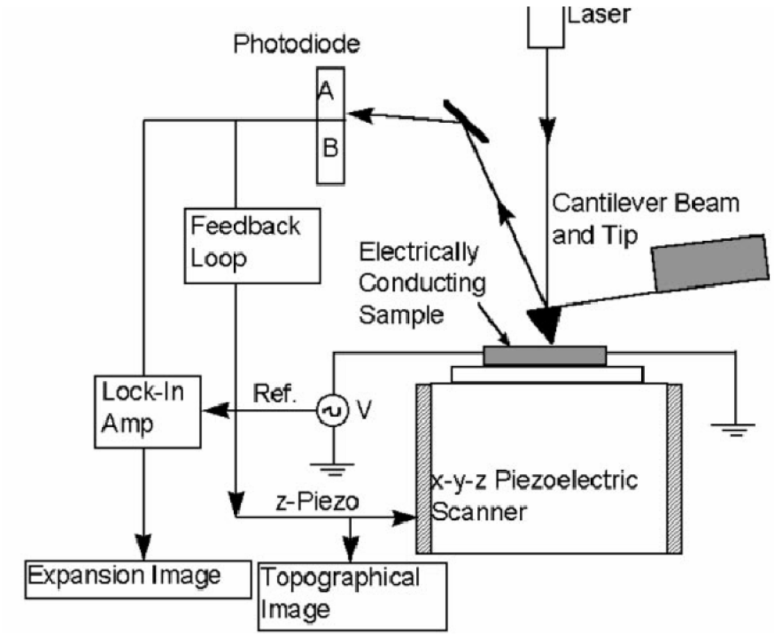
X. Cao, **DH**, H. Zhao, and B. Hu, AIP Advances 5, 053203 (2015)

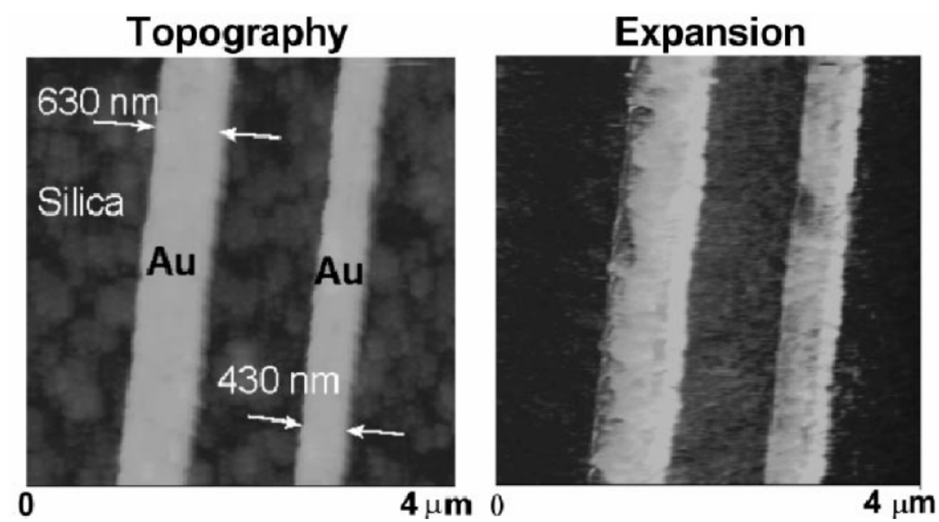
Motivation I

- Recent controversy on the effect of asymmetric interaction potential on normal thermal conduction. (Hong Zhao's and Shunda Chen'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.





Thermal Expansion Thermometry

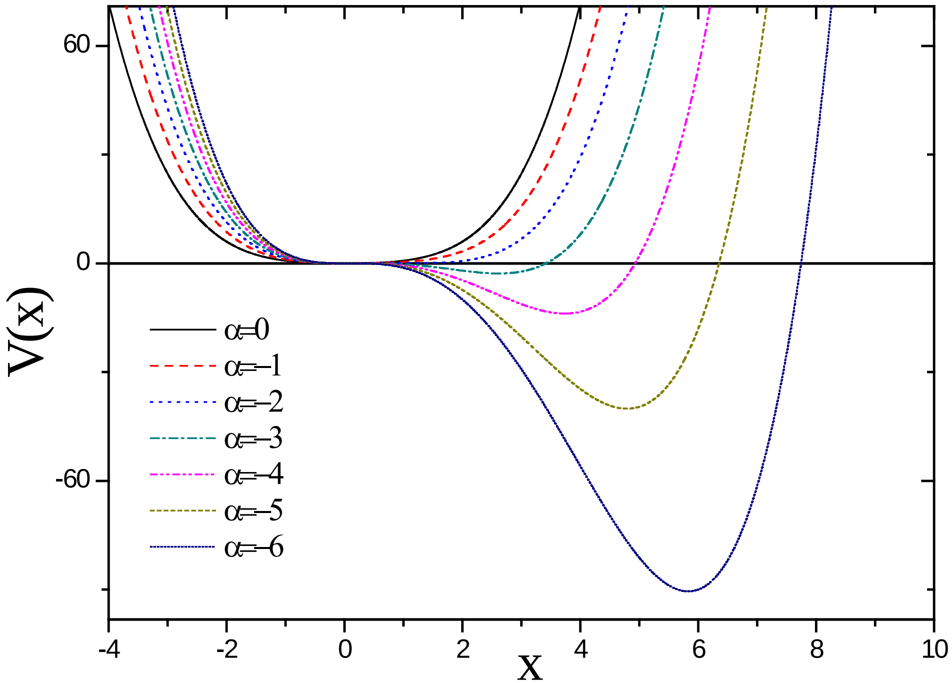
Appl. Phys. Lett. 66, 694

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.

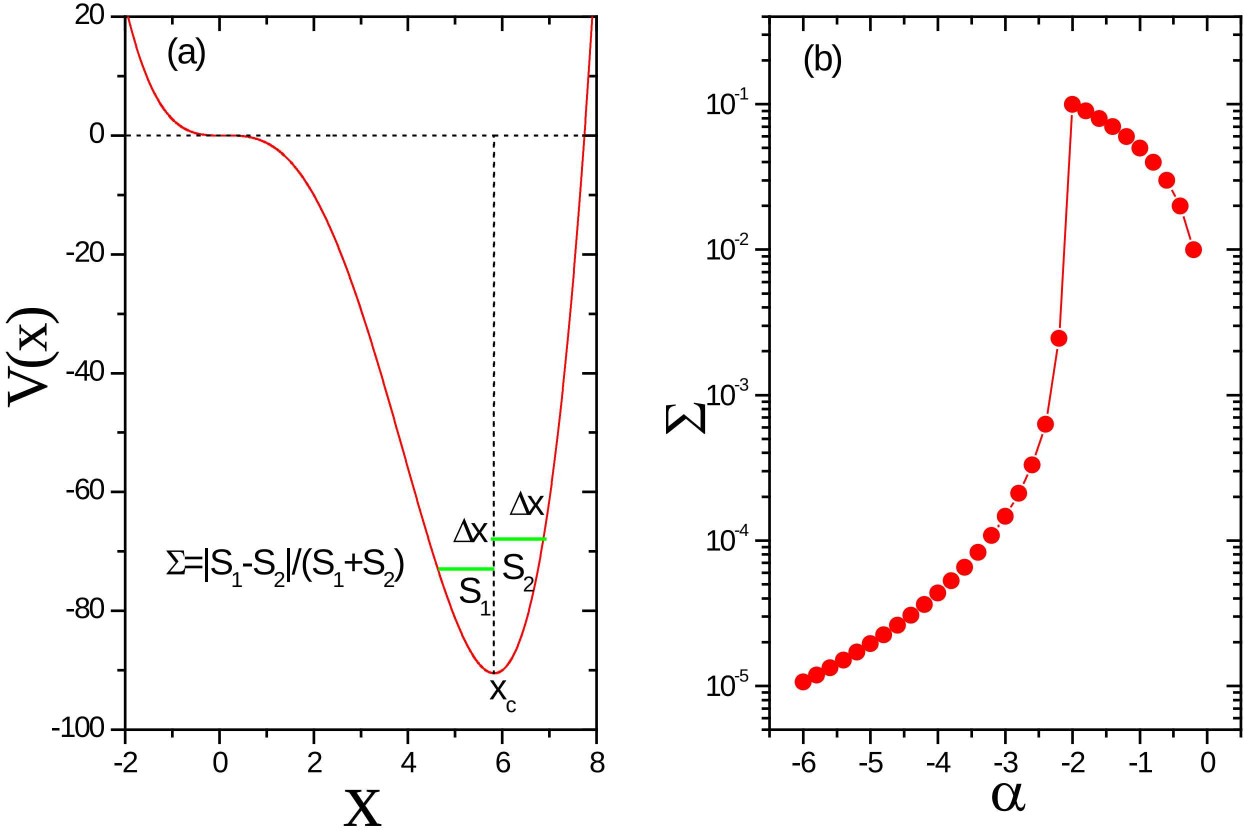
Potential Profile of FPU-ab model

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

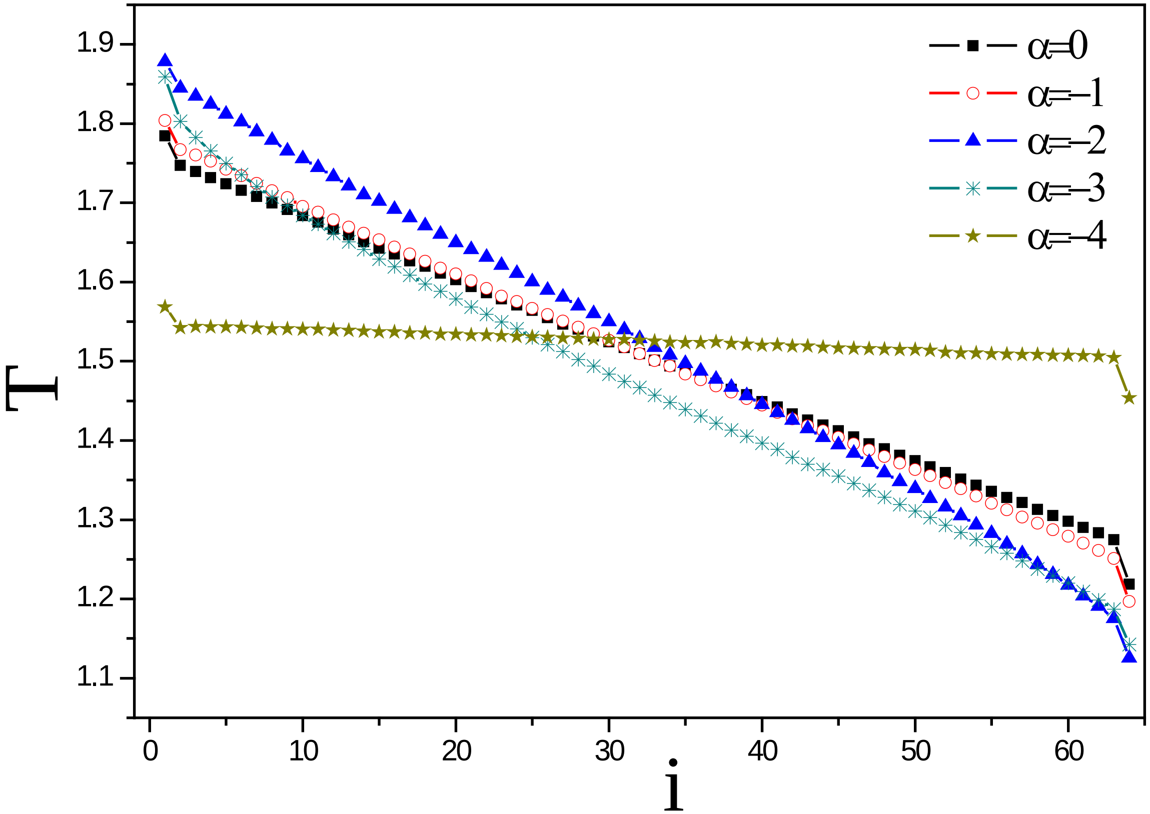


Quantify the asymmetry

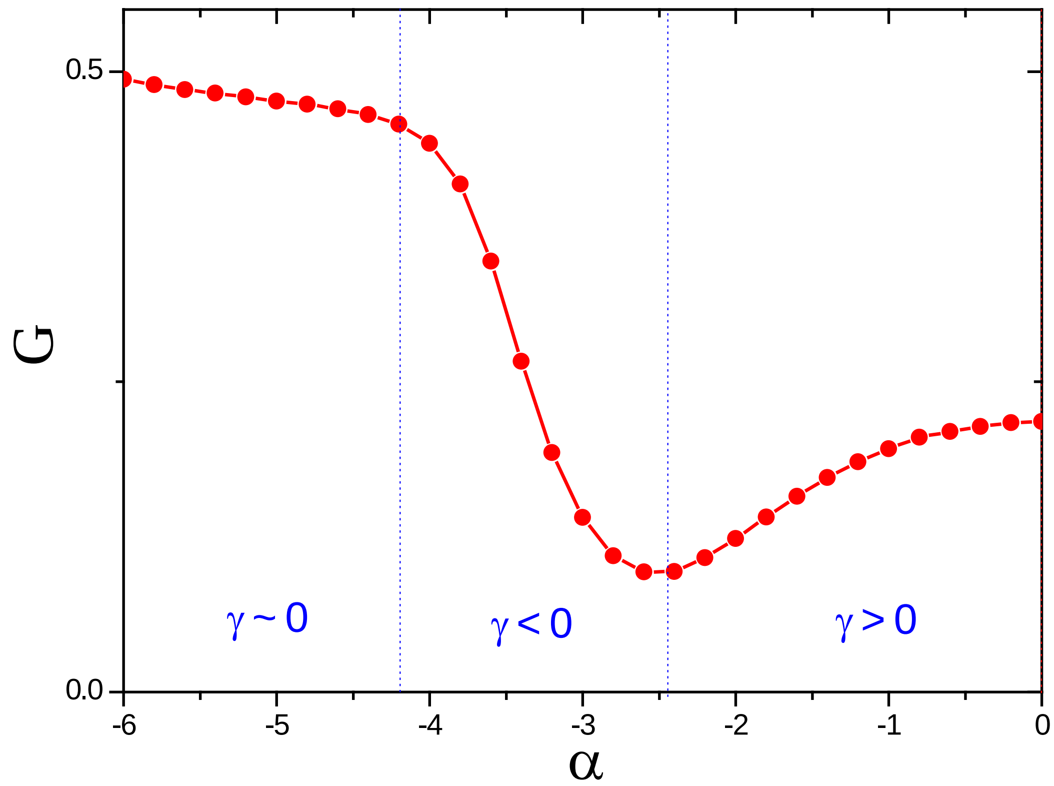
$$\Sigma = |S_1 - S_2|/(S_1 + S_2)$$



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

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

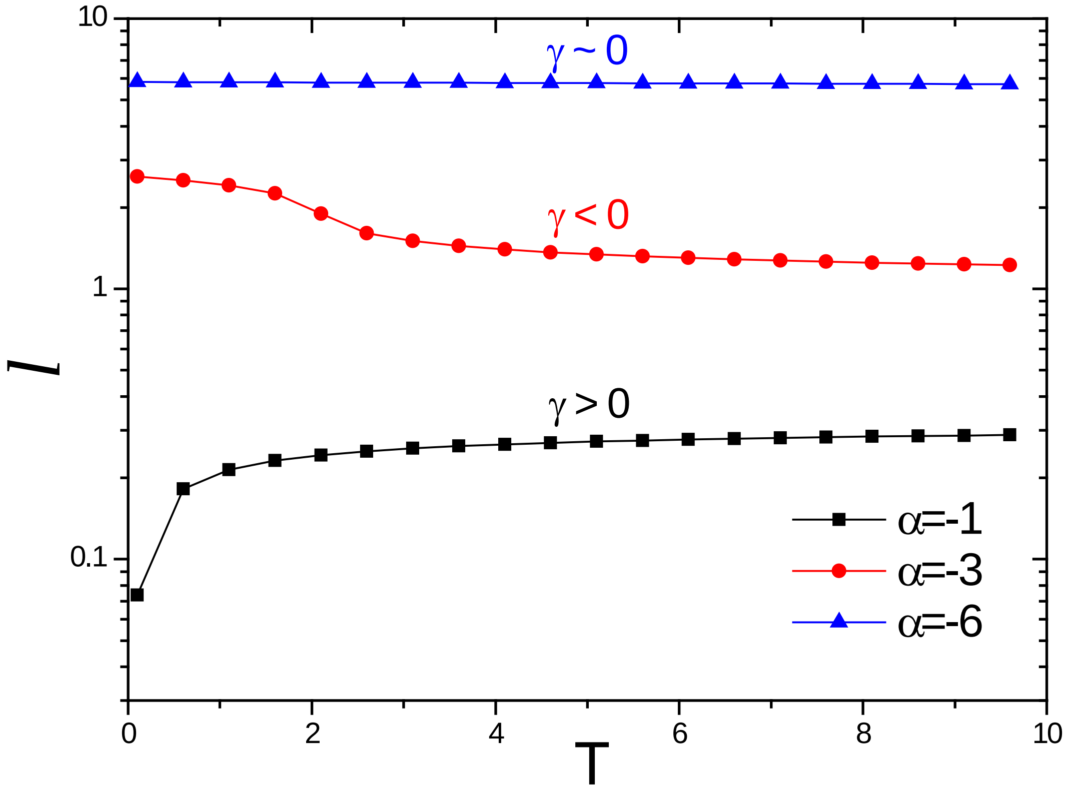
Where the effective harmonic potential coefficient f(T) can be obtained from the self-consistent equations:

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

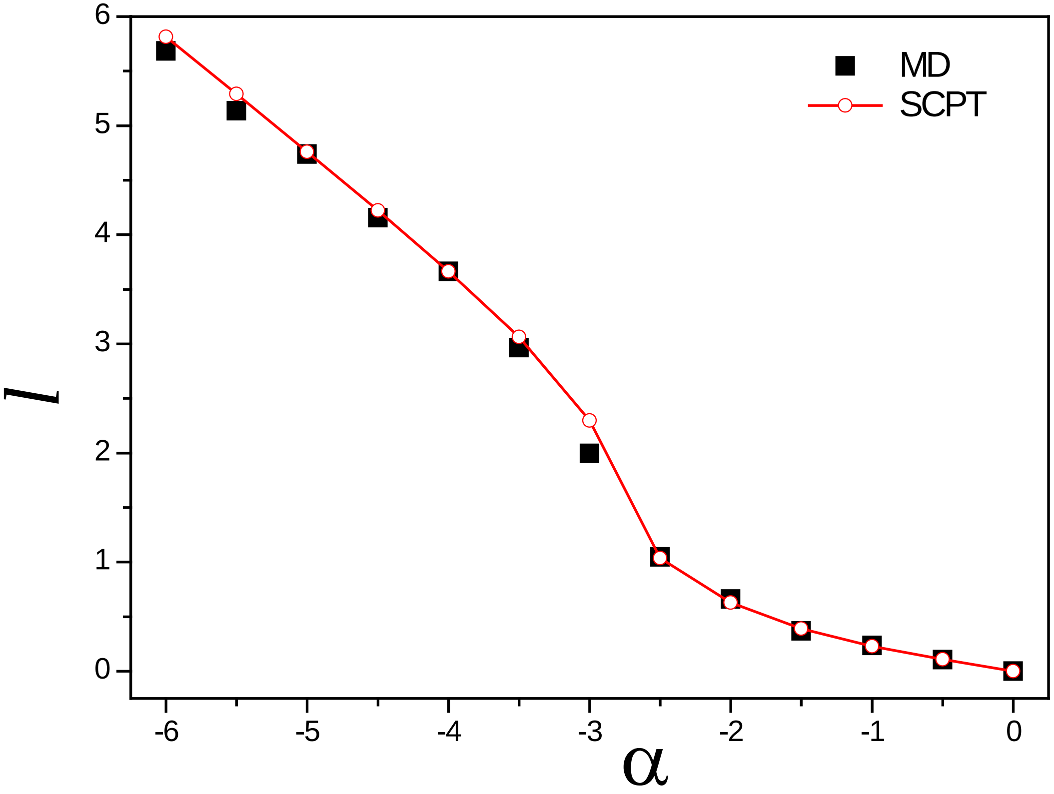
T. Dauxois, et al, *Phys. Rev.* **E** 47, 684(1993)

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

Coefficient of thermal expansion



Effect of nonlinearity on thermal expansion



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

Conclusion

- 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.

Thank You !