TECHNISCHE UNIVERSITÄT DRESDEN

Institute for Materials Science, Chair 'Materials Science and Nanotechnology'

# Thermal conductivity behavior in double-stranded molecular systems

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complex nano materials

DPG, 14 March 2011

# OUTLINE

Introduction

Ladder-model Hamiltonian: Langevin Stochastic Baths

Signatures of normal heat transport

A model of thermal rectifier

Conclusions

# Introduction: Fourier´s Law



## Fourier´s law in one-dimensional systems

$$\mathbf{J}(\mathbf{x},t) = -\kappa\nabla\mathbf{T}(\mathbf{x},\mathbf{t})$$ Diffusive energy transport

$$\mathcal{H} = \sum_{n}^{N} \frac{1}{2} m\dot{y}_n^2 + \frac{k}{2}(y_n - y_{n-1})^2 + V(y_n)$$

| Harmonic | Local - Anharmonic |
|---|---|
| No thermal gradient | Linear thermal gradient |
| Size-dependent κ | *κ remains finite* |
| **Anomalous heat transport** | **Normal heat transport** |

## Thermal rectification: previous models

$V_0$ | $V_1$ | $V_0$

M. Terraneo, M. Peyrard, and G. Casati
PRL 88, 094302 (02)

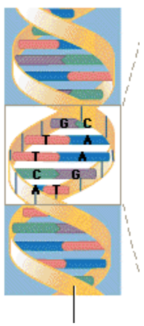
Nonlinearity + Symmetry breaking

$V_0 \longleftrightarrow V_1$

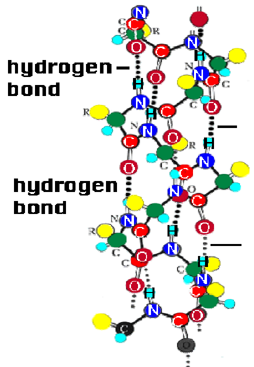
B. Hu, L. Yang, and Y. Zhang
PRL 97, 124302 (06)

## Double-stranded molecular systems

DNA



α- helix in proteins




$V_0$

$\updownarrow \quad \updownarrow \quad \updownarrow \quad \updownarrow \quad \updownarrow$

$V_1 \rightarrow 0$

# Hamiltonian of a ladder-model



$$\mathcal{H} = \mathcal{H}_H + \mathcal{H}_A + \mathcal{H}_{int}$$

$$\mathcal{H}_H = \sum_{n=1}^{N} \frac{1}{2}\dot{y}_n^2 + W(y_n, y_{n-1})$$

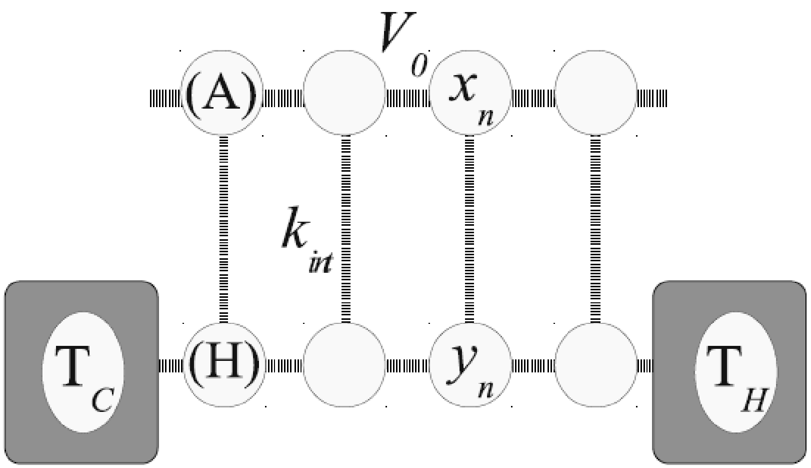
$$\mathcal{H}_{int} = \sum_{n=1}^{N} k_{int} W(x_n, y_n)$$

$$\mathcal{H}_A = \sum_{n=1}^{N} \frac{1}{2}\dot{x}_n^2 + W(x_n, x_{n-1}) + V(x_n)$$

## Potential Terms

$$W(x_n, x_{n-1}) = \frac{1}{2}(x_n - x_{n-1})^2$$

$$V(x_n) = \frac{-V_0}{4\pi^2} \cos 2\pi x_n$$



# Heat Baths – Thermal Properties

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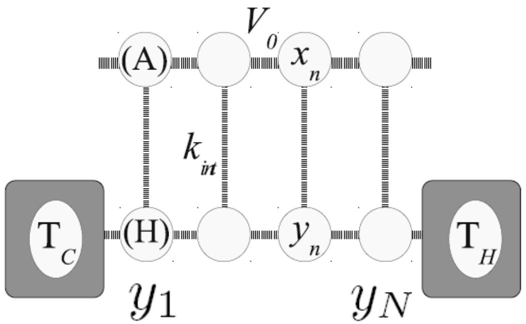
## Heat Reservoirs – Langevin Stochastic Baths

$$\frac{d^2 y_n}{dt^2} = -W'(y_n, y_{n-1}) - W'(y_n, y_{n+1}) \boxed{- \gamma \frac{dy_n}{dt} + f_n(t)}$$

$$\langle f_n(t) f_n(t') \rangle = 2T\gamma\delta(t - t')$$

$$T_{H,C} = T_M \pm 0.05 \qquad \gamma = 0.5$$




## Thermal properties

$$T_n = \langle \dot{x}_n^2 + \dot{y}_n^2 \rangle$$

$$J = \langle J_1 \rangle = \ldots = \langle J_N \rangle$$

$$\kappa = JN/(T_C - T_H)$$

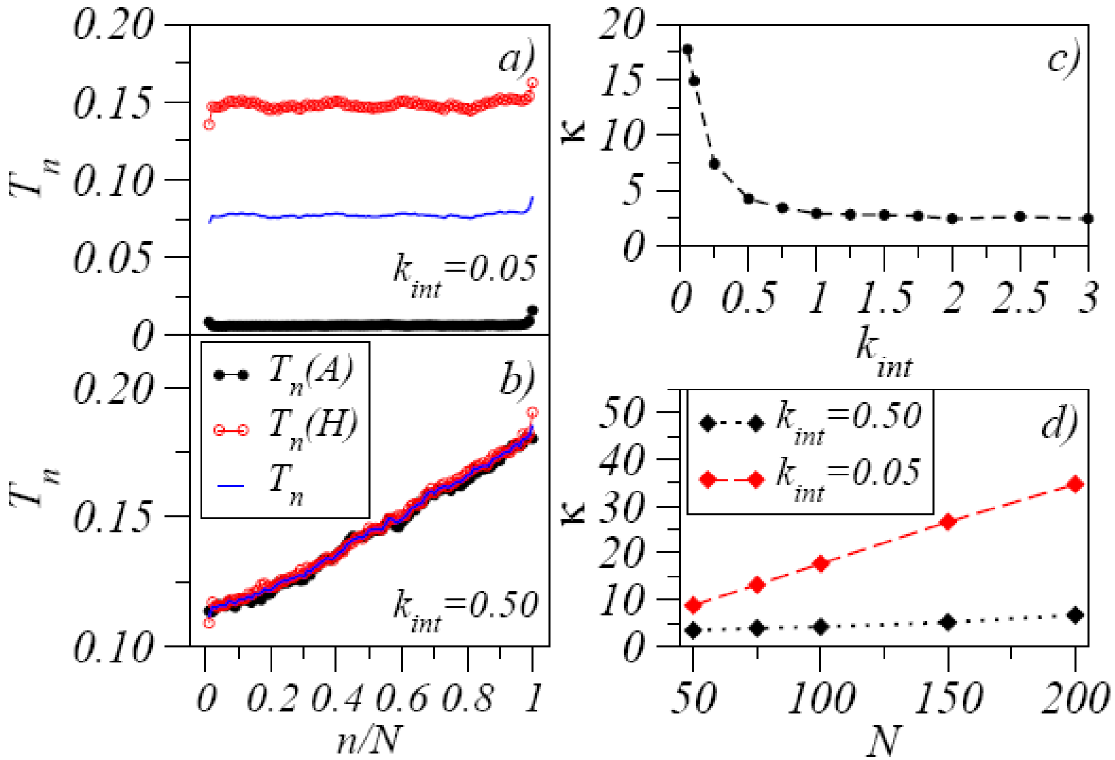
$$J_n = \dot{x}_n \Big( \frac{\partial W'(x_n, x_{n-1})}{\partial x_n} + k_{int} \frac{\partial W'(x_n, y_n)}{\partial x_n} \Big) + \dot{y}_n \Big( \frac{\partial W'(y_n, y_{n-1})}{\partial y_n} + k_{int} \frac{\partial W'(x_n, y_n)}{\partial y_n} \Big)$$

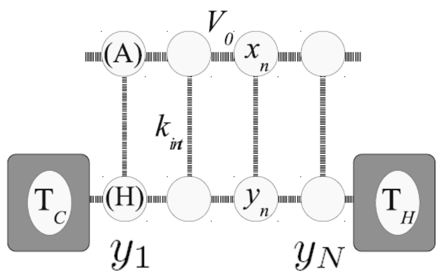
# Interchain Coupling Effects



## Normal heat transport if $k_{int} > k_{int}^*$

$V_0 = 5$




- Well-formed thermal gradient

-The thermal conductivity does not depend on *N*

# Critical Coupling $k_{int}^*$

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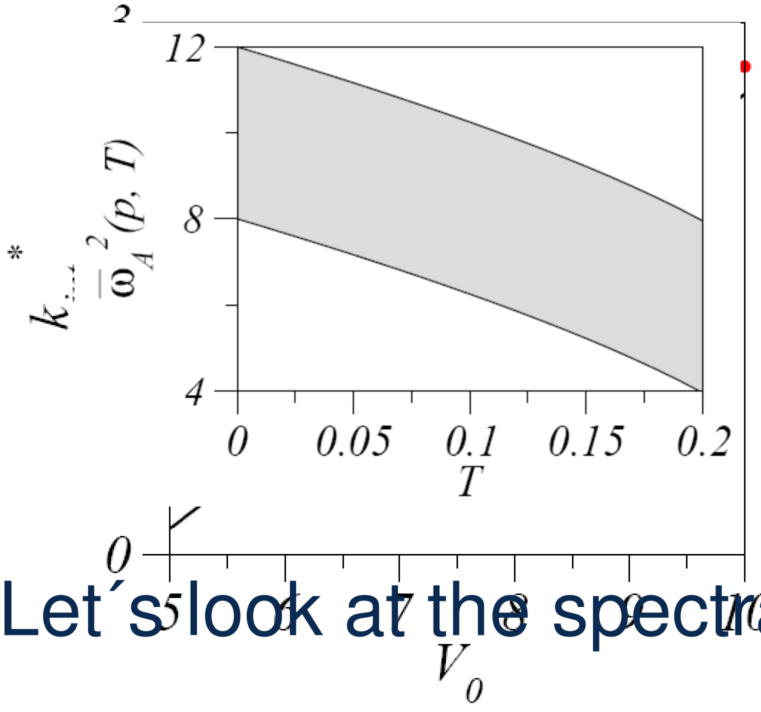
* Anharmonic chain:
self-consistent phonon theory

$$V(x_n) = \frac{-V_0}{4\pi^2}\cos(2\pi x_n) \rightarrow \frac{U(T)}{2}x_n^2$$

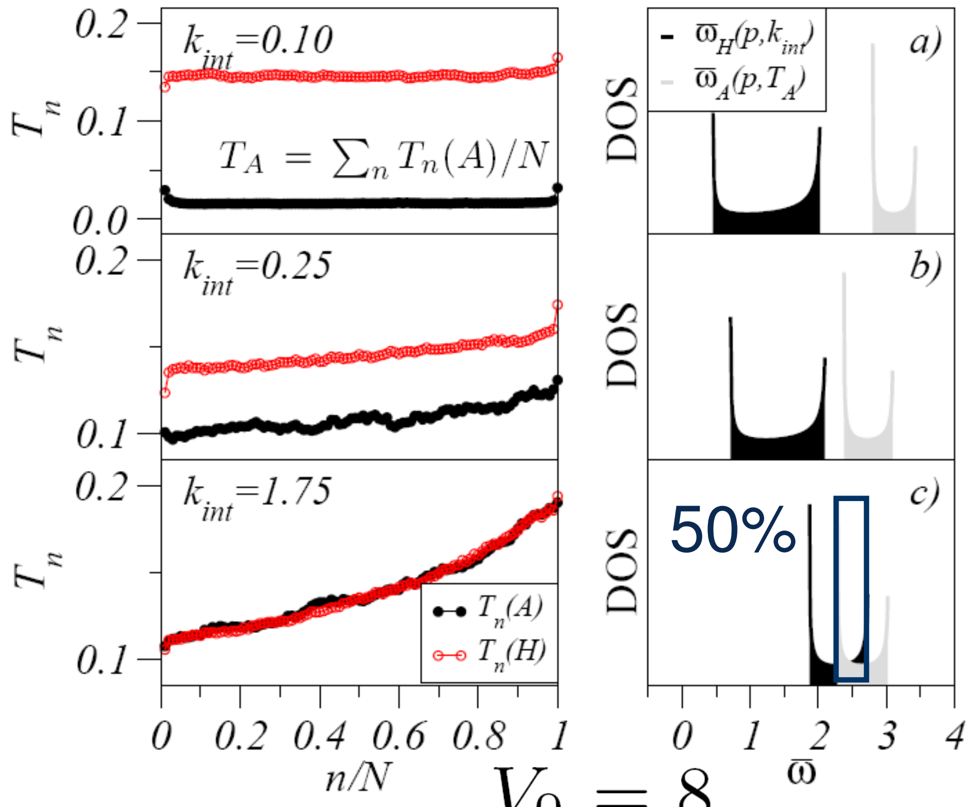
$$\bar{\omega}_A^2(p,T) = U(T) + 2(1 - cos(p))$$




Let´s look at the spectra

* Auxiliary system:
fully harmonic ladder-model

$$\bar{\omega}_H^2(p,k_{int}) = 2k_{int} + 2(1 - cos(p))$$




$V_0 = 8$

# Thermal Rectification

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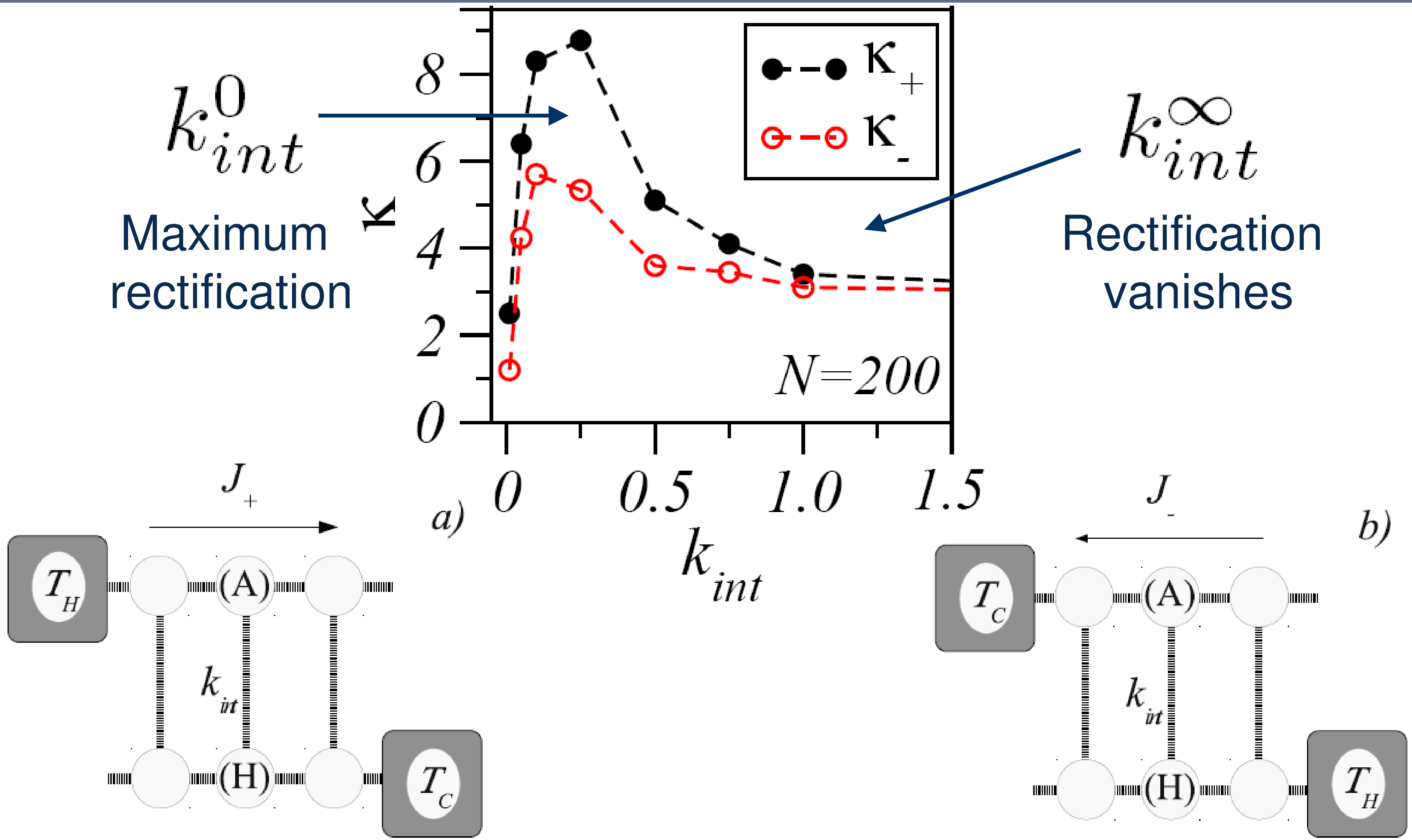
$k_{int}^{0}$

Maximum rectification

$k_{int}^{\infty}$

Rectification vanishes



# Thermal Rectification

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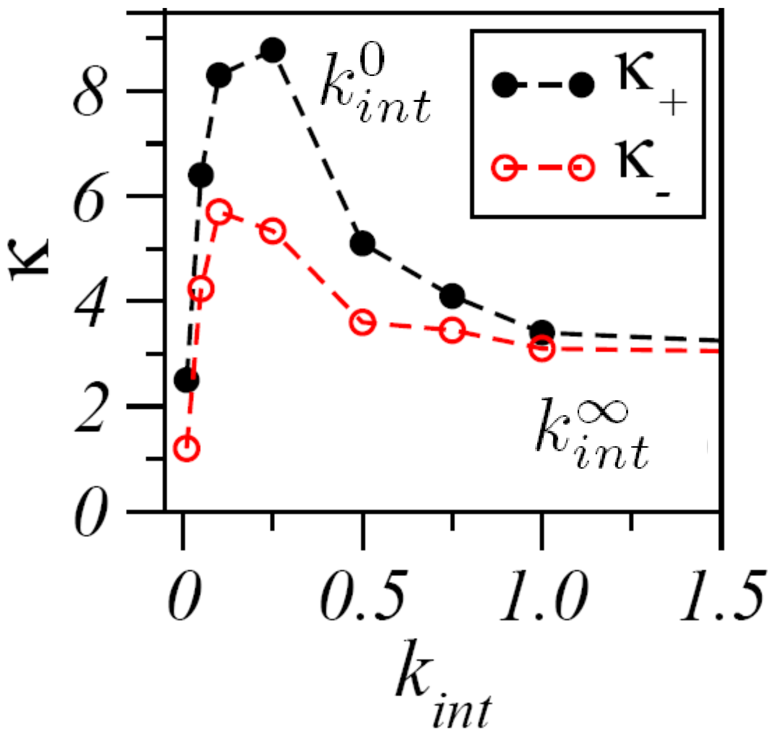
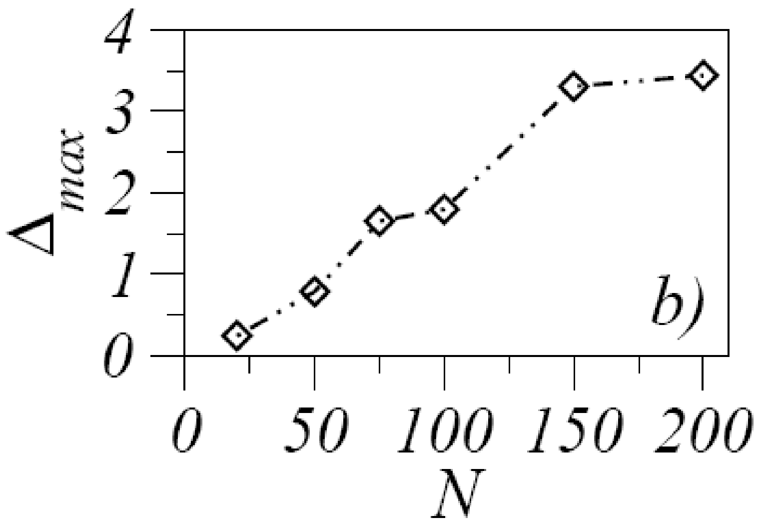
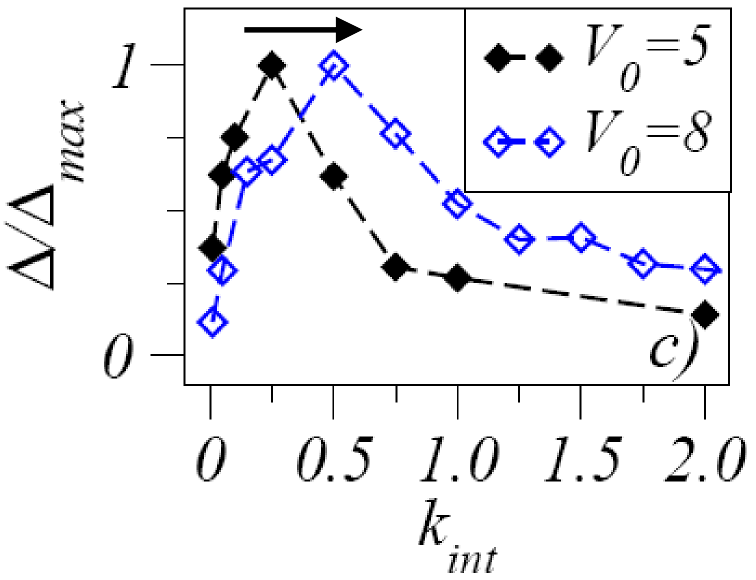
$$\Delta = \kappa_+ - \kappa_-$$




Maximum rectification rates

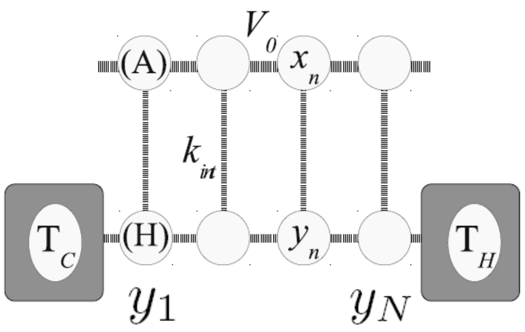
$$k_{int} < k_{int}^*$$

# CONCLUSIONS

* A harmonic lattice supports **normal heat transport** when strongly interacts to an anharmonic one.

SCPT + Harmonic ladder-model

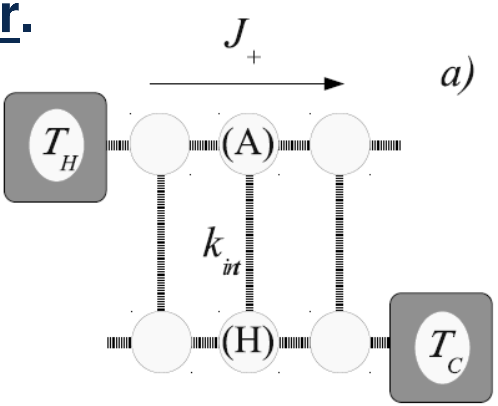
$$k_{int}^{*} = \frac{U(T_M) - 2}{2}$$




* The ladder-system has revealed as a **thermal rectifier.**

The maximum rectification rates:

- increase with the system size
- shift to higher couplings for larger $V_0$




(Submitted to cond-mat-0211630)