Quantum Thermal Conductivity and Brownian Motion in a Harmonic Chain

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Abstract

We want to understand the mechanism of heat conduction microscopically. A chain of harmonic oscillators is the simplest imaginable model. Classical investigations have shown that harmonic chains exhibit anomalous heat conduction: The temperature gradient vanishes and heat flux is independent of the length of the chain (S. Lepri, R. Livi and A. Politi, Phys. Rep. **377**: 1-80, 2003).

Now we are interested in the quantum mechanical regime. Carbon nanotubes are a possible field of application as they show astonishingly high thermal conductivity (Z. Yao, J. Wang, B. Li and G. Liu, Phys. Rev. B **71**: 085417, 2005)

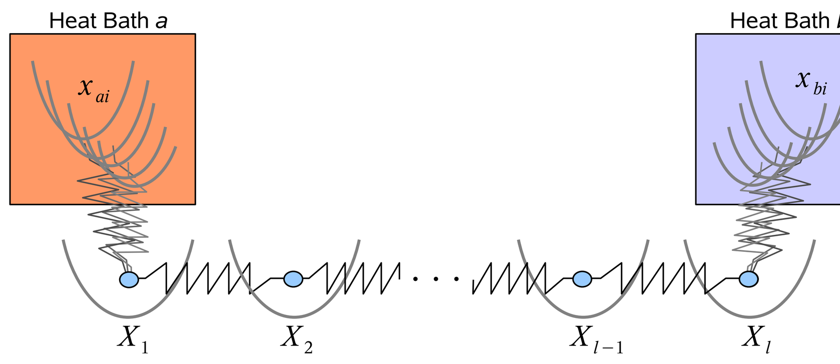
Our ansatz is the Quantum Mechanical Langevin–Equation (Th. M. Nieuwenhuizen and A. E. Allahverdyan, Phys. Rev. E **66**: 036102, 2002)

Ordered Chains – Theory

The Model

We use a chain consisting of l coupled harmonic oscillators with unity mass and frequency ω_0

$$H_c = \sum_{n=1}^{l} \left(\frac{1}{2}P_n^2 + \frac{1}{2}\omega_0^2 X_n^2\right) + \sum_{n=1}^{l-1} \frac{f}{2}(X_{n+1} - X_n)^2$$



Two identical heat baths at different temperatures T_a and T_b are coupled to the first and to the last oscillator of the chain:

$$H_{B\alpha} = \sum_{i=1}^{N} \left[\frac{p_{\alpha i}^2}{2} + \frac{1}{2}\omega_i^2 \left(x_{\alpha i} - \frac{c_i}{\omega_i^2} X_\beta\right)^2\right]$$

Equations of Motion

The Heisenberg equations of motion read

$$\ddot{X}_n(t) = -\left(\omega_0^2 + 2f\right) X_n(t) + f\,(X_{n-1} + X_{n+1})$$

The first and the last oscillator are affected by the baths:

$$\ddot{X}_1(t) = -\left(\omega_0^2 + f + \sum_{i=1}^{N} \frac{c_i^2}{\omega_i^2}\right) X_1(t) + \sum_{i=1}^{N} c_i x_{1i}(t) + f X_2(t)$$

The equation for X_l is analog.

Eliminating the baths' degrees of freedom leads to **coupled Langevin equations** with quantum mechanical damping $\gamma(t)$ and noise $\eta_k(t)$

$$\ddot{X}_1(t) = -\left(\omega_0^2 + f\right) X_1(t) + f X_2(t) - \gamma(t) X_1(0) - \int_0^t dt' \gamma(t - t') \dot{X}_1(t') + \eta_a(t)$$

$$\ddot{X}_2(t) = -(\omega_0^2 + 2f) X_2 + f X_1 + f X_3, \ \ldots \qquad \text{(Langevin equations)}$$

These can be solved by:

- Transforming to the normal coordinates Y_i (standing waves) of the pure chain to get rid of the coupling f
- Transforming to Laplace space:
  - The convolution transforms to a product $s\hat{\gamma}(s)\hat{X}_1(s)$.
  - The differential equation becomes an algebraic equation.

The Solution of the Langevin Equations

The solution of the Langevin–equations reads

$$Y_j(t) = \sum_{k=1}^{l} \left[\dot{A}_{jk}(t) Y_k(0) + A_{jk}(t) Q_k(0)\right] + \int_0^t dt' \left[F_j^a(t - t')\eta_a(t') + F_j^b(t - t')\eta_b(t')\right]$$

With the response functions $F_j(t)$ for the noise and the response functions $A_{jk}(t)$ for the initial conditions of the chain.

In the limit of infinite baths with Drude–Ullersma–coupling–constants

- The response functions $R(t) \in \{F_j(t), A_{jk}(t)\}$ read

  $$R(t) = \sum_k r_k e^{\lambda_k t} + c.c.$$

  and decay exponentially with time.
- In the stationary case only the noise integrals are relevant.

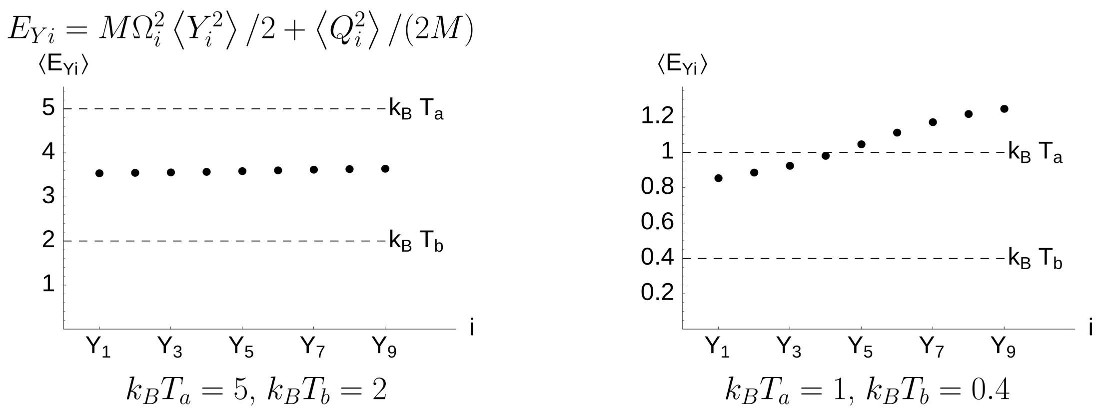
Due to symmetry arguments there is no mixing between even and odd normal coordinates.

Now we can calculate any correlation between the normal coordinates Y_i and their momenta Q_i

Ordered Chains – Results

Energy in Normal Modes

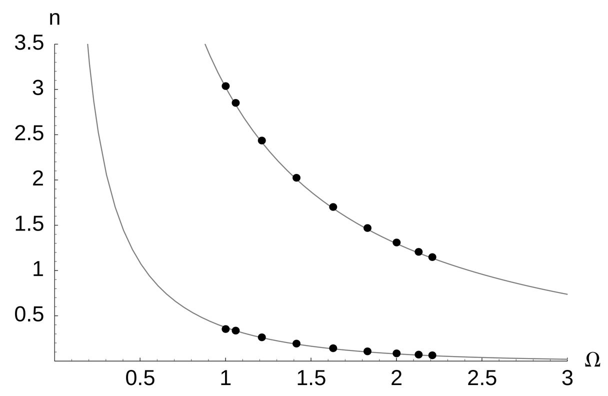
$E_{Yi} = M\Omega_i^2 \left\langle Y_i^2 \right\rangle/2 + \left\langle Q_i^2 \right\rangle/(2M)$



$k_B T_a = 5$, $k_B T_b = 2$ | $k_B T_a = 1$, $k_B T_b = 0.4$

- Equipartition at high temperatures: $\langle E_{Yi} \rangle \approx k_B \frac{1}{2}(T_a + T_b)$
- Zero point energy dominate at low temperatures: $\Rightarrow \langle E_{Yi} \rangle \approx \hbar\Omega_i/2$

Occupation Numbers $n_i = E_{Yi}/(\hbar\Omega_i) - 1/2$



The occupation numbers for the normal modes.

Upper curve: $k_B T_a = 5$, $k_B T_b = 2$.

Lower curve: $k_B T_a = 1$, $k_B T_b = 0.4$

The occupation numbers fit on a Bose–Einstein–distribution $n_i = \left[\exp\left(\frac{\hbar\Omega_i}{k_B T}\right) - 1\right]^{-1}$

I.e. normal modes have got a common temperature.

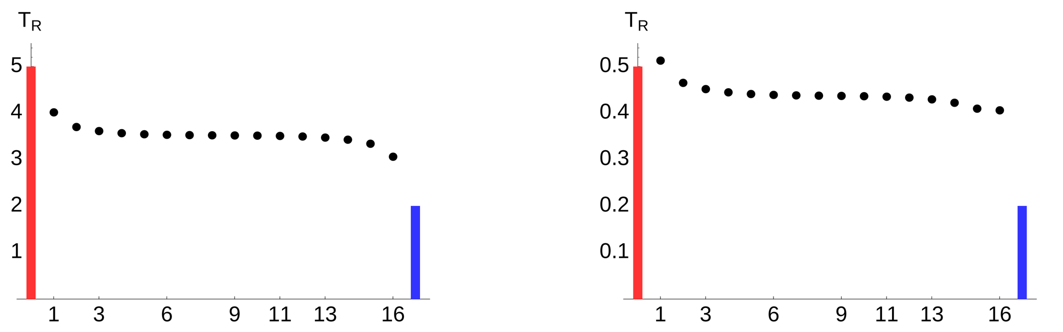
Temperature Profiles

We calculate the energy per lattice site i

$$\langle E_i \rangle = \frac{1}{2}(\omega_0^2 + 2f)\left\langle X_i^2 \right\rangle - \frac{1}{2}f\left(\langle X_i X_{i+1} \rangle + \langle X_i X_{i-1} \rangle\right) + \frac{1}{2}\left\langle P_i^2 \right\rangle$$

Then we reconstruct the temperature using

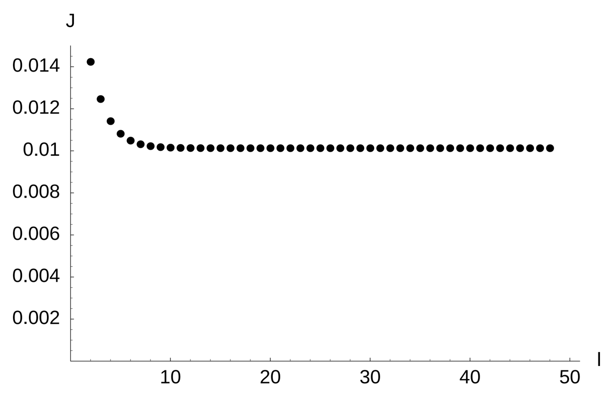
$$\langle E \rangle = \frac{1}{2}\hbar\omega \coth\left(\frac{\hbar\omega}{2k_B T}\right)$$



$T_a = 5$, $T_b = 2$ | $T_a = 0.5$, $T_b = 0.2$

The temperature gradient vanishes both in the classical and in the quantum mechanical regime. $\Rightarrow$ anomalous heat conduction

Heat Current and the Chain Length

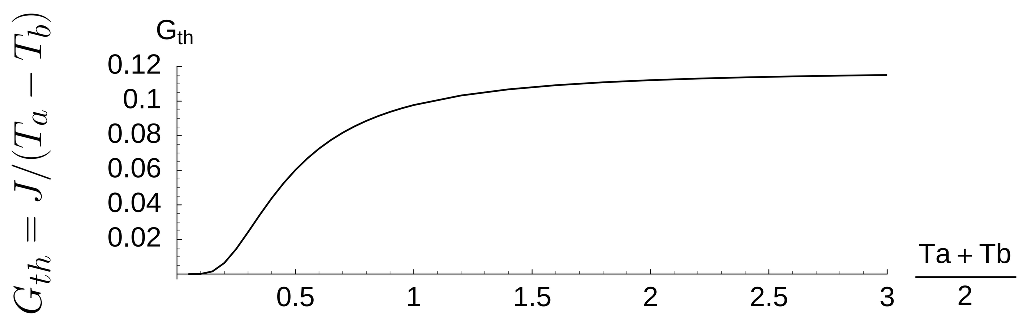


Stationary energy current for different chain lengths l

Parameter: $\gamma = 0.35$, $f = 1$, $k_B T_a = 0.5$, $k_B T_b = 0.2$

- The energy current is independent of the length of the chain. $\Rightarrow$ anomalous heat conduction

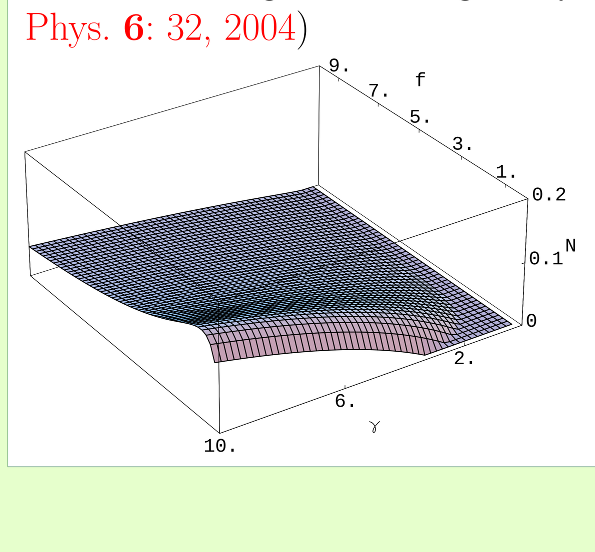
Thermal Conductivity as a Function of Temperature



- In the classical regime $k_b T \gg \hbar\Omega_i$ the thermal conductivity is constant.
- In the low temperature regime the thermal conductivity behaves like the occupation number $\propto e^{-\frac{k_B T}{\hbar\Omega}}$

Entanglement

From the correlations between the coordinates and momenta we can calculate the logarithmic negativity (Plenio, Hartley and Eisert, New J. Phys. **6**: 32, 2004)



Example: The Logarithmic Negativity between the Center–of–Mass–Motion and the other Normal Modes as a function of γ and f. Parameter: $l = 3$, $T_a = 0.5$, $T_b = 0.2$

Disordered Chains

Motivation for Disorder

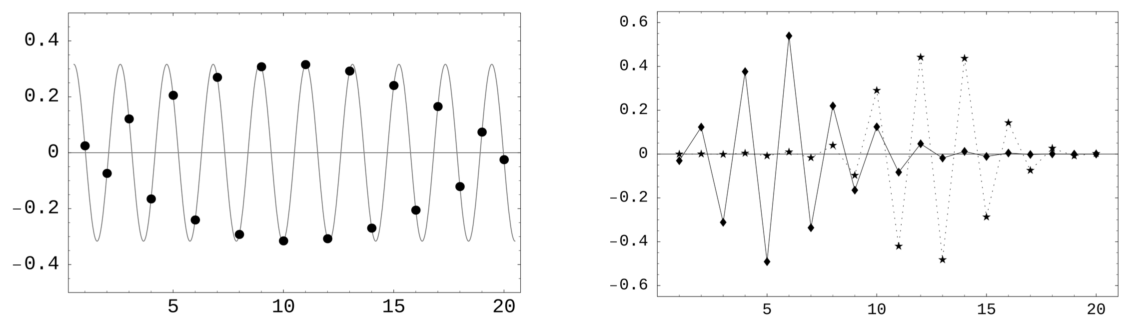
From classical considerations it is known that harmonic chains show diverging heat conductivity, because anharmonicities are necessary for diffusion due to Umklapp–Processes. An alternative which conserves the linearity of the system is the introduction of disorder.

Modifications to the ordered chain

- We choose either the onsite potentials randomly: $\omega_0 \to \omega_i$ or the coupling constants: $f \to f_i$
- The inversion symmetry of the system breaks down.

Localization of the Normal Modes

Disorder changes the character of the normal modes:



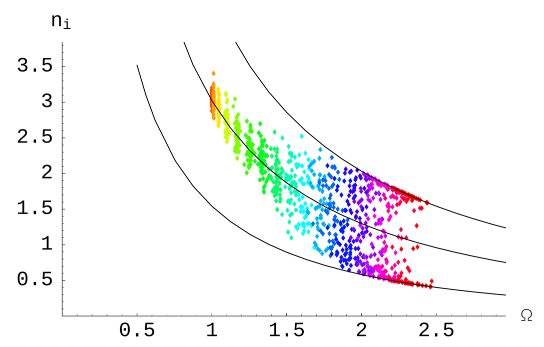
(a) Ordered chain | (b) Disorder: $f_i = 1 \pm 0.2$

The highest normal modes (Disorder: Two typical realizations)

- Normal modes have lower amplitudes at the ends of the chain
- Normal modes have different amplitudes at left and right end of the chain

  $\Rightarrow$ Strong coupling to one bath, weak coupling to the other bath

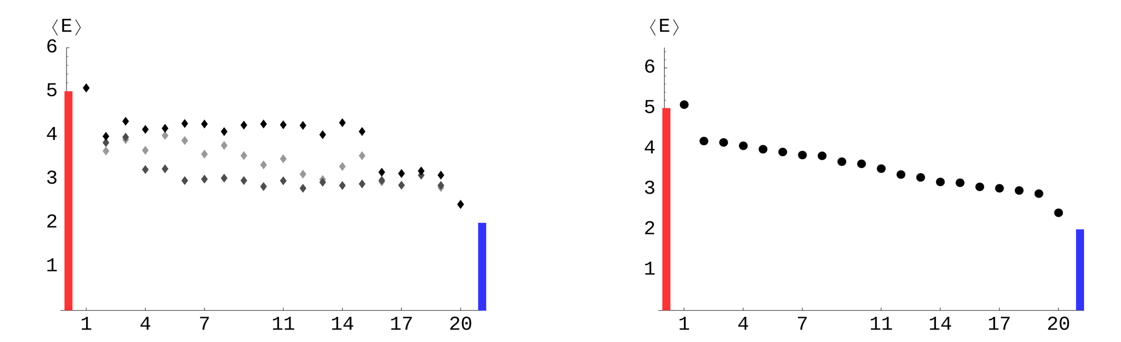
Occupation Numbers



Occupation numbers of a disordered chain, 50 realizations. $l = 20$, $\gamma = 2$, $k_B T_a = 5$, $k_B T_b = 2$

- Modes with high frequency are strongly localized
- Localized modes are coupled more strongly to one bath than to the other.
- Low frequency modes are coupled more or less equally to both baths.

Temperature Profiles

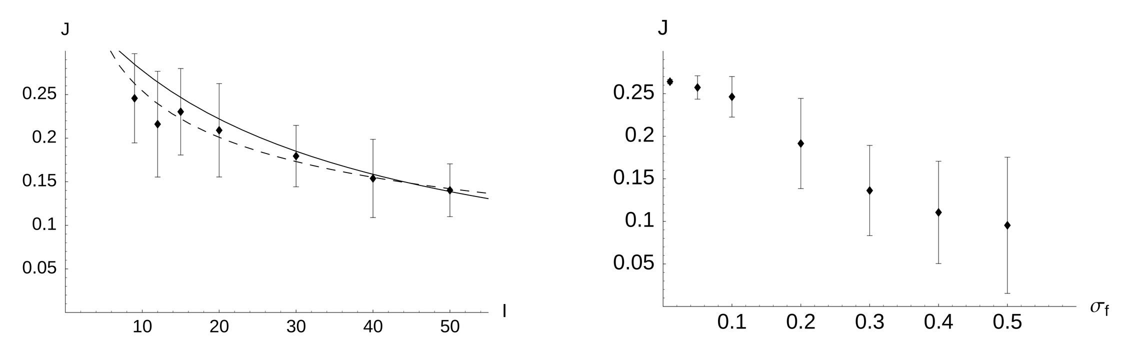


(a) Some single realizations | (b) Average over 50 realizations

Parameters: $f_i = 1 \pm 0.2$, $k_B T_a = 5$, $k_B T_b = 2$

The temperature gradient increases.

The Heat Current



as a function of the chain length l ($f_i = 1 \pm 0.2$) | as a function of the standarddeviation of σ_f ($l = 12$)

The heat current reduces with the strength of disorder and with the length of the chain. $\Rightarrow$ finite heat conductivity.

Unfortunately the asymptotic behavior cannot be figured out with the achieved chain lengths.

Conclusions

- Like in classical systems the heat conduction is anomalous in the ordered quantum mechanical case.
- We see several new features in the quantum mechanical regime:
  - The heat conductivity breaks down in the low temperature regime.
  - One can observe entanglement inside the chain.
  - Energies are dominated by zero point energies
- In the disordered case we find finite heat conduction like in the classical case. Investigations with longer chains are to be done to determine the asymptotic behavior.