Fundamentals of thermal rectification

Giuliano Benenti
Center for Nonlinear and Complex Systems,
Univ. Insubria, Como, Italy
INFN, Milano, Italy

G. B., G. Casati, C. Mejia-Monasterio, M. Peyrard, arXiv: 1512.06889, in Lecture Notes in Physics vol. 921 "*Thermal transport in low dimensions: from statistical physics to nanoscale heat transfer*", ed. by S. Lepri (2016)

Outline

Dynamical foundations of Fourier law: Can we derive the Fourier law of heat conduction from dynamical equations of motion, without any a priori statistical assumptions? And in quantum mechanics?

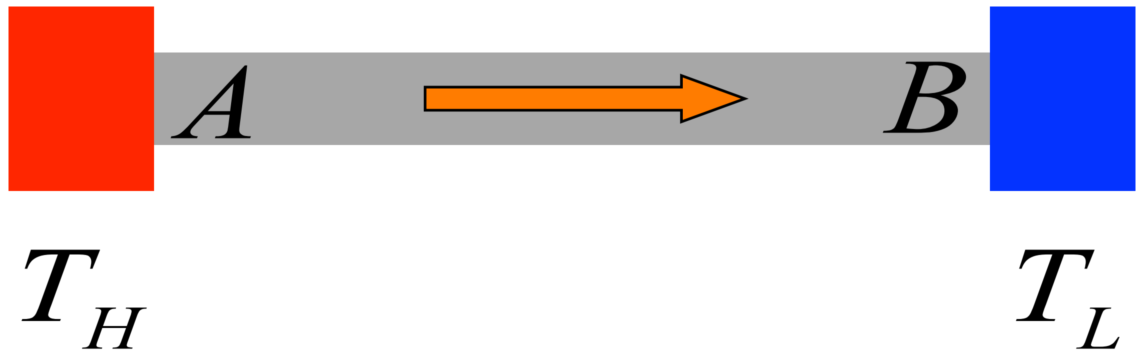
Can we control the heat current? Towards thermal diodes and thermal transistors

Basic **ingredients for a thermal diode**

Thermal rectification with a ballistic spacer (work in progress)

Fourier Heat Conduction Law (1808)

"Théorie de la Propagation de la Chaleur dans les Solides"



$$\boxed{\boldsymbol{J} = -\kappa \nabla T}$$

$\boldsymbol{J}$: heat flux

∇T: temperature gradient

κ : thermal conductivity

An old problem, and a long history

1808 - J.J. Fourier: study of the earth thermal gradient

19 century: Clausius, Maxwell, Boltzmann,
kinetic theory of gas, Boltzmann transport equation

1914 - P. Debye: conjectured the role of nonlinearity to ensure finite transport coefficients

1936 - R. Peierls: reconsidered Debye's conjecture

1953 - E. Fermi, J. Pasta and S.Ulam: **(FPU) numerical experiment** to verify Debye's conjecture

"It seems there is no problem in modern physics for which there are on record as many false starts, and as many theories which overlook some essential feature, as in the problem of the thermal conductivity of (electrically) nonconducting crystals."

R. E. Peierls (1961),
Theoretical Physics in the Twentieth Century.

QUESTION:

Can one derive the Fourier law of heat conduction from dynamical equations of motion without any statistical assumption?

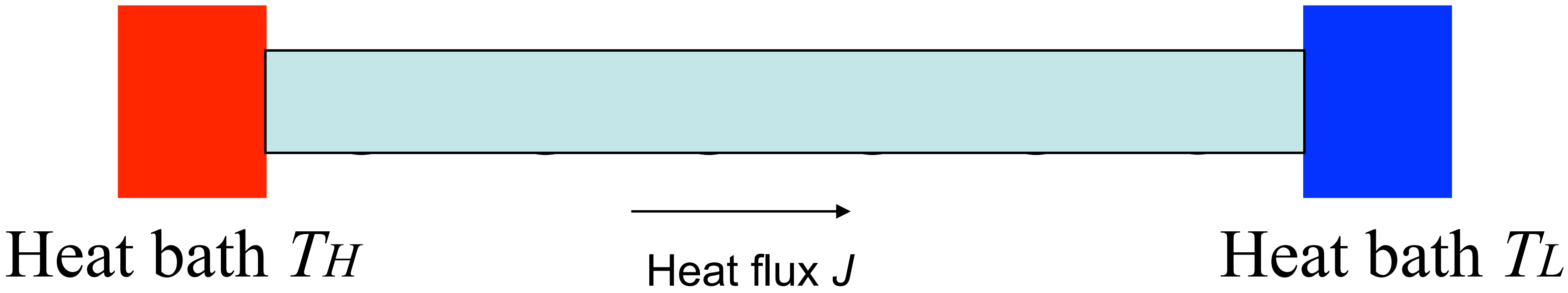
REMARK:

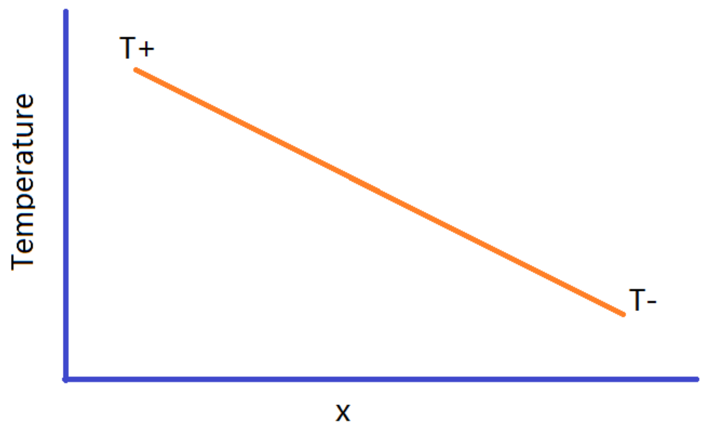
(Normal) heat flow obeys a simple diffusion equation which can be regarded as a continuous limit of a discrete random walk

Randomness should be an essential ingredient of thermal conductivity

deterministically random systems are tacitly required by the transport theory

Methods: nonequilibrium simulations





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

S. Lepri, et al, Phys. Rep. 377, 1 (2003); A. Dhar, Adv. Phys. 57, 457 (2008)

Ding-a-ling model

chaos for $\omega^2/E \gg 1$

Free electron gases at the reservoirs with Maxwellian distribution of velocities

$$f(v) = \frac{m\,|v|}{T} \exp\left(-\frac{mv^2}{2T}\right)$$

Heat flux $\quad J = \lim_{t\to\infty} \frac{1}{t} \sum_i \Delta E_i$

Internal temperature $T_i = \langle v_i^2 \rangle \qquad (m = k_B = 1)$

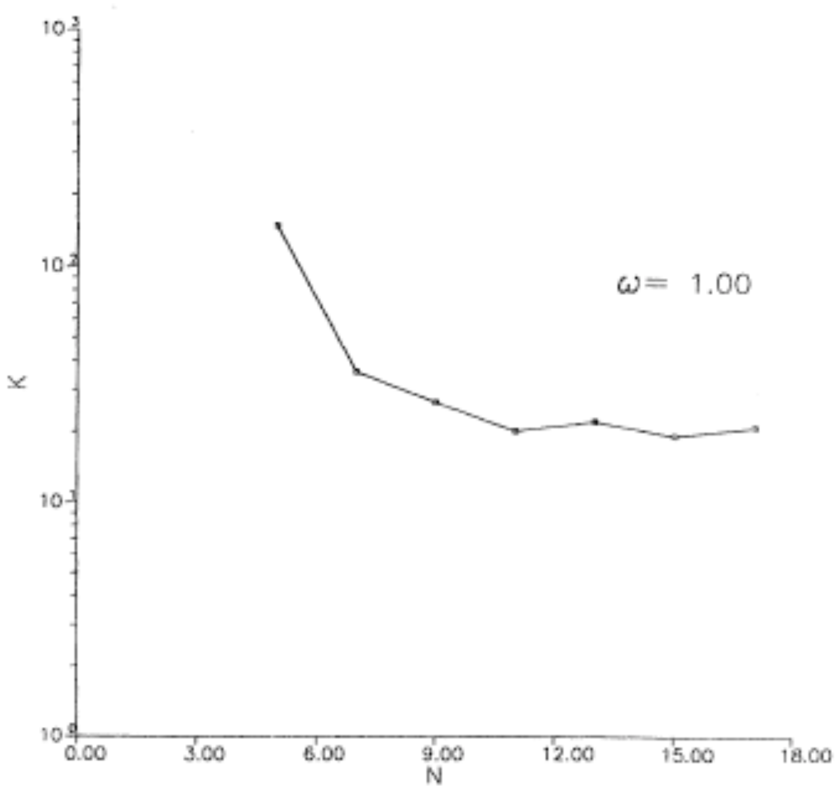


FIG. 3. Behavior of the coefficient of thermal conductivity as a function of the particle number N.

(G. Casati, J. Ford, F. Vivaldi, W.M. Visscher, PRL **52**, 1861 (1984))

Methods: equilibrium simulations

Green-Kubo formula:

$$\kappa_{GK} = \lim_{\tau\to\infty}\lim_{N\to\infty}\frac{1}{T^2 N}\int_0^{\tau} < J(t)J(0) > dt \ ,$$

$$J(t) = \sum_{i=1}^{N} J_i(t)$$

$$< J(t)J(0) > /N \sim t^{-\gamma} \quad \begin{cases} 0 \le \gamma \le 1 & \text{anomalous heat conduction} \\ \gamma > 1 & \text{normal heat conduction} \end{cases}$$

S. Lepri, et al, Phys. Rep. 377, 1 (2003); A. Dhar, Adv. Phys. 57, 457 (2008)

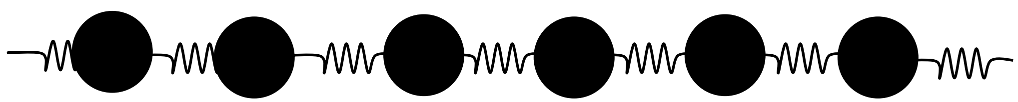
Momentum-conserving systems

Slow decay of correlation functions, diverging transport coefficients

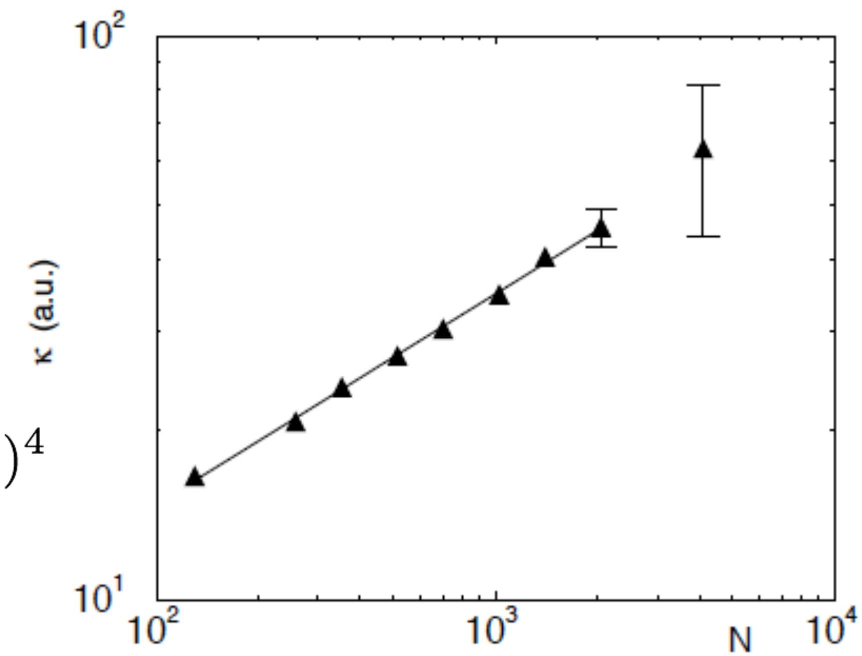
(Alder and Wainwright, PRA **1**, 18 (1970))

FPU revisited: chaos is not sufficient to obtain Fourier law

(Lepri, Livi, Politi, EPL **43**, 271 (1998))



$$V(y_n - y_{n-1}) = \frac{1}{2}K(y_n - y_{n-1})^2 + \frac{1}{4}g(y_n - y_{n-1})^4$$



For momentum-conserving systems

3D $\kappa \sim L^0$ (**normal** heat conduction)

2D $\kappa \sim \ln(L)$ (**anomalous** heat conduction)

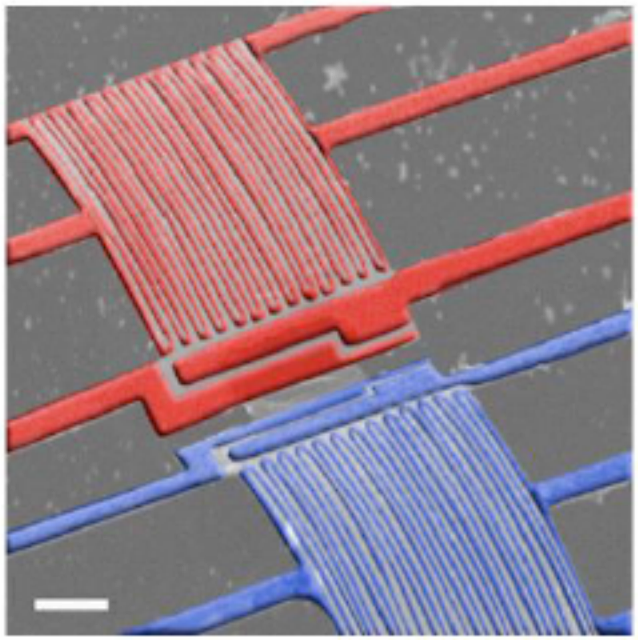
1D $\kappa \sim L^\alpha$ (**anomalous** heat conduction)

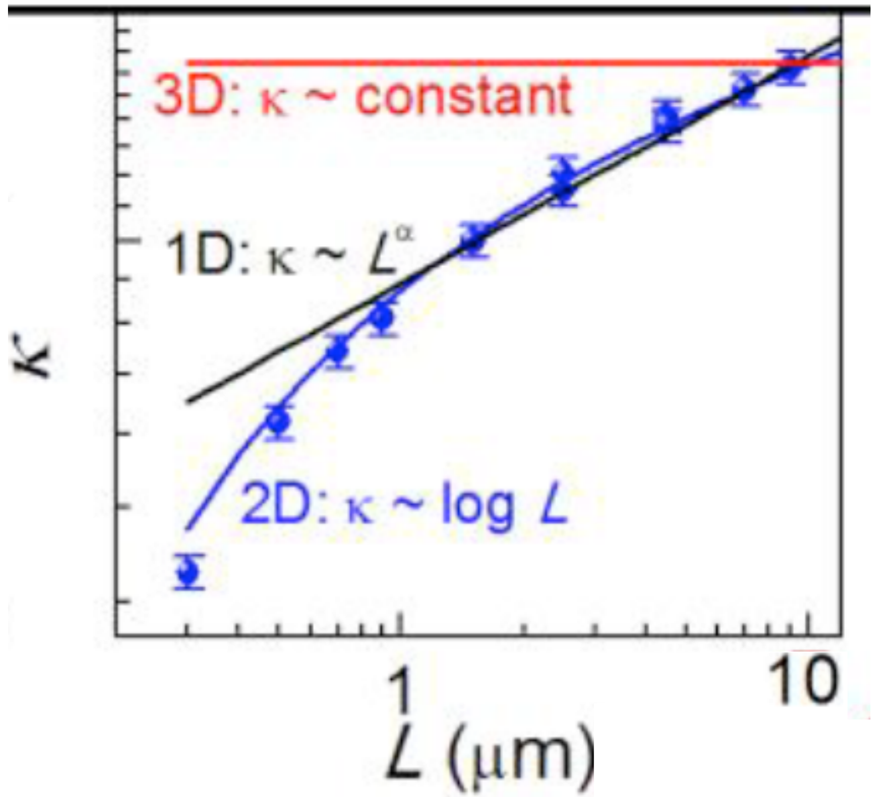
From hydrodynamic theory: $\alpha = 1/3$

Length-dependent thermal conductivity in suspended single-layer graphene

Xiangfan Xu, Luiz F. C. Pereira, Yu Wang, Jing Wu, Kaiwen Zhang, Xiangming Zhao, Sukang Bae, Cong Tinh Bui, Rongguo Xie, John T. L. Thong, Byung Hee Hong, Kian Ping Loh, Davide Donadio, Baowen Li & Barbaros Özyilmaz

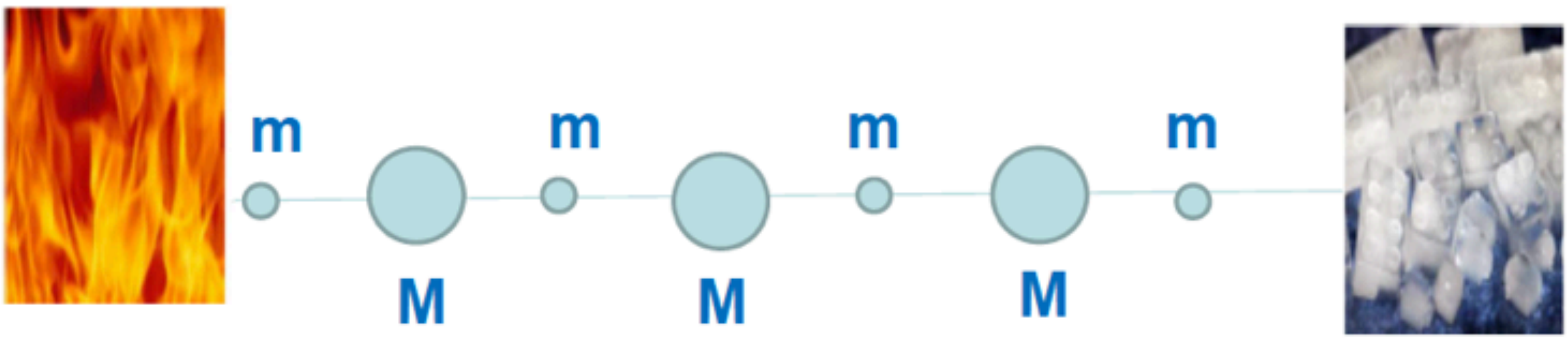
Nature Communications 5, Article number: 3689 doi:10.1038/ncomms4689
Received 09 October 2013 Accepted 19 March 2014 Published 16 April 2014





The red and blue Pt coils are the heater and sensor thermally connected by suspended graphene (grey sheet in the middle)

1-d hard point gas with alternative masses, m, M



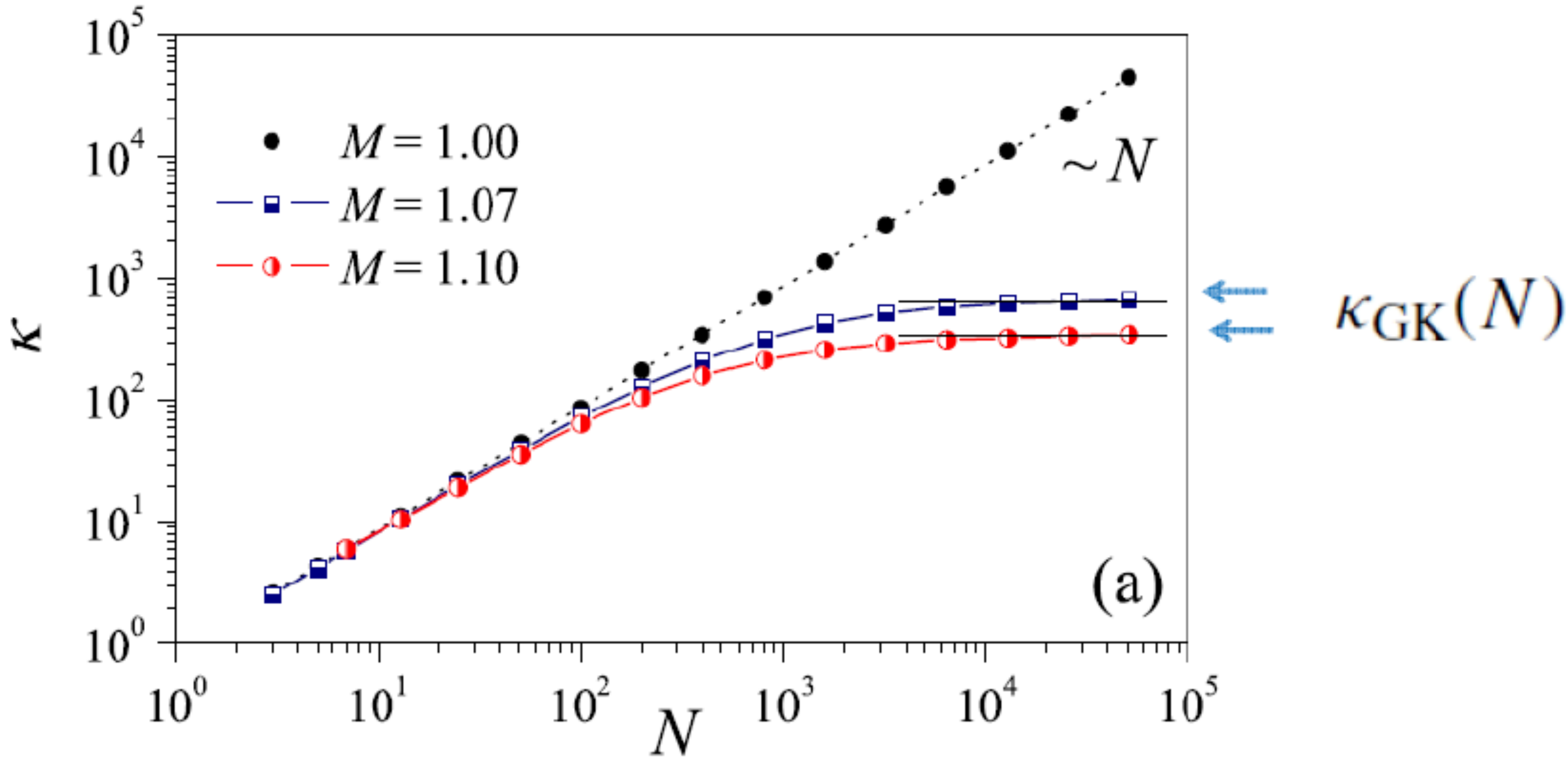
In the equal mass case, m=M:

$$\boxed{\kappa_{\text{int}} = N\sqrt{\frac{2k_B^3}{m\pi}} \Big/ \left(\frac{1}{\sqrt{T_L}} + \frac{1}{\sqrt{T_R}}\right)}$$

balistic

Fourier law close to the integrable limit?

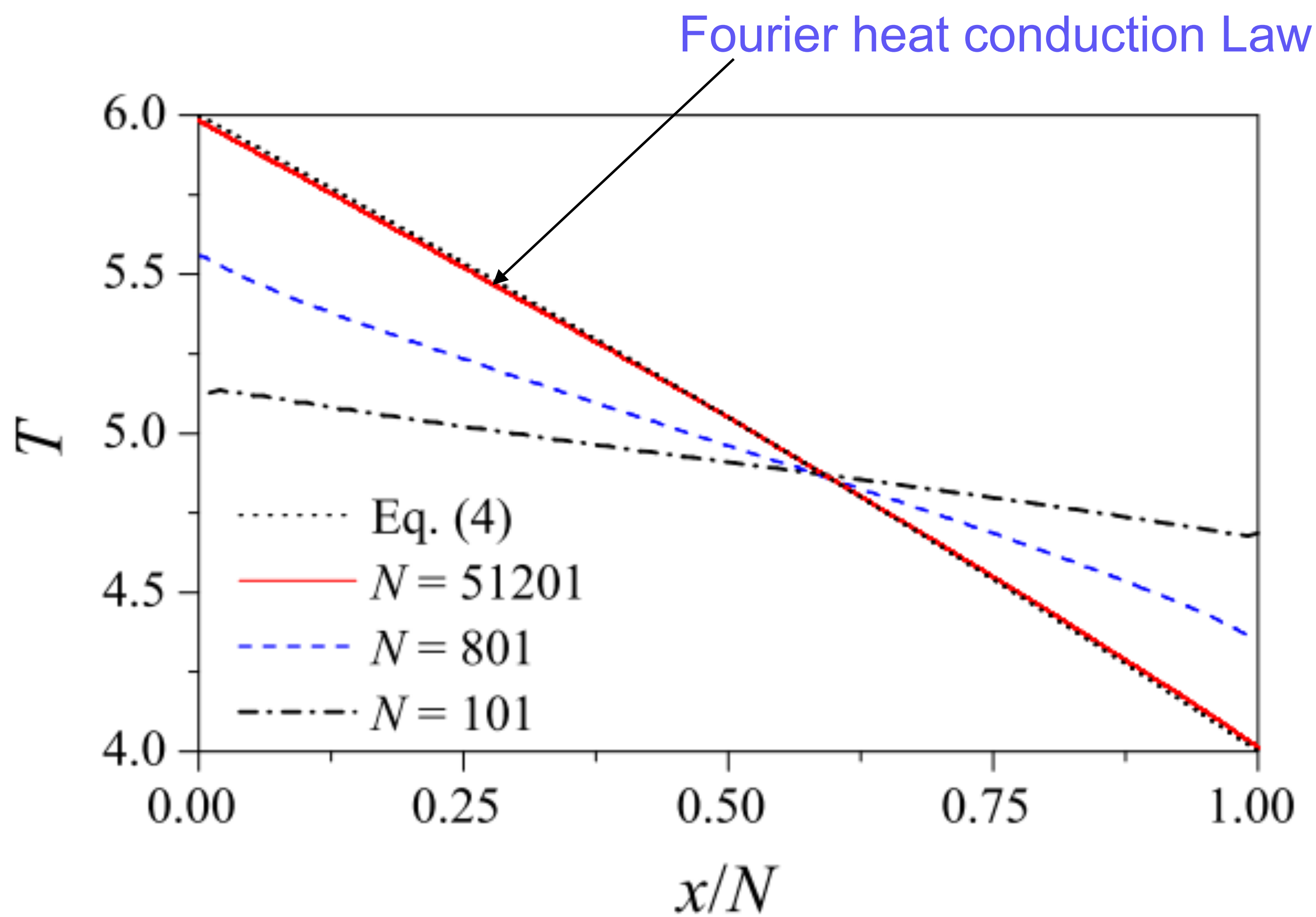
Results of nonequilibrium simulations for the hard-point gas model:



$$\kappa_{\mathrm{int}} = N\sqrt{\frac{2k_B^3}{m\pi}} \Big/ \left(\frac{1}{\sqrt{T_L}} + \frac{1}{\sqrt{T_R}}\right)$$

(S. Chen, J. Wang ,
G. Casati, G.B.,
PRE **90**, 032134 (2014))

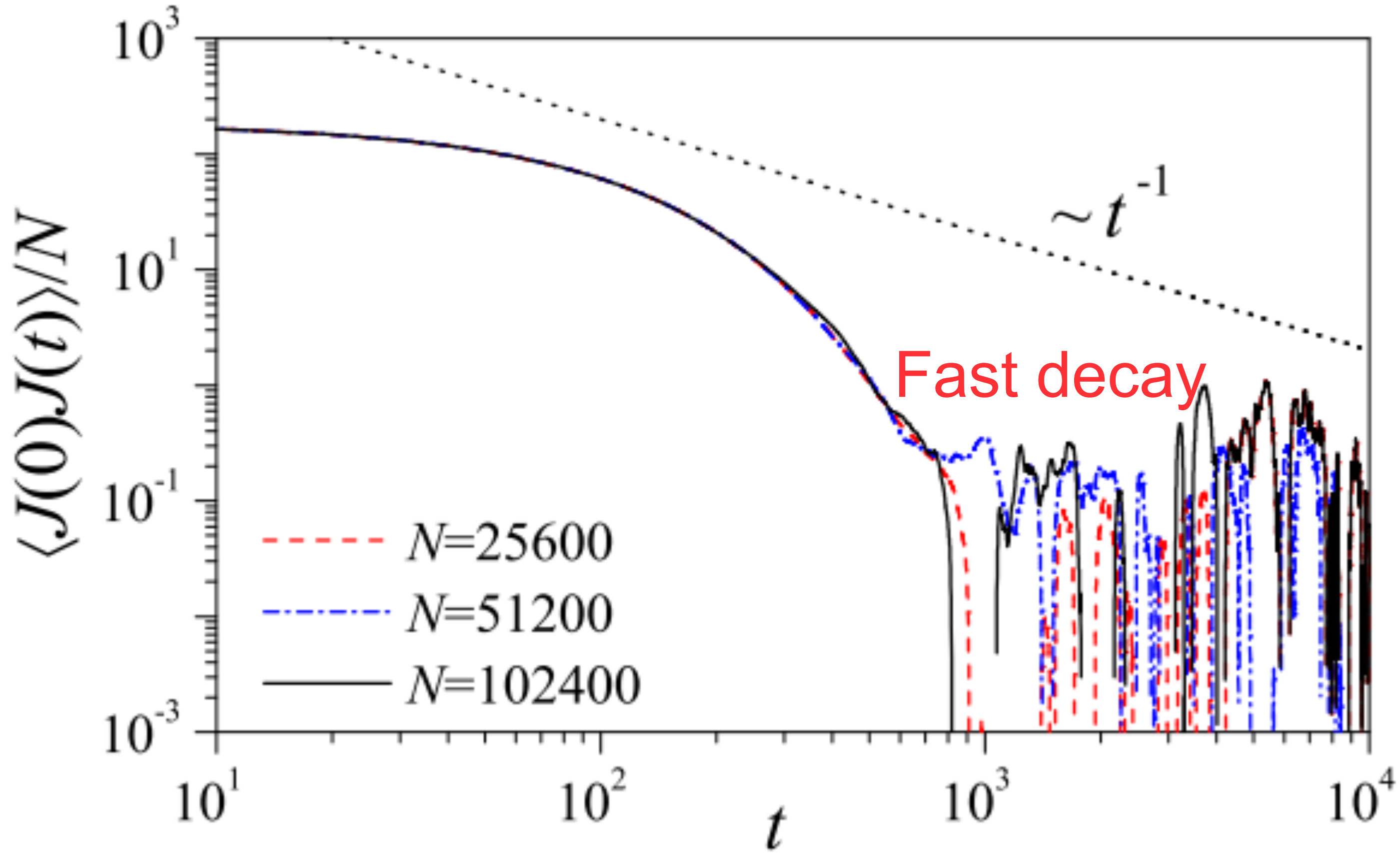
Temperature profiles



$$T(x) = \left[T_L^{3/2} \left(1 - \frac{x}{N} \right) + T_R^{3/2} \frac{x}{N} \right]^{2/3} \qquad (4)$$

Heat current correlation function

Results of equilibrium simulations for the diatomic hard-point gas model:



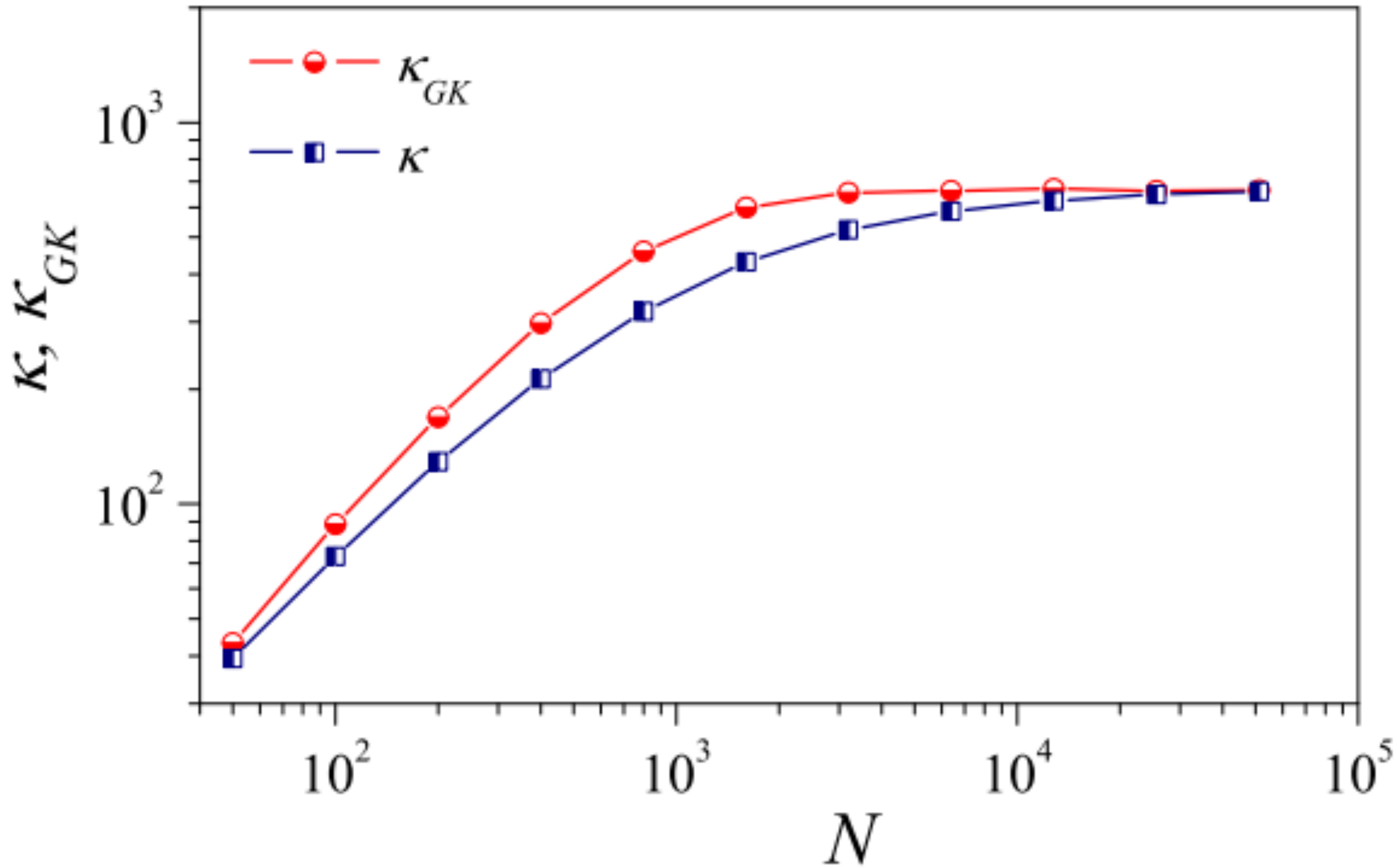
M=1.07

(m=1)

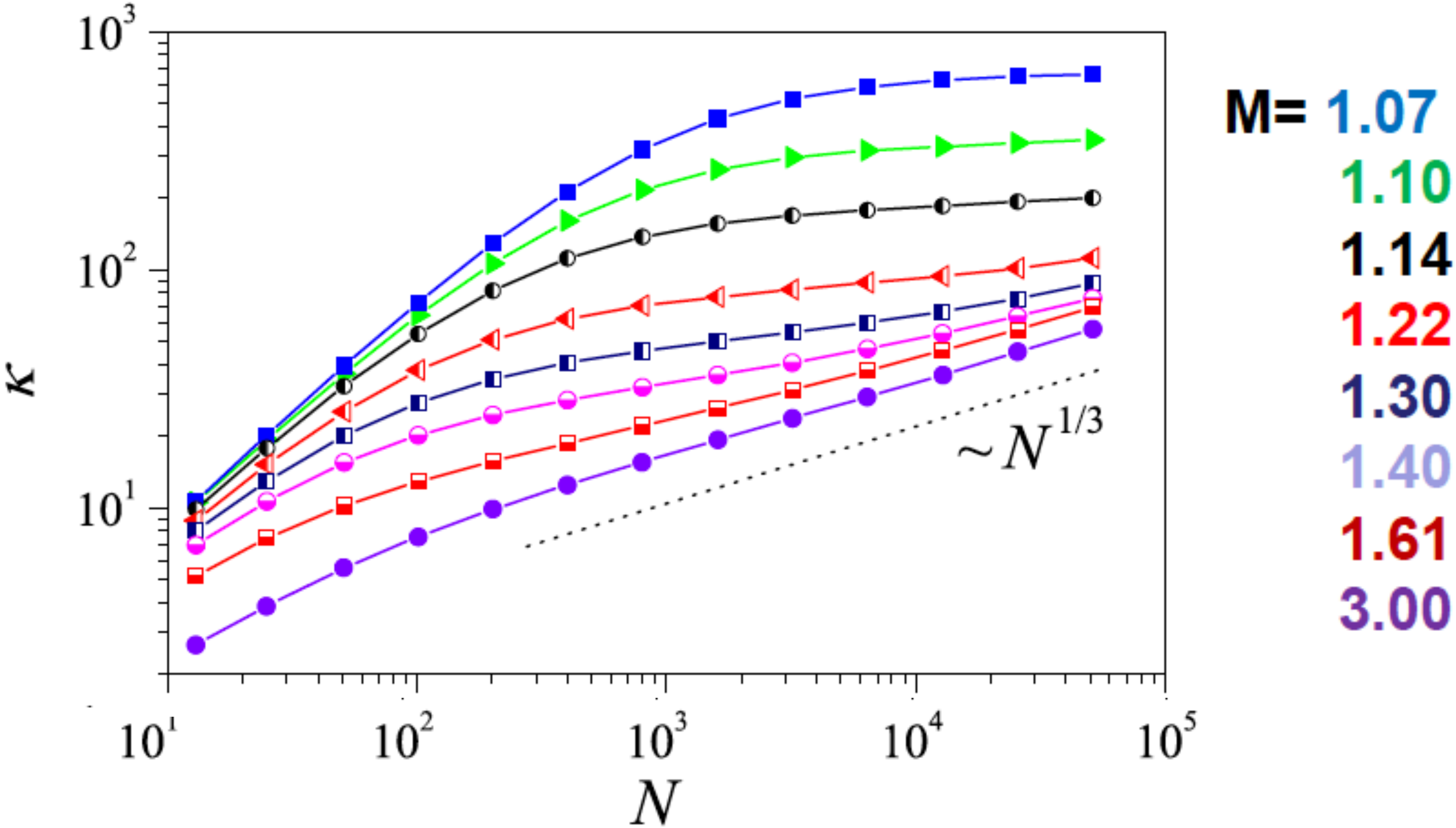
Total heat current $J \equiv \sum_i \mu_i v_i^3/2$

$$\kappa_{\rm GK}(N) = \frac{1}{k_B T^2 N}\int_0^{\tau_{\rm tr}} dt \langle J(0)J(t)\rangle \qquad \tau_{\rm tr} = N/(2v_s)$$

Confirmation of Fourier law close to the integrable limit?



Is the Fourier-like regime asymptotic?



The Fourier-like behavior, seen in both equilibrium and nonequilibrium simulation, might be a finite-size effects

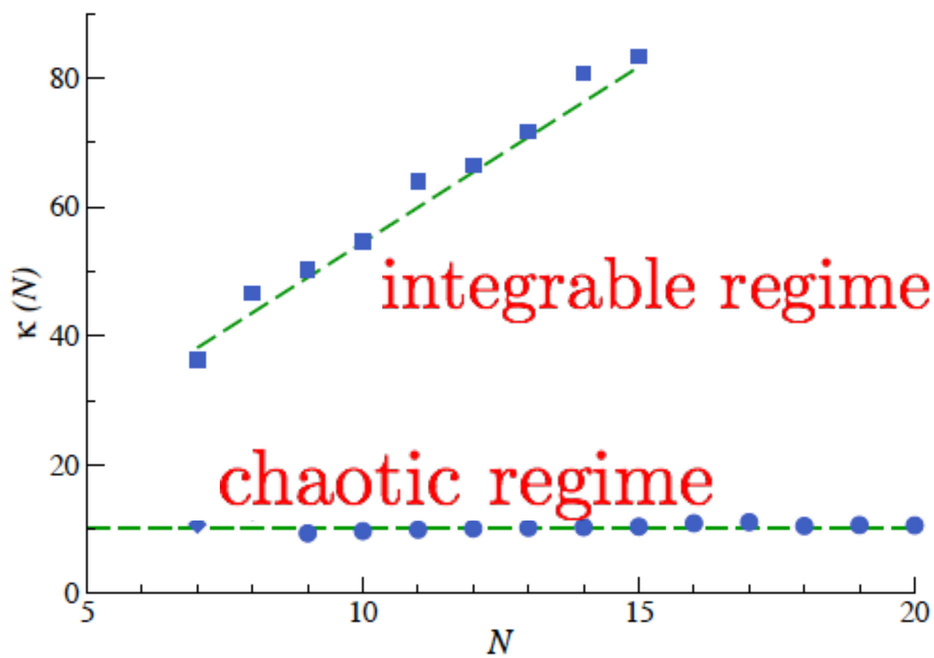
Fourier law in quantum mechanics

Quantum chaos ensures diffusive heat transport and decay of ``dynamical'' (energy-energy) correlation functions.

Exponential sensitivity to errors absent in quantum mechanics but not necessary to obtain the Fourier law

$$\mathscr{H} = \sum_{n=0}^{N-2} H_n + \frac{h}{2}(\sigma_L + \sigma_R) \, ,$$

$$H_n = -Q\sigma_n^z\sigma_{n+1}^z + \frac{\mathbf{h}}{2} \cdot (\sigma_n + \sigma_{n+1})$$



Can we control the heat current?

Towards thermal diodes and thermal transistors

Thermal rectification: everyday's experience when there is thermal convection (transfer of matter, e.g.: heating a fluid from below or from the top surface)

Thermal recifiers much less intuitive in solid-state devices, but not forbidden by thermodynamics

Let us focus on electrical insulators (heat carried by lattice vibrations: phonons)

Rectification factor

Ratio between reverse and forward heat flow

$$R = \left| \frac{j_r}{j_f} \right| \qquad (\text{assuming } j_r > j_f)$$

Why can these flows be different?

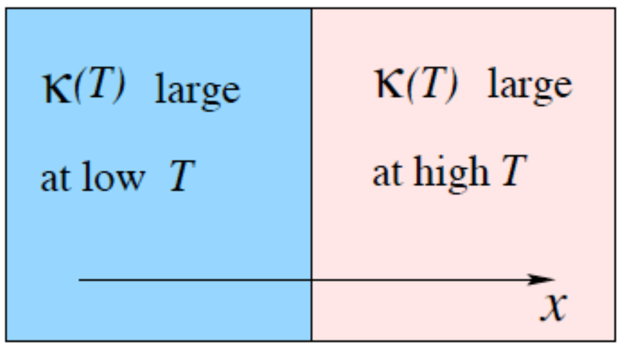
Assuming the Fourier law:

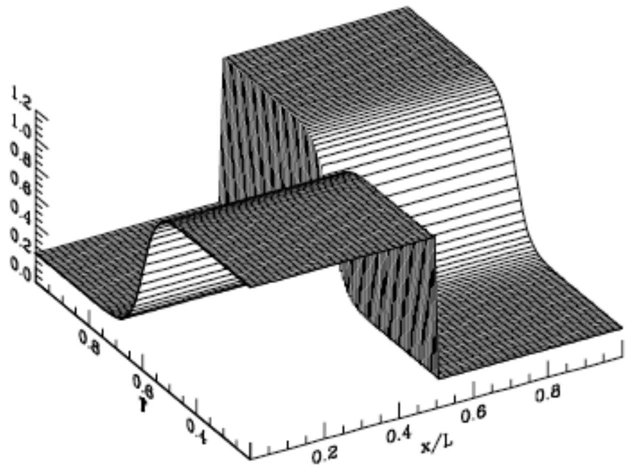
$$T(x) = T_1 + \int_0^x \frac{j_f}{\kappa[\xi, T(\xi)]} d\xi \qquad T(x=L) = T_2$$

reversing boundary conditions we can change temperature and local thermal conductivity distributions

Two ingredients are needed:

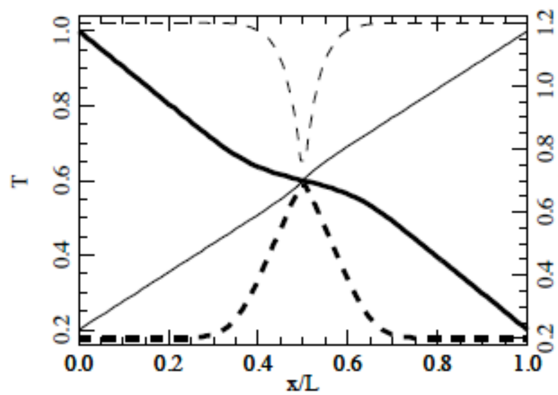
- Temperature-dependent thermal conductivity (nonlinearity needed)
- breaking of the inversion symmetry of the device in the direction of the flow





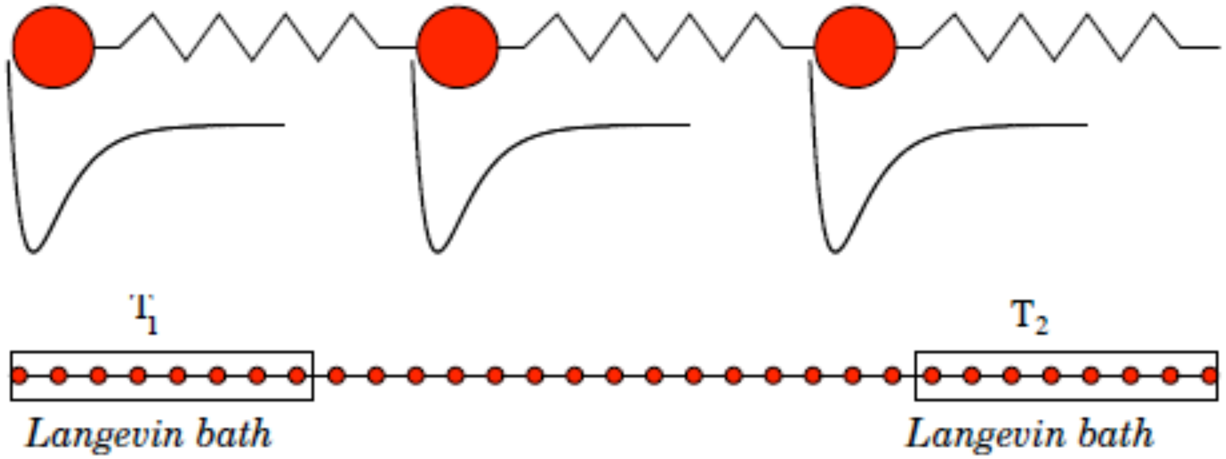
Full curves:
temperature profiles

Dashed curves:
local conductivity



$$R = |j_r / j_f| = 4.75$$

Microscopic model



$$\mathcal{H} = \sum_{n=1}^{N} H_n = \sum_{n=1}^{N} \left[\frac{p_n^2}{2m} + \frac{1}{2} K (y_n - y_{n-1})^2 + D_n (e^{-\alpha_n y_n} - 1)^2 \right]$$

Morse on-site potential: Nonlinearity needed to have temperature-dependent phonon bands

Linearized model (around the equilibrium position):

$$H = \sum_n \frac{p_n^2}{2m} + \tilde{D}_n y_n^2 + \frac{1}{2} K (y_n - y_{n-1})^2$$

$$\tilde{D}_n = D_n \alpha_n^2$$

$$y_n(t) = e^{ikn - i\omega t}$$

Plane waves solutions

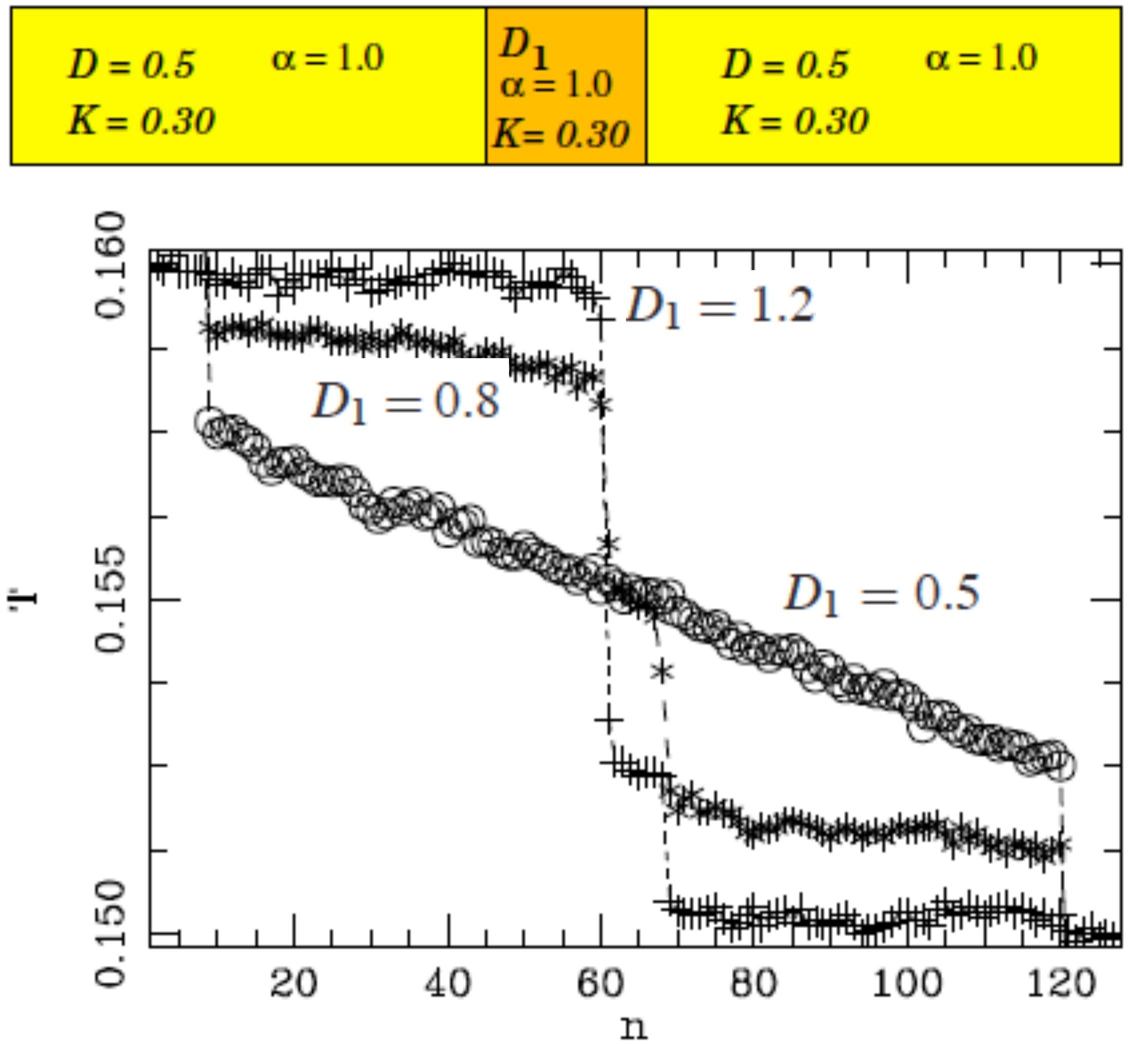
$$\omega^2 = 2K + 2\tilde{D} - 2K \cos k$$

Dispersion relations

$$2\tilde{D} \leq \omega^2 \leq 2\tilde{D} + 4K$$

Phonon band

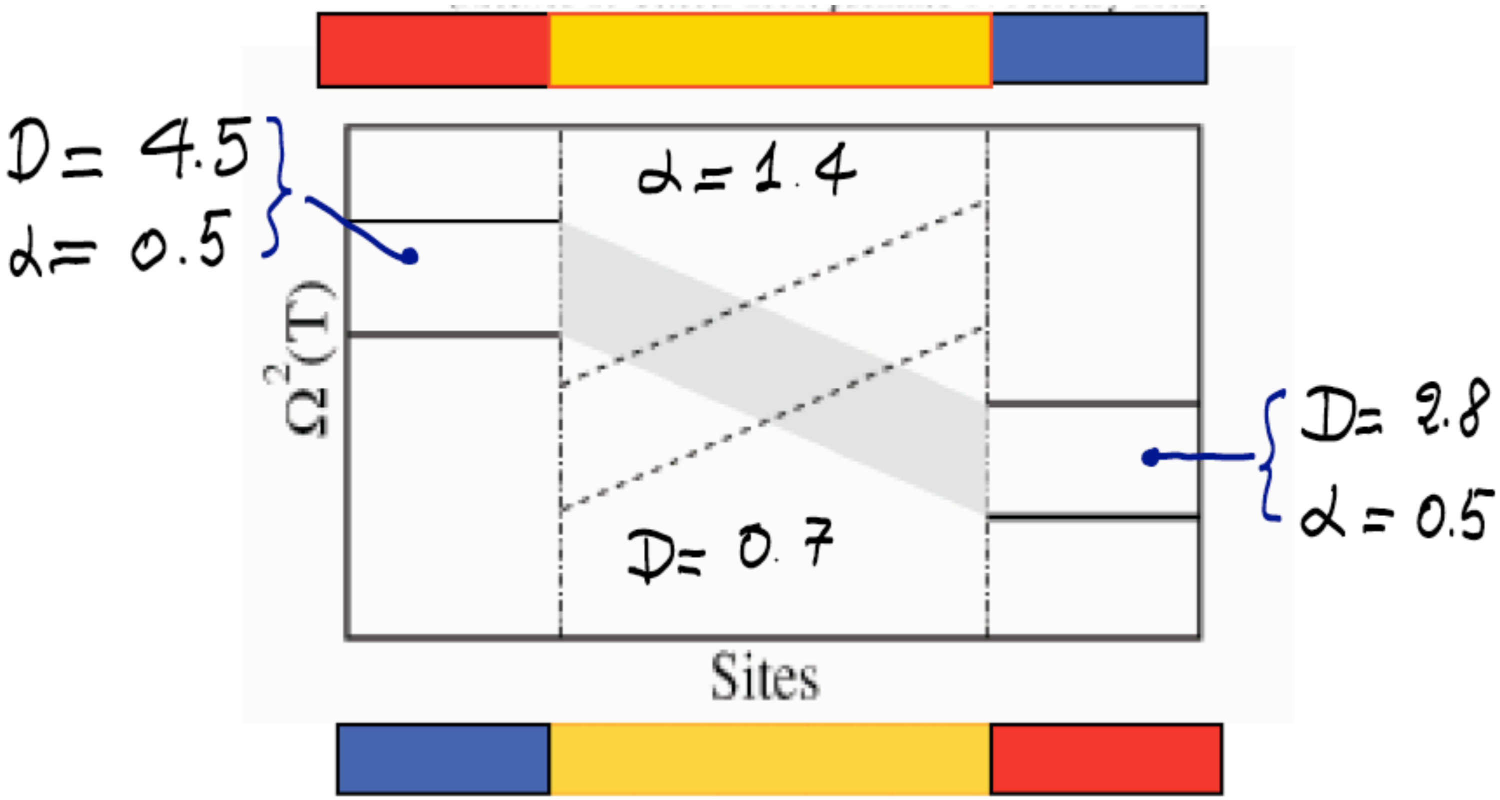
phonon-band mismatch:



Effective (temperature-dependent) harmonic model:

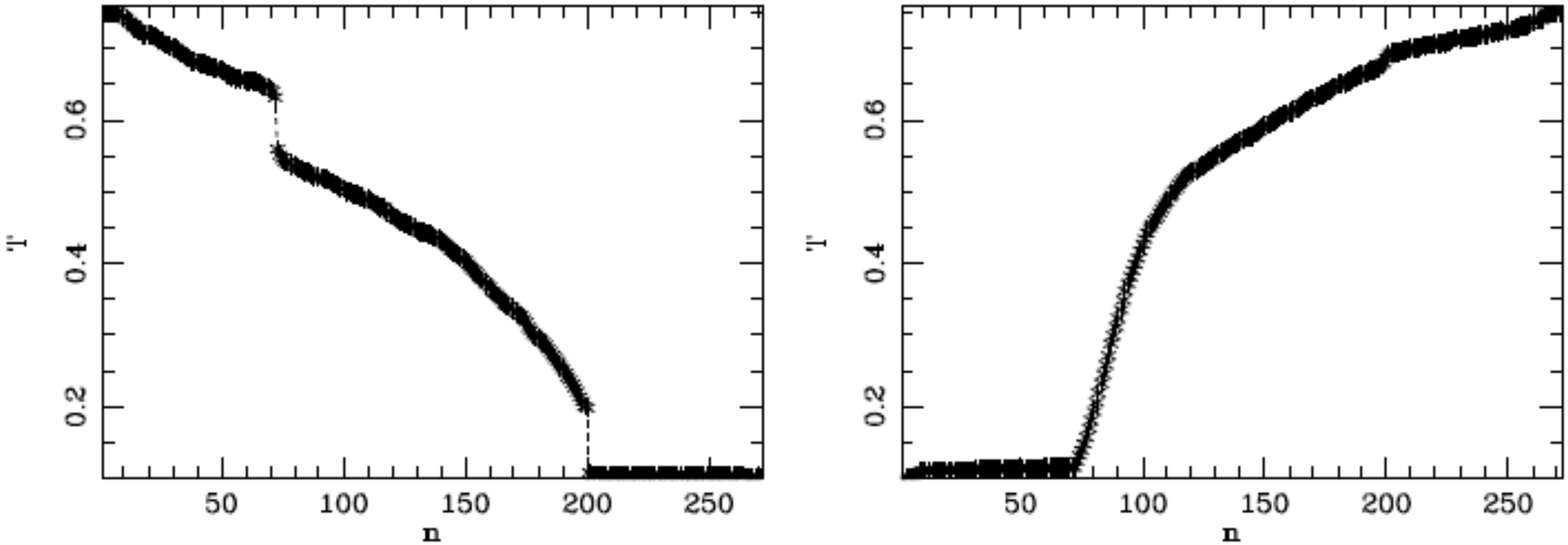
$$H_0 = \sum_{n=1,N} \frac{p_n^2}{2m} + \Omega^2(T) y_n^2 + \frac{1}{2}\Phi(T)\,(y_n - y_{n-1})^2$$

$\Phi(T) = K$ $\qquad$ $\Omega(T)$ decreases as T increases



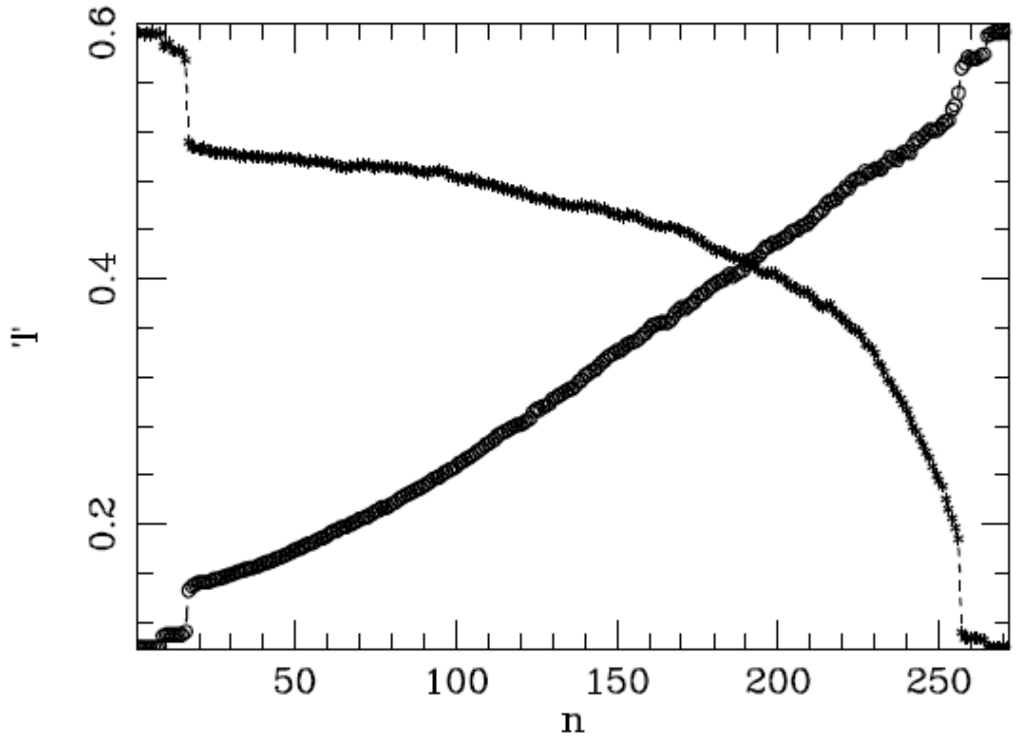
(M. Terraneo, M. Peyrard, G. Casati, PRL **88**, 094302 (2002))

large interface (Kapitza) resistance



$$|j_{\mathrm{right}\to\mathrm{left}}|/j_{\mathrm{left}\to\mathrm{right}} = 2.4$$

With continuos variation of the vibrational properties versus space (it amounts to stacking an infinity of interfaces):



rectifying coefficient $R = 4.95$

(for a pedagogical review, see G. B., G. Casati, C. Mejia-Monasterio, M. Peyrard, arXiv:1512.06889, in Lecture Notes in Physics vol. 921)

Solid-State Thermal Rectifier

C. W. Chang,[1,4] D. Okawa,[1] A. Majumdar,[2,3,4] A. Zettl[1,3,4*]

SCIENCE VOL 314 17 NOVEMBER 2006

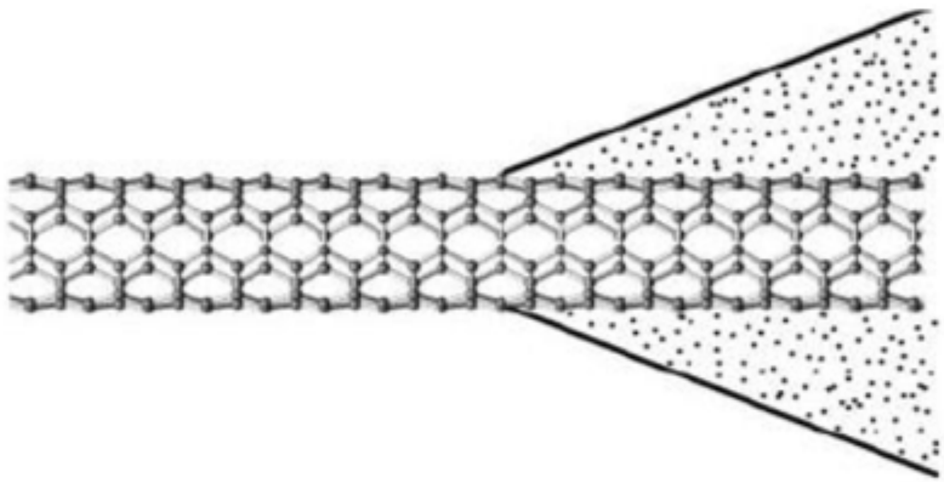


Fig. 1. A schematic description of depositing amorphous $C_9H_{16}Pt$ (black dots) on a nanotube (lattice structure).

For uniform mass distribution, thermal conduction is symmetric.

For mass loading geometry higher thermal conductance was observed when heat flowed from the high-mass region to the low –mass region.

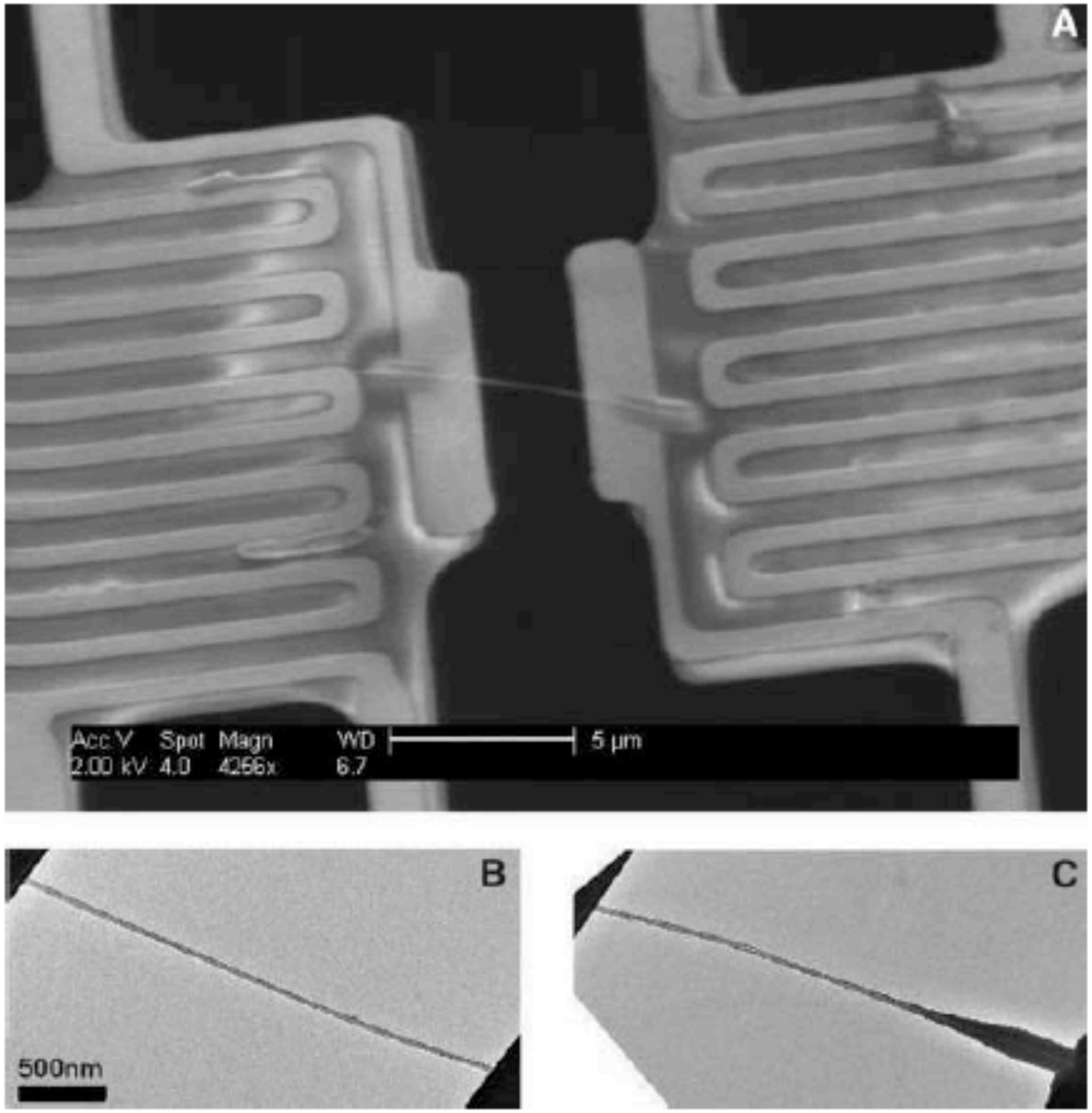


Fig. 2. (**A**) The SEM image of a CNT (light gray line in center) connected to the electrodes. Scale bar, 5 µm. (**B** and **C**) The corresponding low-magnification TEM images of the same CNT in (A), before (B) and after (C) $C_9H_{16}Pt$ was deposited.

thermal rectifications

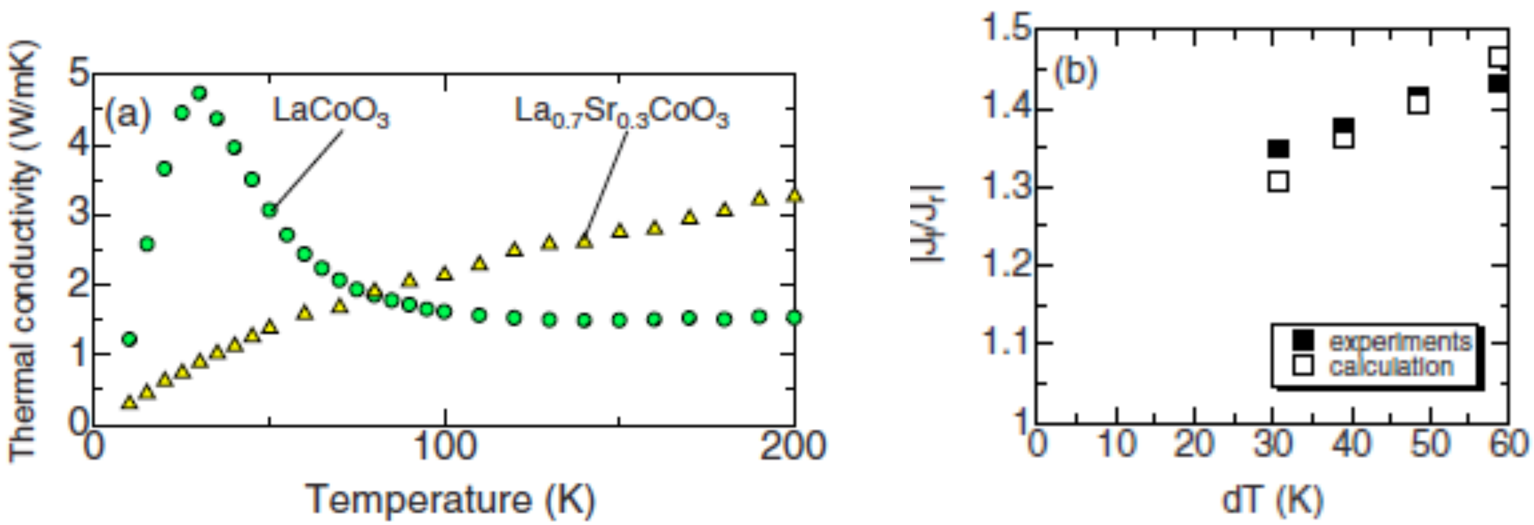
7, 4, and 3%

An oxide thermal rectifier

W. Kobayashi,[1,a)] Y. Teraoka,[2] and I. Terasaki[3]
[1]*Waseda Institute for Advanced Study, Waseda University, Tokyo 169-8050, Japan and PRESTO, Japan Science and Technology Agency, Saitama 332-0012, Japan*
[2]*Department of Physics, Waseda University, Tokyo 169-8555, Japan*
[3]*Department of Applied Physics, Waseda University, Tokyo 169-8555, Japan*

(Received 13 June 2009; accepted 2 October 2009; published online 29 October 2009)

We have experimentally demonstrated thermal rectification as bulk effect. According to a theoretical design of a thermal rectifier, we have prepared an oxide thermal rectifier made of two cobalt oxides with different thermal conductivities, and have made an experimental system to detect the thermal rectification. The rectifying coefficient of the device is found to be 1.43, which is in good agreement with the numerical calculation. [doi:10.1063/1.3253712]



Applied Physics Express 5 (2012) 027302
DOI: 10.1143/APEX.5.027302

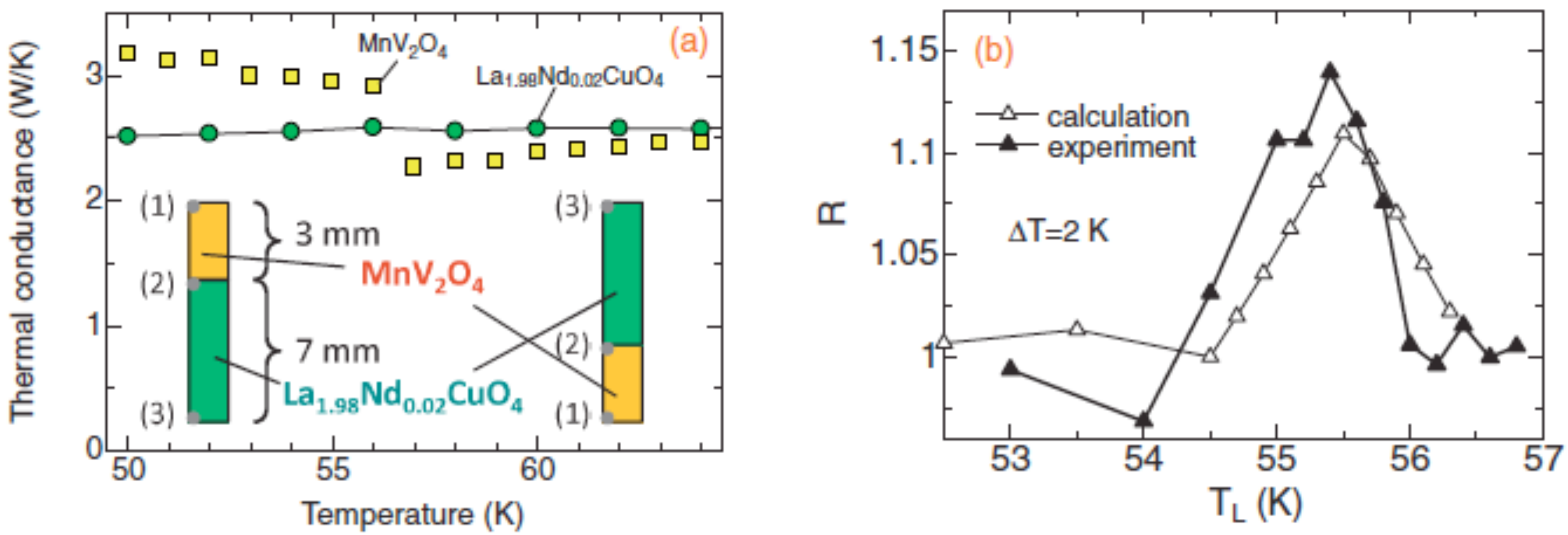
Thermal Rectification in the Vicinity of a Structural Phase Transition

Wataru Kobayashi[1,2,3*], Daisuke Sawaki[4], Tsubasa Omura[4], Takuro Katsufuji[4], Yutaka Moritomo[1,2], and Ichiro Terasaki[5]

[1] *Graduate School of Pure and Applied Sciences, University of Tsukuba, Ibaraki 305-8571, Japan*
[2] *Tsukuba Research Center for Interdisciplinary Materials Science (TIMS), University of Tsukuba, Ibaraki 305-8571, Japan*
[3] *PRESTO, Japan Science and Technology Agency, Kawaguchi, Saitama 332-0012, Japan*
[4] *Department of Physics, Waseda University, Shinjuku, Tokyo 169-8555, Japan*
[5] *Department of Physics, Nagoya University, Nagoya 464-8602, Japan*

Received December 7, 2011; accepted January 5, 2012; published online January 25, 2012

We have fabricated an oxide thermal rectifier made of $La_{1.98}Nd_{0.02}CuO_4$ and MnV_2O_4. By utilizing a jump of a thermal conductivity originated in the structural phase transition accompanied by the orbital ordering in MnV_2O_4, a rectifying coefficient of 1.14 has been achieved in the presence of a small temperature difference of 2 K. A thermal rectifier operating under a small temperature difference will play an important role for realizing heat-current control in electronic devices.

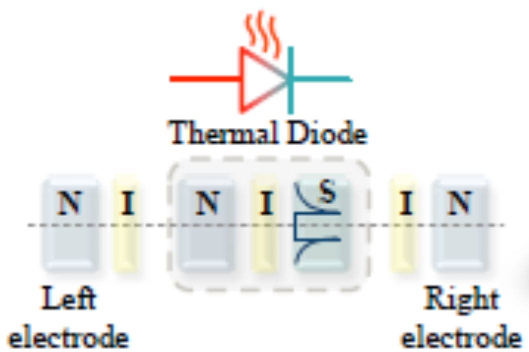


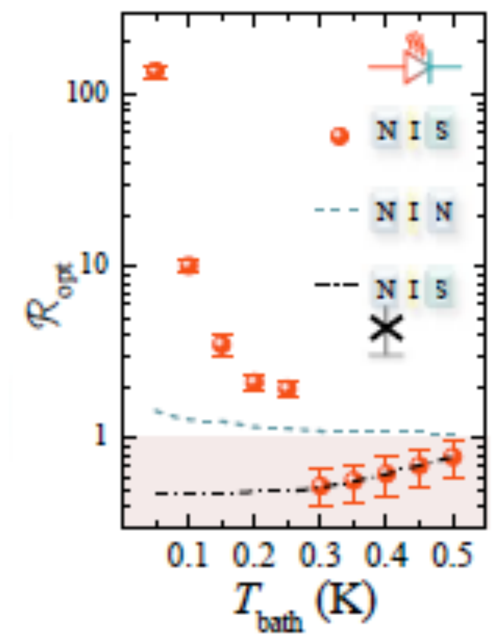
Rectification of electronic heat current by a hybrid thermal diode

Maria José Martínez-Pérez, Antonio Fornieri & Francesco Giazotto

Affiliations | Contributions | Corresponding author

Nature Nanotechnology **10**, 303–307 (2015) | doi:10.1038/nnano.2015.11





Several proposals of a thermal diode are based on the sequential coupling of segments with different anharmonic potentials, with practical problems:

Difficult to be experimentally implemented (necessary to implement large asymmetry and temperature gradients on small scales)

The **rectification factor is small**

The **rectification factor decays to zero with increasing the system size** (i.e., going to the linear response regime)

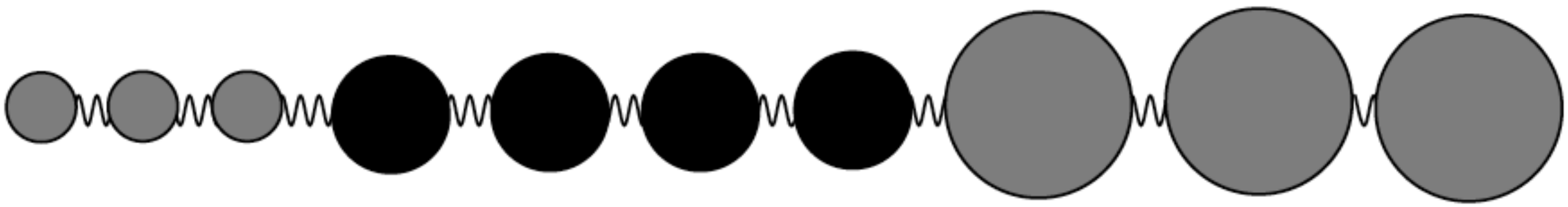
Lack of efficient and feasible diodes

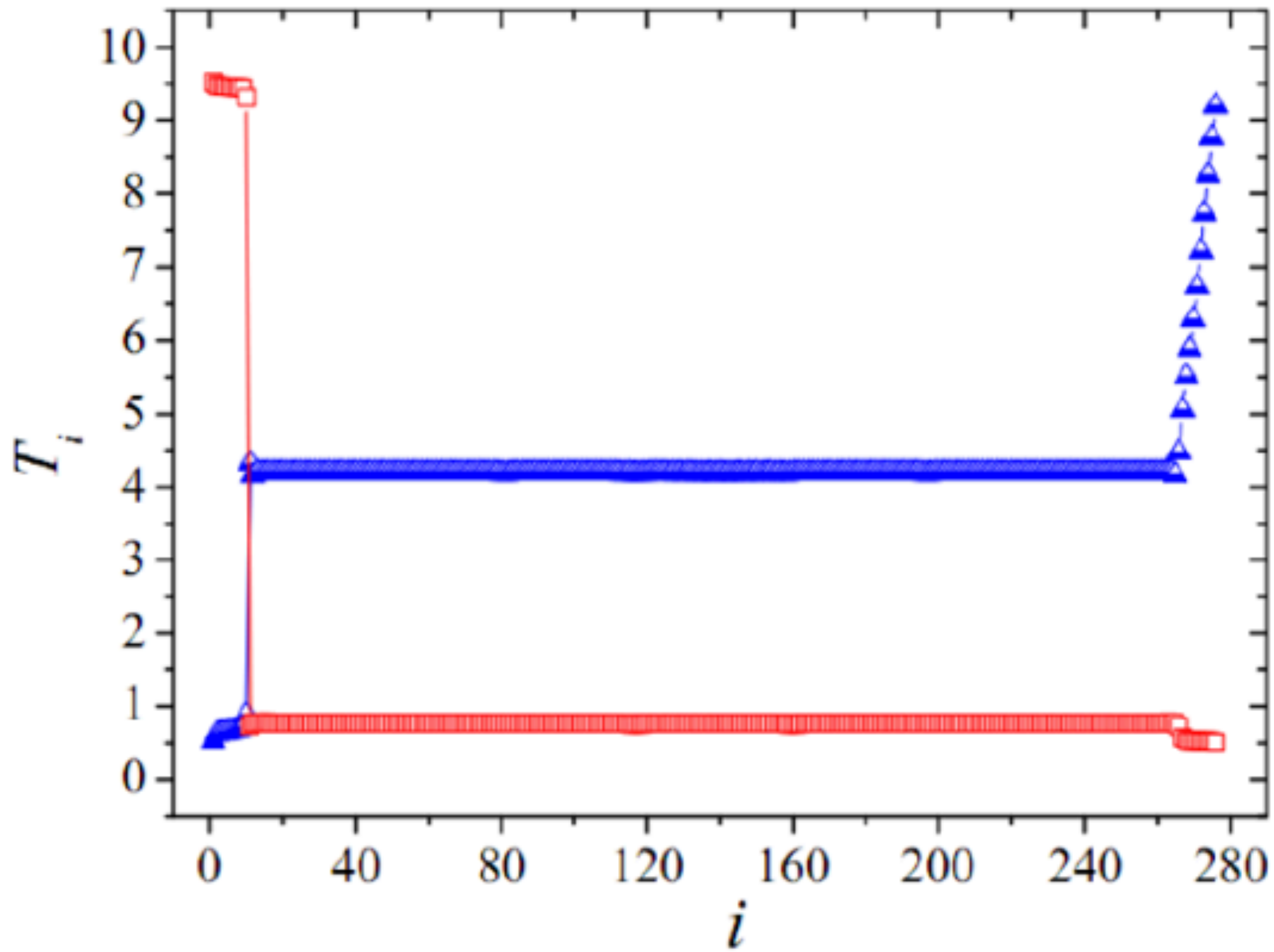
Graded-mass system + ballistic channel

$$H = H_L + H_C + H_R + \frac{1}{2}(x_{N_L+1} - x_{N_L})^2 + \frac{1}{2}(x_{N_L+N_C+1} - x_{N_L+N_C})^2$$

$$H_{L,R} = \sum_i \left(\frac{p_i^2}{2m_{L,R}} + \frac{1}{2}(x_i - x_{i-1})^2 + \frac{\gamma_{L,R}}{4} x_i^4 \right)$$

$$H_C = \sum_i \left(\frac{p_i^2}{2m_C} + \frac{1}{2}(x_i - x_{i-1})^2 \right)$$

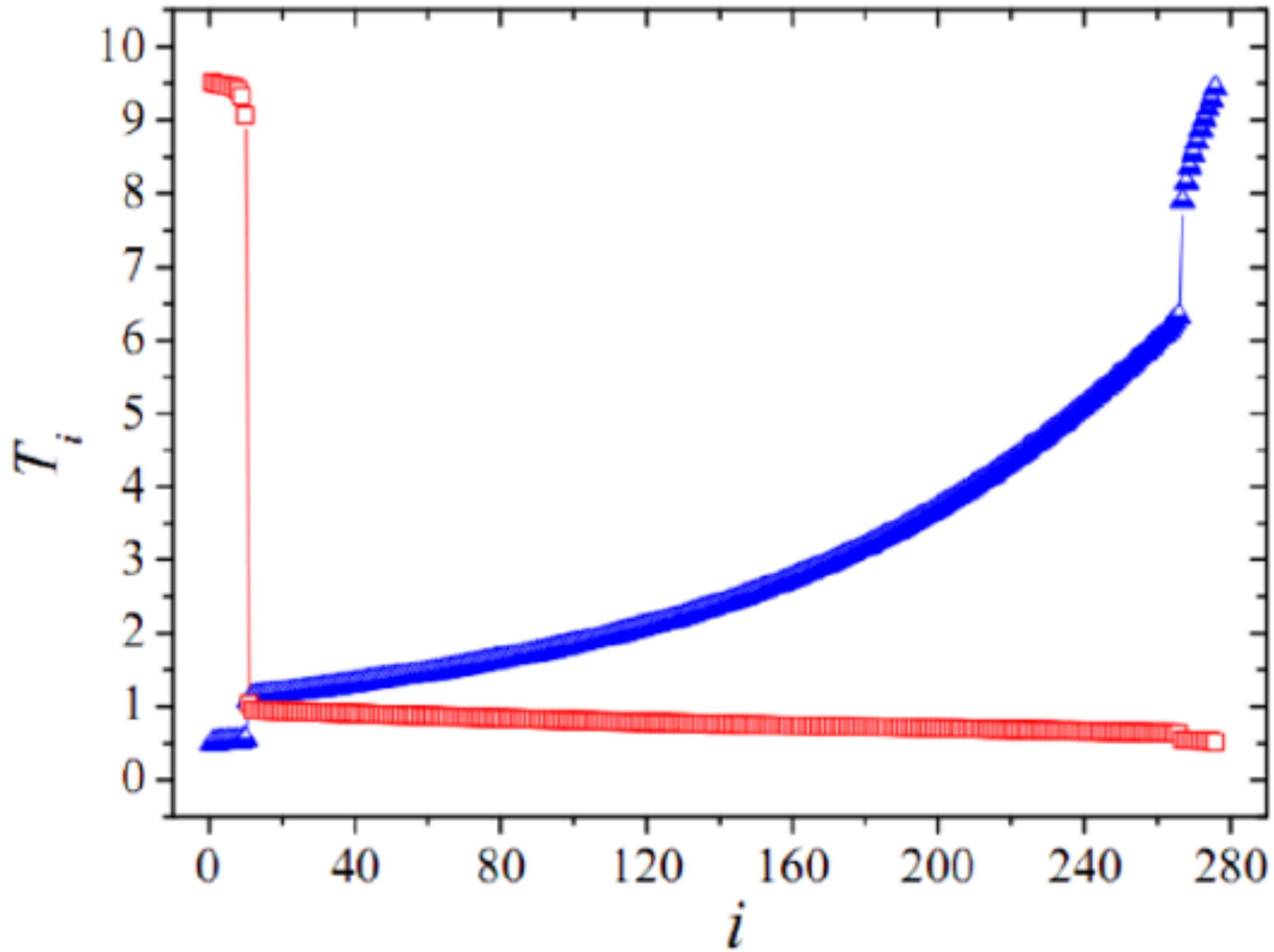




(simulations by Shunda Chen, UC Davis)

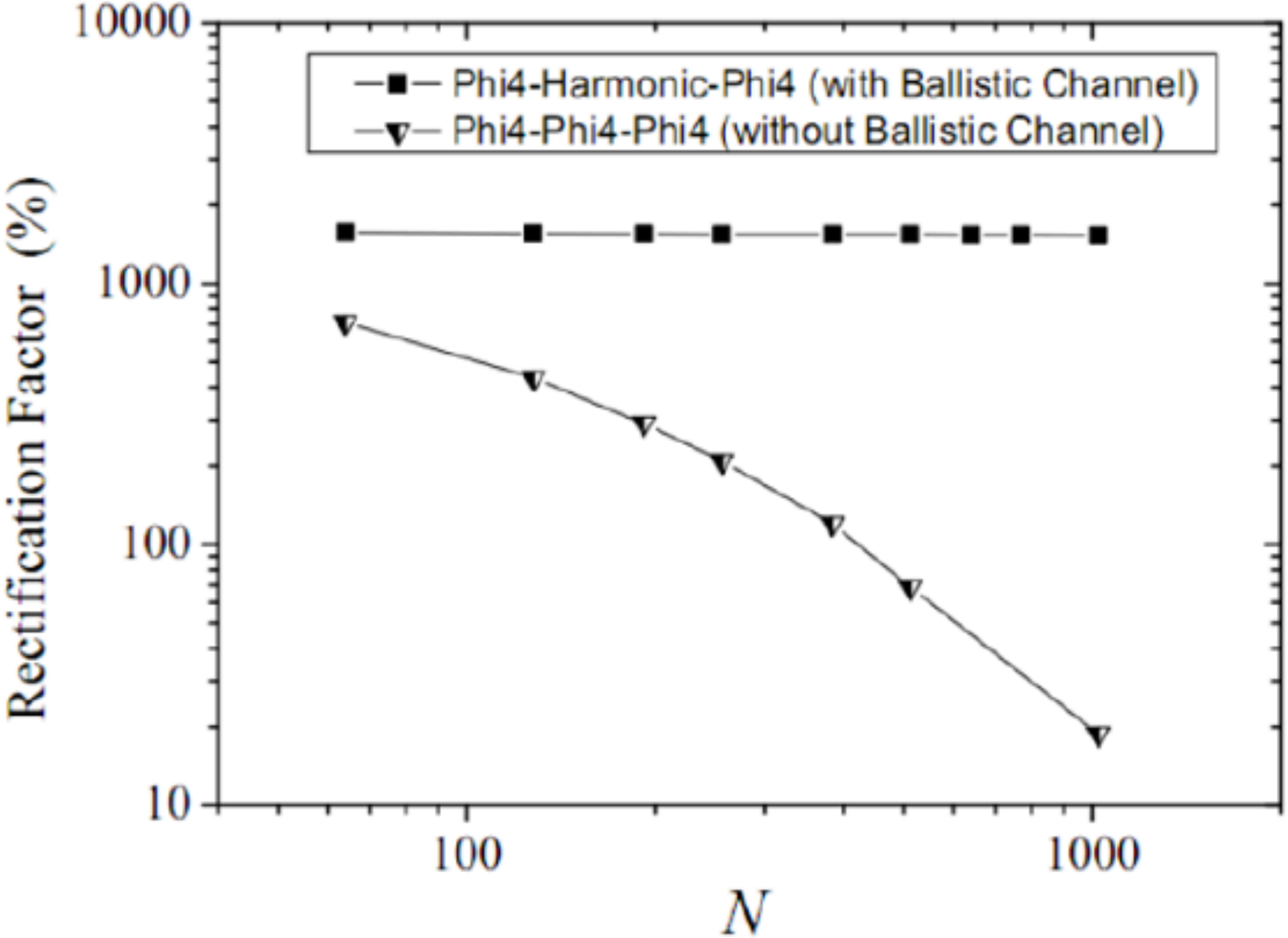
Temperature profiles: **NC=256, Ntot=276.**

(T+=9.5, T-=0.5, NL=NR=10, mL=1, mC=4.5, mR=10)



Temperature profiles: **Phi4-Phi4-Phi4 model,**

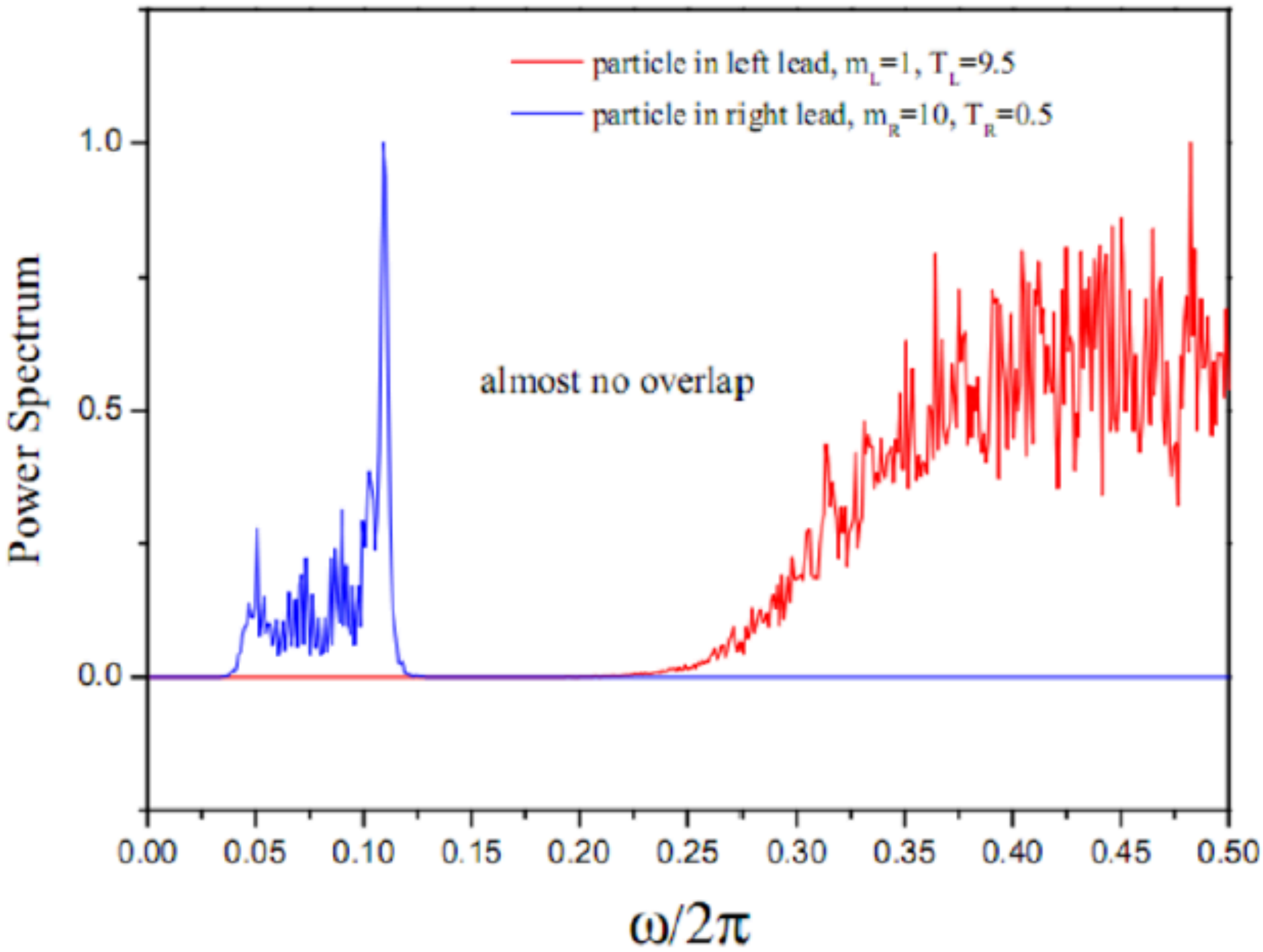
T+=9.5, T-=0.5, NL=NR=10, mL=1, mC=4.5, mR=10



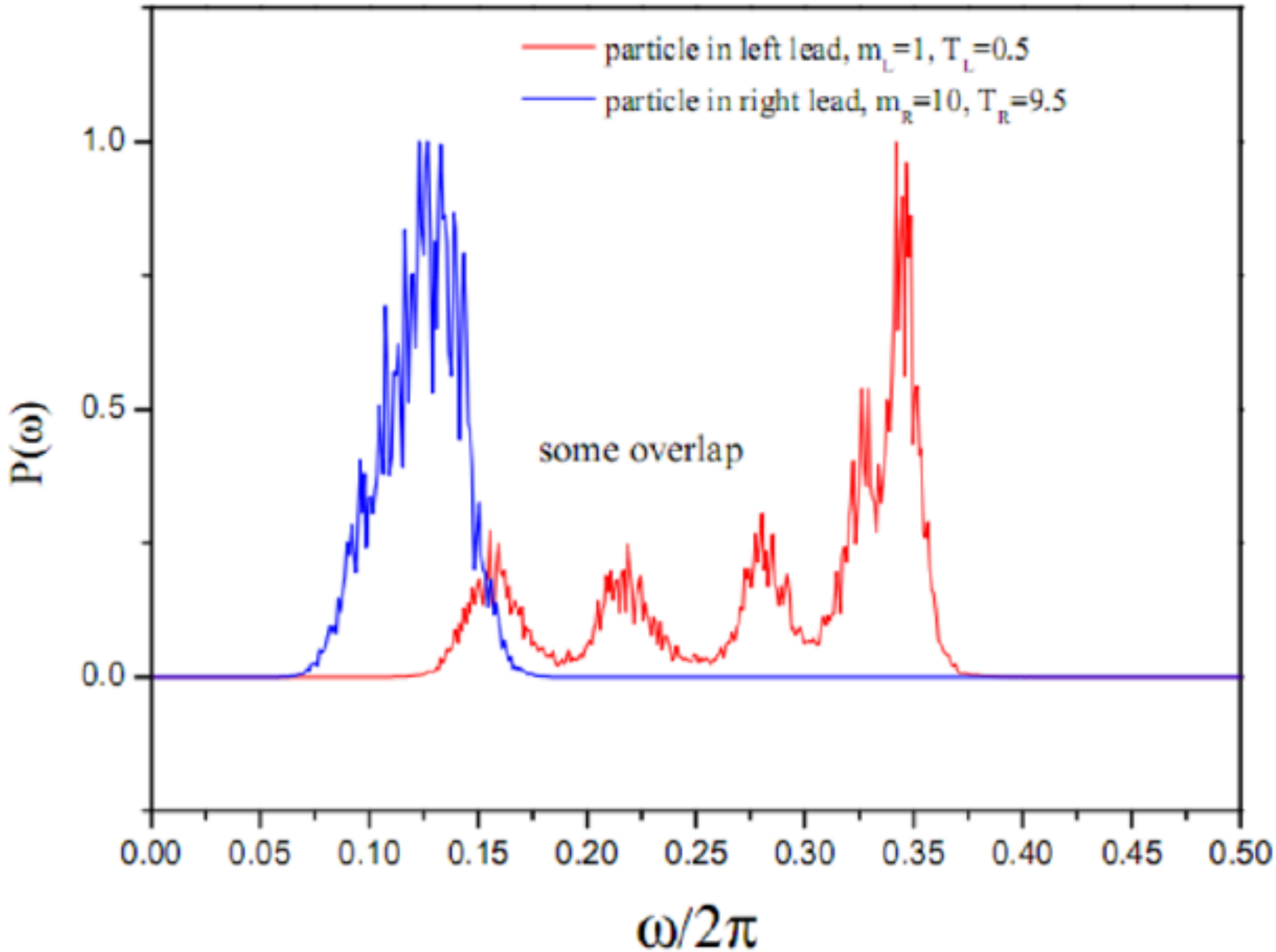
$$\boxed{f_r = \frac{(J_+ - J_-)}{J_-} \times 100\%}$$

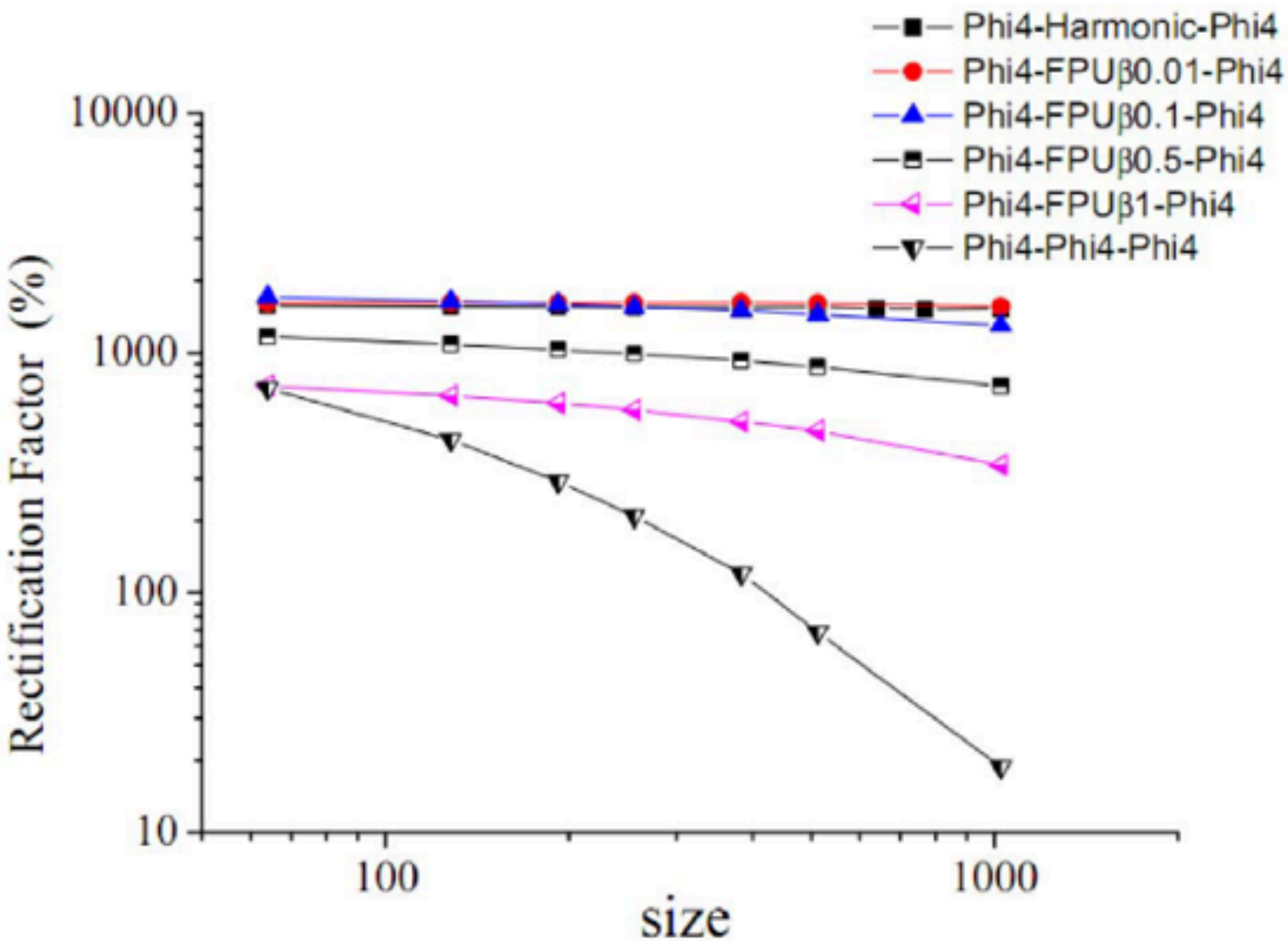
T+=9.5, T-=0.5, NL=NR=10, mL=1, mC=4.5, mR=10

High temperature on the left lighter lead



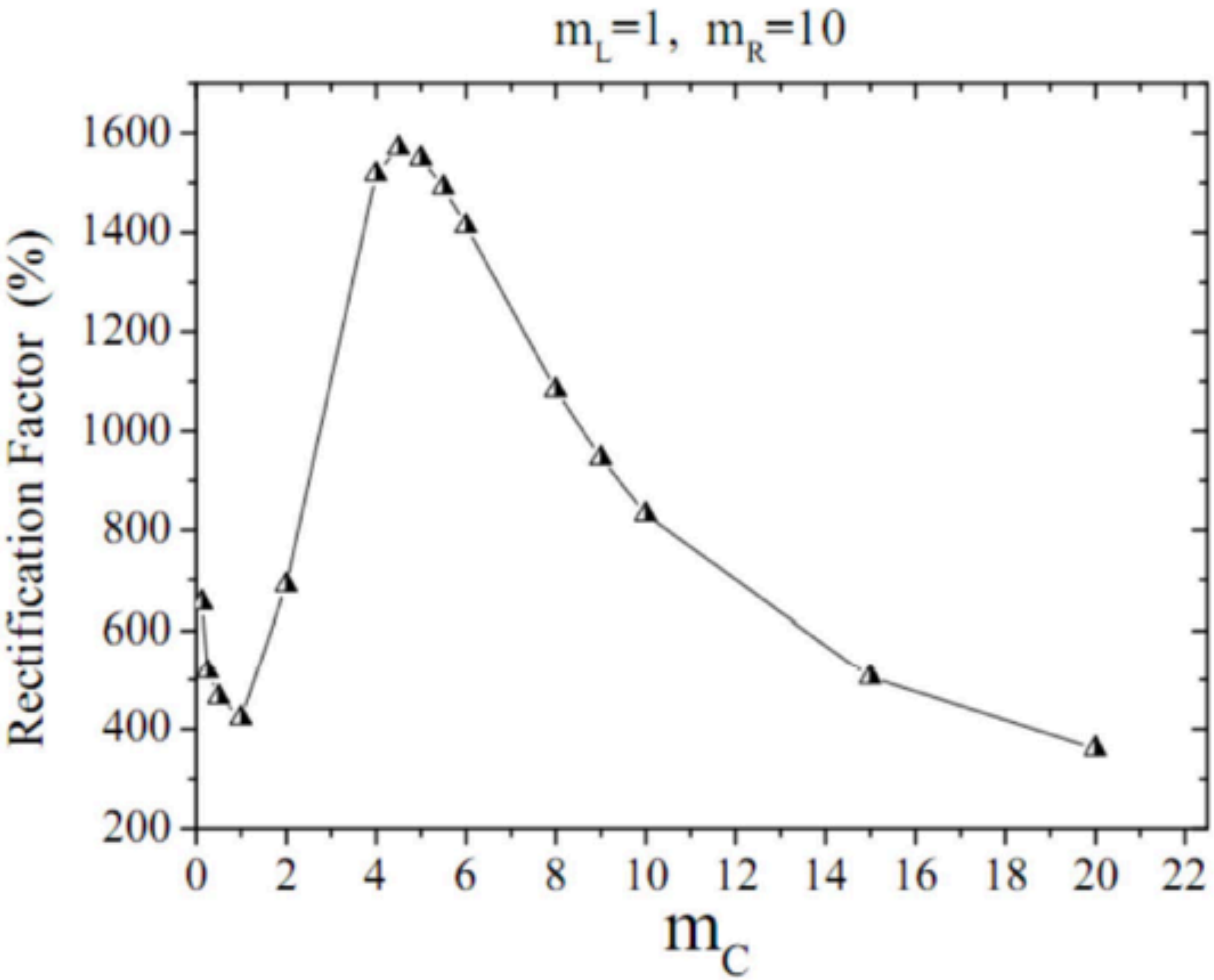
High temperture on the right heavier lead





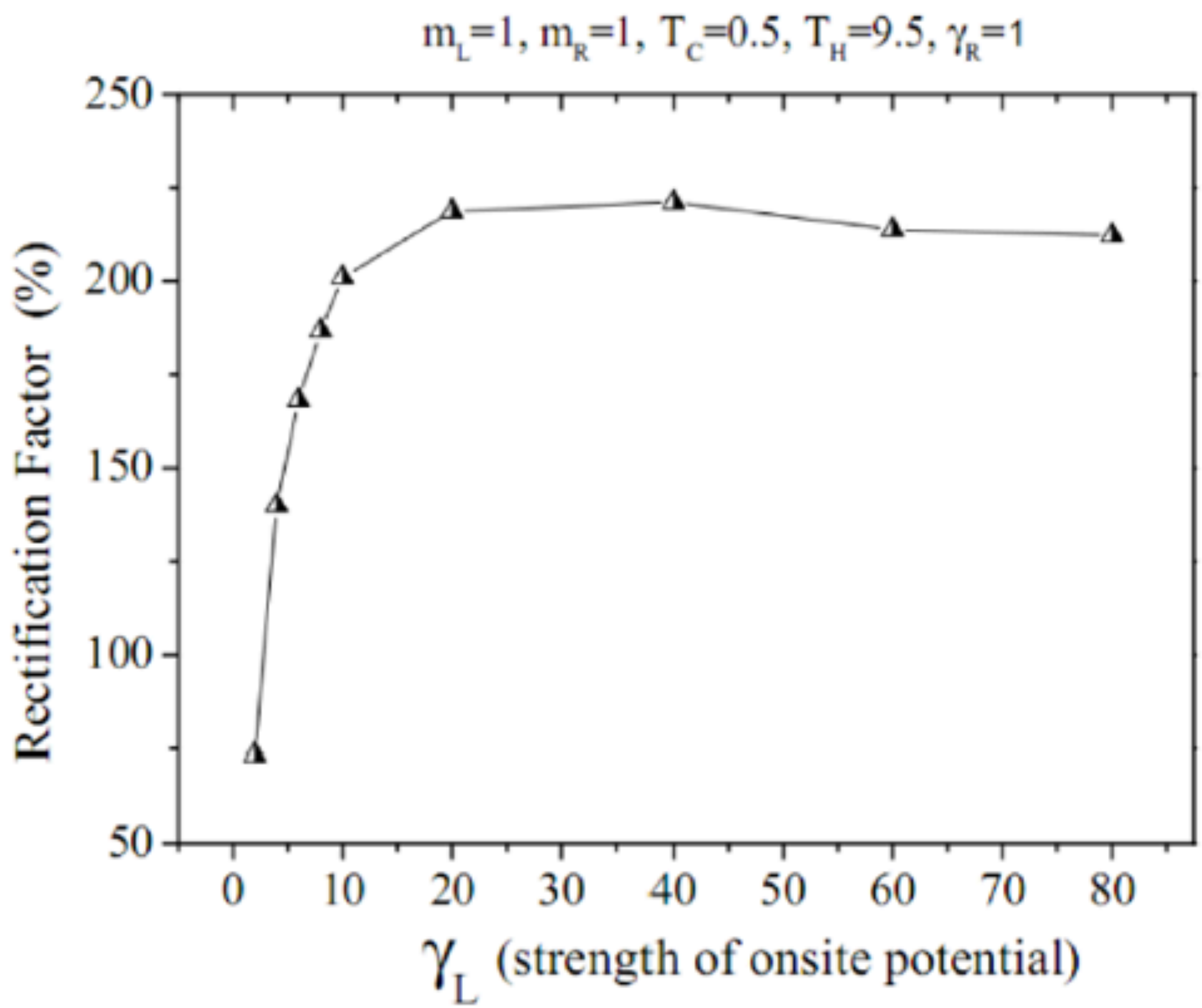
Dependence on anharmonicity

FPU-beta in the central part with different value of beta

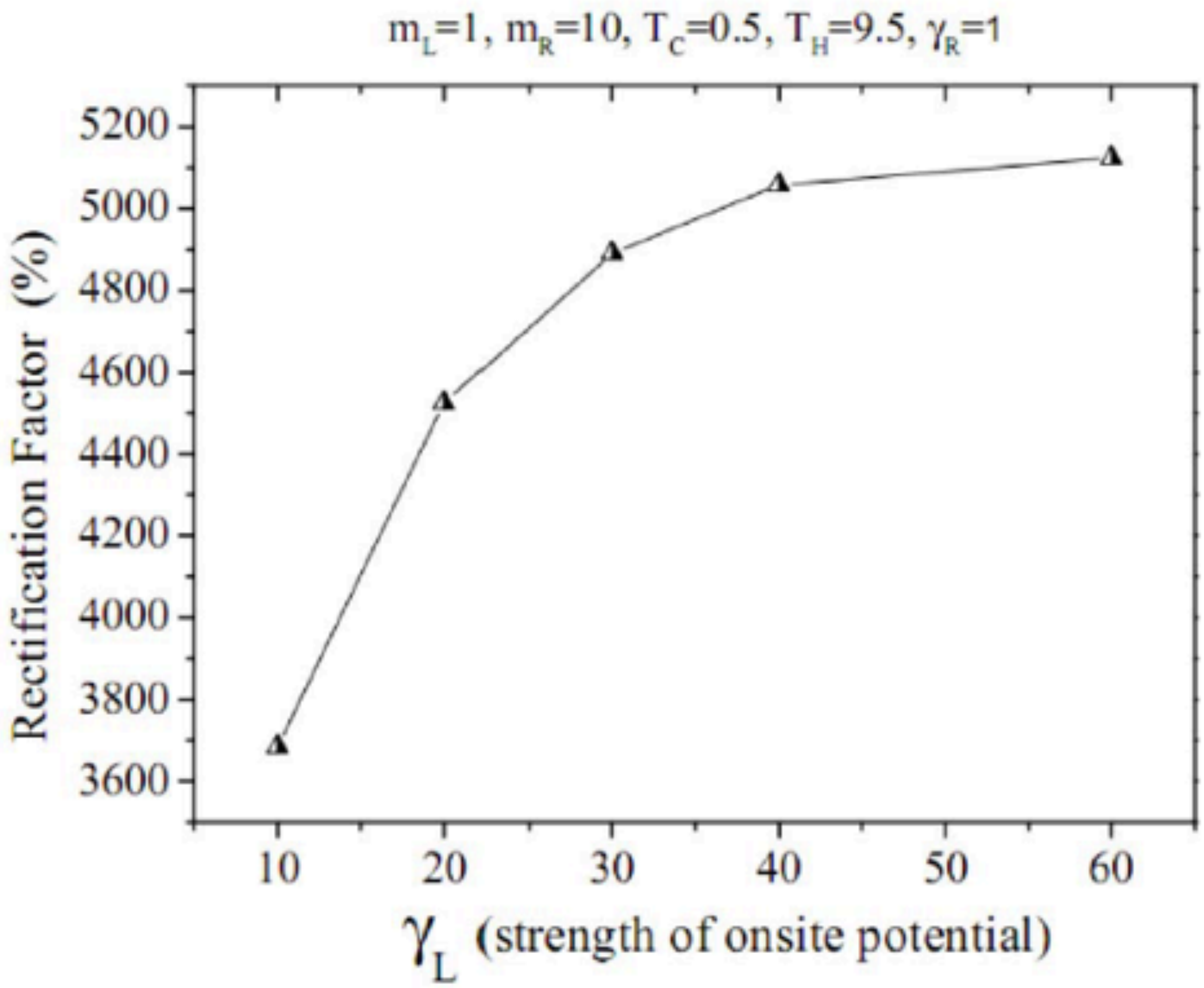


Dependence on mass of the central channel mC.

mL=1, mR=10,



Dependence on onsite potential coefficient gamma_L (onsite potential gradient) for equal-mass system.
gamma_R=1,



Dependence on onsite potential coefficient gamma_L (onsite potential gradient) for mass-graded system. mL=1, =mR=10, mC=(mL+mR)/2=5.5, gamma_R=1,

Conclusions

Basic ingredients for a thermal diode:

- Temperature-dependent thermal conductivity (nonlinearity needed)
- breaking of the inversion symmetry of the device in the direction of the flow

Problems for an efficient practical implementation still remain

Thermal rectification with a ballistic spacer might be a promising model, but more realistic calculations are needed.