Thermal transport in one-dimensional systems: Some numerical results

Gabriel STOLTZ

CERMICS & MICMAC project team, Ecole des Ponts ParisTech

`http://cermics.enpc.fr/~stoltz/`

Outline of the talk

Anomalous transport properties of one-dimensional systems, studied in two cases:

- Thermal transport in the Toda chain (anharmonic potential but integrable system) with a noise preserving energy and momentum

  (joint work with A. Iacobucci (CEREMADE), F. Legoll (Ecole des Ponts) and S. Olla)

- Quantum thermal transport in harmonic carbon nanotubes with mass disorder

  (joint work with F. Mauri, M. Lazzeri (IMPMC, Paris 6&7) and N. Mingo (CEA Grenoble))

Thermal transport in the Toda chain with a noise preserving energy and momentum

Description of the system

- Configuration $\{q_i, p_i, i = 1, \ldots, n\} \in \mathbb{R}^{2n}$ (q_i displacement with respect to equilibrium, p_i momentum)
- Equal masses, first particle fixed ($q_0 = 0$)
- Hamiltonian $\mathcal{H} = \displaystyle\sum_{i=1}^{n} \frac{p_i^2}{2} + \sum_{i=1}^{n} V(q_i - q_{i-1})$ with $V(r) = \dfrac{\mathrm{e}^{-br} + br - 1}{b^2}$
- The corresponding Hamiltonian system is completely integrable
- Hamiltonian dynamics + Langevin at the boundaries:

$$\begin{cases} dq_i = p_i \, dt, \\ dp_i = \Big(v'(q_{i+1} - q_i) - v'(q_i - q_{i-1}) \Big) dt \\ \qquad + \delta_{i,1} \Big(- \xi p_1 \, dt + \sqrt{2\xi T_{\mathrm{L}}} \, dW_{1,t} \Big) + \delta_{i,N} \Big(- \xi p_N \, dt + \sqrt{2\xi T_{\mathrm{R}}} \, dW_{N,t} \Big) \end{cases}$$

and the convention $v'(q_{N+1} - q_N) = 0$

Energy and momentum preserving noise

- Additional jump process: random exchanges of momenta between nearest neighbor atoms (at random exponential times, mean time γ^{-1})[a]
- Destruction of all invariants except energy and momentum
- Local energies $\mathcal{E}_i = \frac{p_i^2}{2} + \frac{1}{2}\Big(V(q_i - q_{i-1}) + V(q_{i+1} - q_i)\Big)$ and total momentum $\sum_{j=1}^N p_j$ preserved
- Energy variations $d\mathcal{E}_i(t) = dJ_{i-1,i}(t) - dJ_{i,i+1}(t)$
- Decomposition of the currents as

$$J_{i,i+1}(t) = \int_0^t \left(j_{i,i+1}^{\rm ham} + \gamma\, j_{i,i+1}^{\rm sto}\right) ds + M_{i,i+1}^{\gamma}(t)\,,$$

where $M_{i,i+1}^{\gamma}(t)$ is a martingale, and

$$j_{i,i+1}^{\rm ham} = -\frac{1}{2}(p_i + p_{i+1})V'(q_{i+1} - q_i), \qquad j_{i,i+1}^{\rm sto} = \frac{1}{2}\left(p_i^2 - p_{i+1}^2\right)$$

[a] Basile/Bernardin/Olla 2006 & 2009

- Question: scaling of the thermal conductivity with the system size n

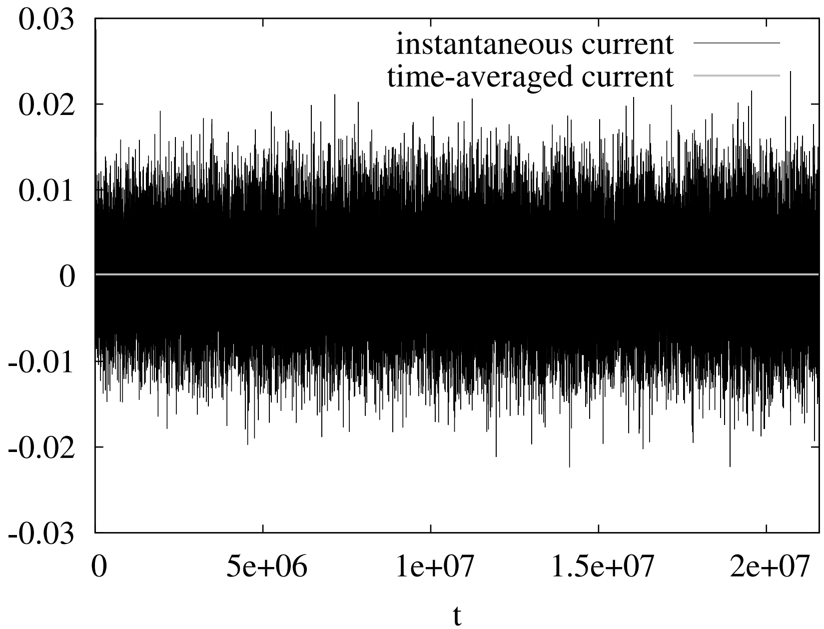
$$\kappa_n^{\mathrm{ham}}(T,\tau) = \lim_{\substack{T_{\mathrm{L}}-T_{\mathrm{R}}\to 0 \\ T_{\mathrm{R}}\to T}} \frac{n\langle J_n^{\mathrm{ham}}\rangle_{\mathrm{ss}}}{T_{\mathrm{L}}-T_{\mathrm{R}}}, \qquad nJ_n^{\mathrm{ham}} = \sum_{i=0}^{n-1} j_{i,i+1}^{\mathrm{ham}}$$

- In general, $\kappa_n \sim n^\alpha$ with $0 < \alpha < 1$ when no on-site potential and no stochastic destruction of the momentum conservation
- For the Toda chain with no noise[a] ($\gamma = 0$): $\kappa_n \sim n$
- For the noise considered here: theoretical bound $0 \le \kappa_n \le C\sqrt{n}$
- Numerical simulations with $T_{\mathrm{L}} = 1.05$ and $T_{\mathrm{R}} = 0.95$
- Numerical scheme: splitting between Hamiltonian part (Verlet scheme), thermalization at the boundaries, and random exchanges of momenta
- Time step $\Delta t = 0.025 - 0.05$ (important parameter: when it is too large, energy accumulation in the middle of the chain)

[a] Zotos 2002

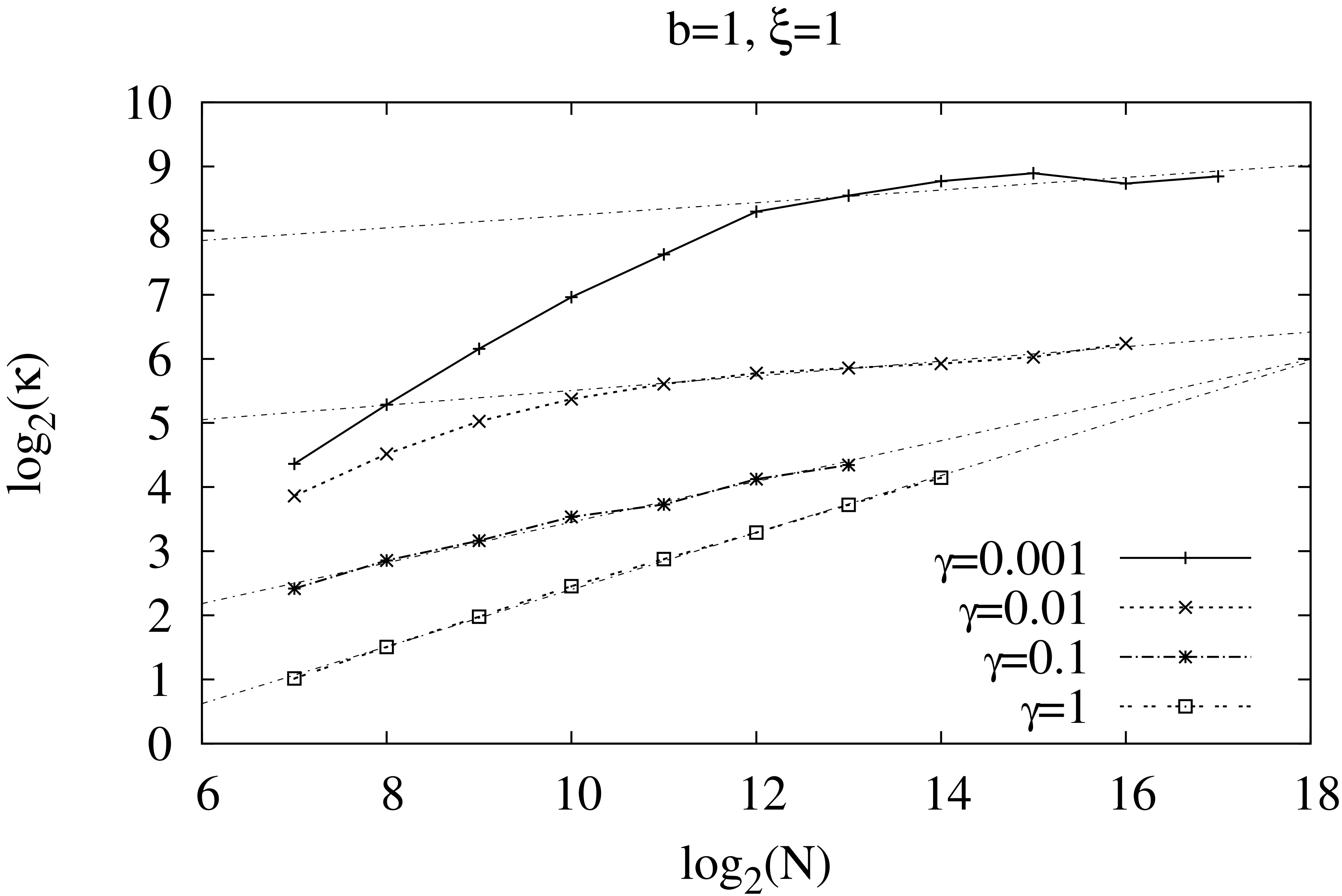
Large statistical errors...

- Test case $n = 16,384$, $b = 1$, $\gamma = 1$, $\xi = 1$
- Instantaneous current: standard deviation $\sigma \sim 0.02$, average $\mu \sim 10^{-4}$, correlation time $\tau_{\rm corr} \sim 10^3$.
- 1% relative accuracy when $\dfrac{\sigma}{\sqrt{t_{\rm req}/\tau_{\rm corr}}} = 0.01\,\mu$, *i.e.* $t_{\rm req} \sim 4 \times 10^{11}$...
- Simulations results not completely reliable since $t_{\rm simu} = 10^6 - 10^8$

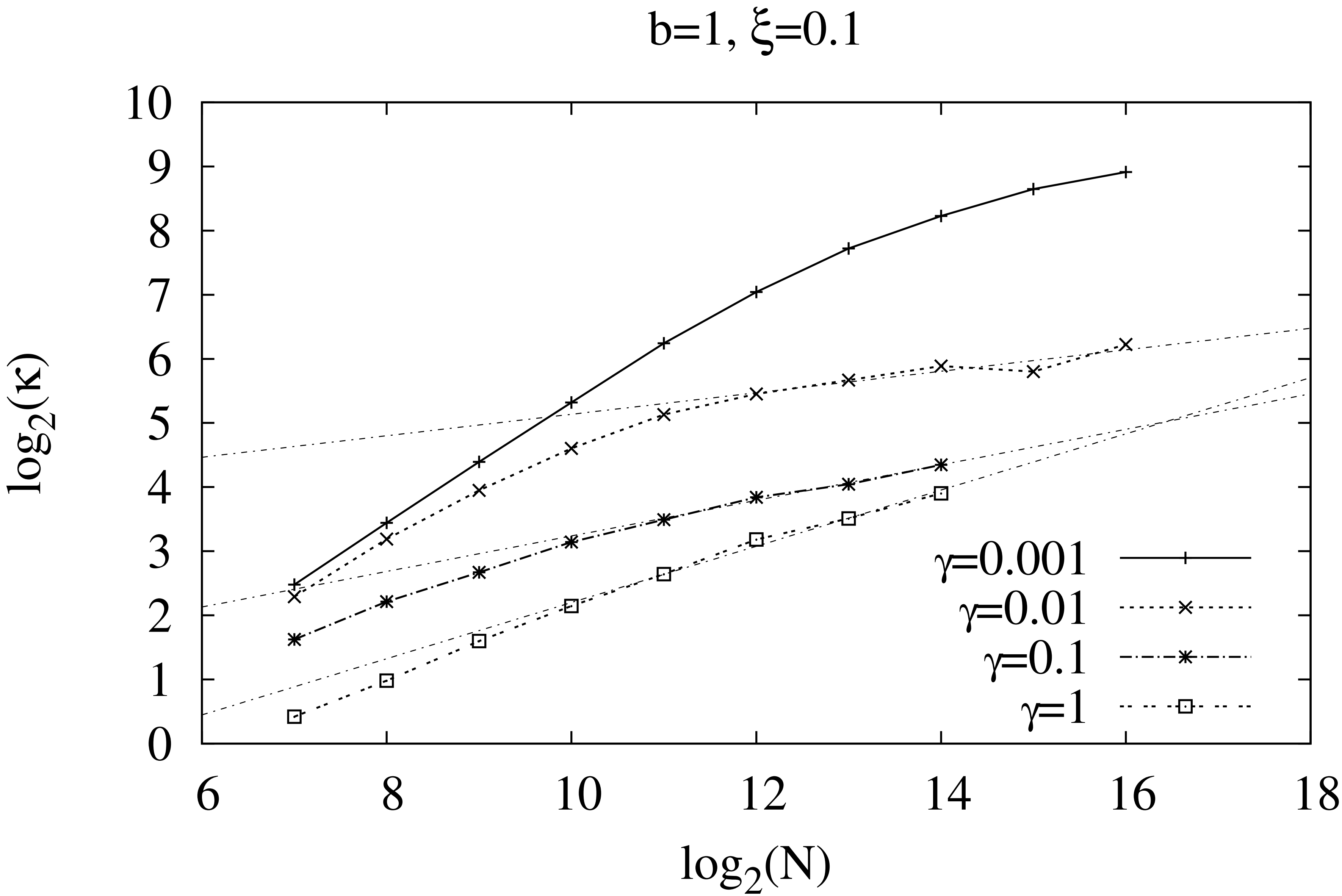


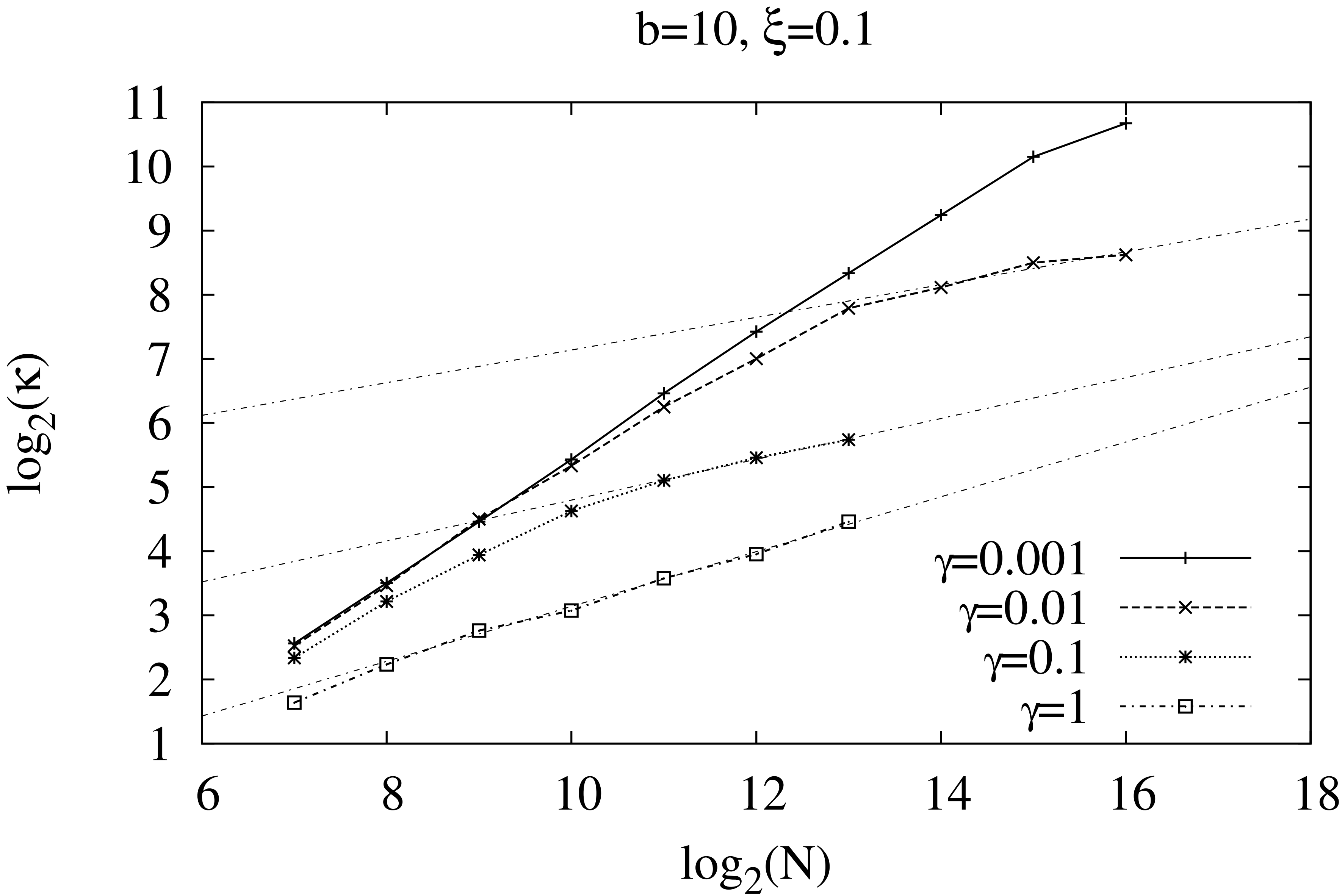
- This should motivate some work on variance reduction techniques...

Case $b = 1$, $\xi = 1$



b=1, ξ=1
log2(κ)
log2(N)
γ=0.001
γ=0.01
γ=0.1
γ=1
0
1
2
3
4
5
6
7
8
9
10
6
8
10
12
14
16
18


b=1, ξ=0.1
log2(κ)
log2(N)
γ=0.001
γ=0.01
γ=0.1
γ=1
10
9
8
7
6
5
4
3
2
1
0
6
8
10
12
14
16
18


b=10, ξ=0.1
log2(κ)
log2(N)
11
10
9
8
7
6
5
4
3
2
1
6
8
10
12
14
16
18
γ=0.001
γ=0.01
γ=0.1
γ=1

Discussion of the results

γ	α $(b=1,\ \xi=1)$	α $(b=1,\ \xi=0.1)$	α $(b=10,\ \xi=0.1)$
0.001	0.10	–	–
0.01	0.11	0.17	0.25
0.1	0.32	0.30	0.32
1	0.44	0.44	0.43

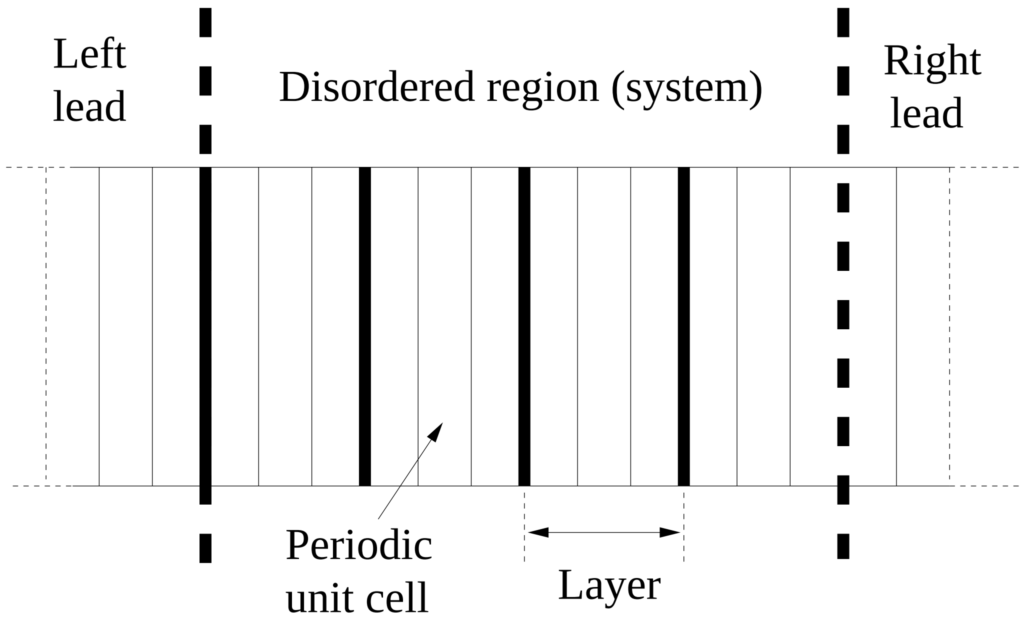
Conclusions:[a]

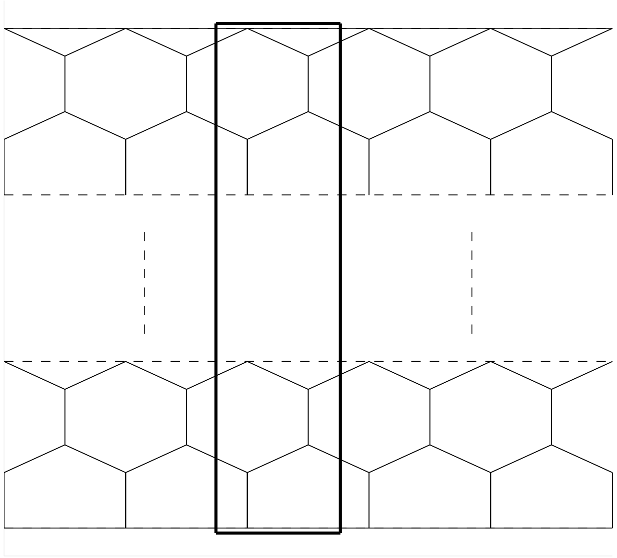
- Destruction of the ballistic transport (although the asymptotic regimes are difficult to obtain when $\gamma \to 0$)
- No universality of α (depends on γ)
- The value of α seems to depend on the noise strength γ in a monotonically increasing way. Counter-intuitive! (suppression of some scattering effects of the nonlinearities)

[a] Iacobucci/Legoll/Olla/Stoltz 2010

Quantum thermal transport in harmonic carbon nanotubes with mass disorder

Description of the system





- N degrees of freedom in the geometric unit cell, infinite system
- Displacements $q = (\dots, q_{i,1}, \dots, q_{i,N}, q_{i+1,1}, \dots)^t$ and momenta $p = (\dots, p_{i,1}, \dots, p_{i,N}, p_{i+1,1}, \dots)^t$
- Harmonic system $H(q,p) = \frac{1}{2} q^t K q + \frac{1}{2} p^t M^{-1} p$
- K estimated from quantum mechanical computations
- Harmonic matrix $A = M^{-1/2} K M^{-1/2}$ where M diagonal mass matrix

Conduction channels for the perfect system

- For perfect systems, the harmonic matrix reads ($a_j = a_j^T \in \mathbb{R}^{N\times N}$)

$$\begin{pmatrix} & & & & \ddots & & & & & & & & \\ \dots & 0 & a_{-K} & \dots & a_{-1} & a_0 & a_1 & \dots & a_K & 0 & \dots & & \\ & \dots & 0 & a_{-K} & \dots & a_{-1} & a_0 & a_1 & \dots & a_K & 0 & \dots & \\ & & \dots & 0 & a_{-K} & \dots & a_{-1} & a_0 & a_1 & \dots & a_K & 0 & \dots \\ & & & & & & & & \ddots & & & & \end{pmatrix}$$

- Dynamical matrix $D(k) = \sum_{j=-K}^{K} a_j \mathrm{e}^{\mathrm{i}jk}$ for $k \in [0, \pi]$ (phonons)
- (Generalized) Eigenvalues $\omega_n(k)^2$ ($1 \leq n \leq N$)
- The number of conduction channels at a given pulsation ω is defined as

$$T(\omega) = \mathrm{Card}\left\{(k,n) \in [0,\pi] \times \{1,\dots,N\} \,\middle|\, \omega_n(k)^2 = \omega^2\right\}.$$

Computation of the thermal current (exact)

- Decomposition $A = \begin{pmatrix} A_L & \mathfrak{T}_L & 0 \\ \mathfrak{T}_L^t & A_{\text{sys}} & \mathfrak{T}_R \\ 0 & \mathfrak{T}_R^t & A_R \end{pmatrix}$ since $M = \begin{pmatrix} M & 0 & 0 \\ 0 & M_{\text{sys}} & 0 \\ 0 & 0 & M \end{pmatrix}$
- Effective Green function

$$G_{\text{sys}}^{+}(\omega) = \lim_{\eta \to 0} \left(\omega^2 + \mathrm{i}\eta - A_{\text{sys}} - \Sigma_L^{+}(\omega) - \Sigma_R^{+}(\omega)\right)^{-1}$$

where the self-energies are $\Sigma_\alpha^{+}(\omega) = \lim_{\eta \to 0} \mathfrak{T}_\alpha^t (\omega^2 + \mathrm{i}\eta - A_\alpha)^{-1} \mathfrak{T}_\alpha$

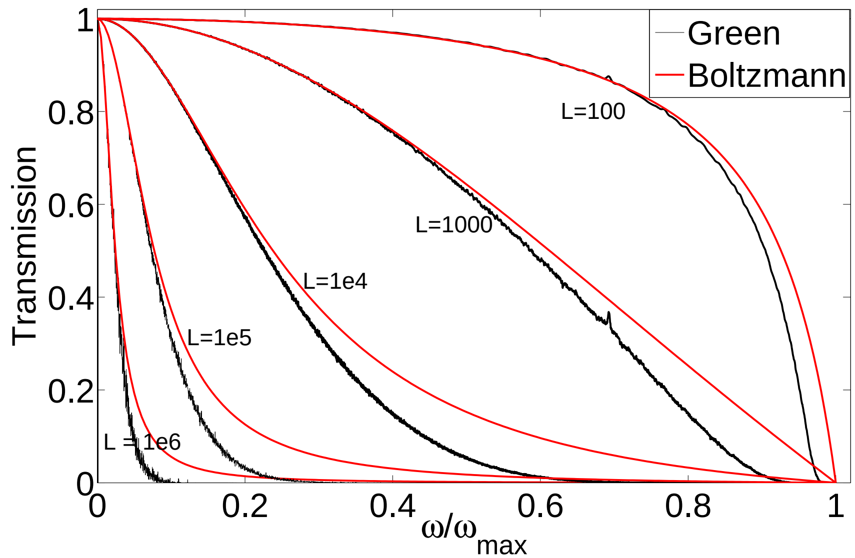
- Transmission function ($\Gamma_\alpha^{+}(\omega) = -2\,\text{Im}\,(\Sigma_\alpha^{+}(\omega))$)

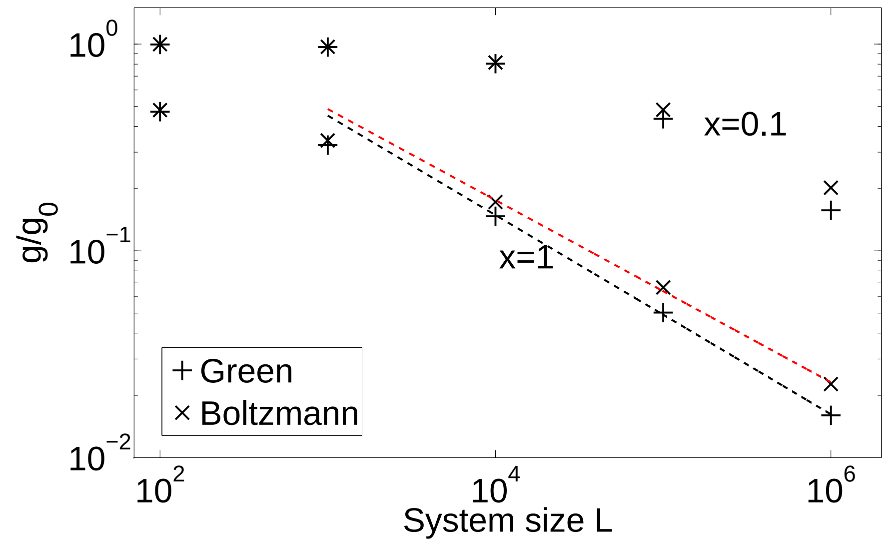
$$0 \leq \mathcal{T}(\omega) = \mathrm{Tr}\left[\Gamma_L^{+}(\omega) G_{\text{sys}}^{+}(\omega) \Gamma_R^{+}(\omega) \left(G_{\text{sys}}^{+}(\omega)\right)^{\dagger}\right] \leq T(\omega)$$

- Landauer-Büttiker formula (f_T Bose-Einstein distributions)

$$J(T_L, T_R) = \int_0^{+\infty} \frac{\hbar\omega}{2\pi} \mathcal{T}(\omega)(f_{T_L}(\omega) - f_{T_R}(\omega))\, d\omega$$

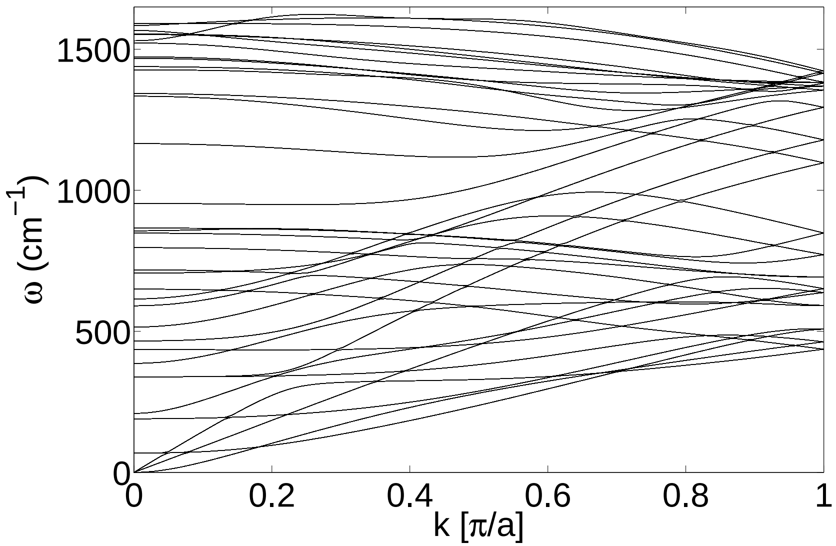
Results for the one-dimensional chain

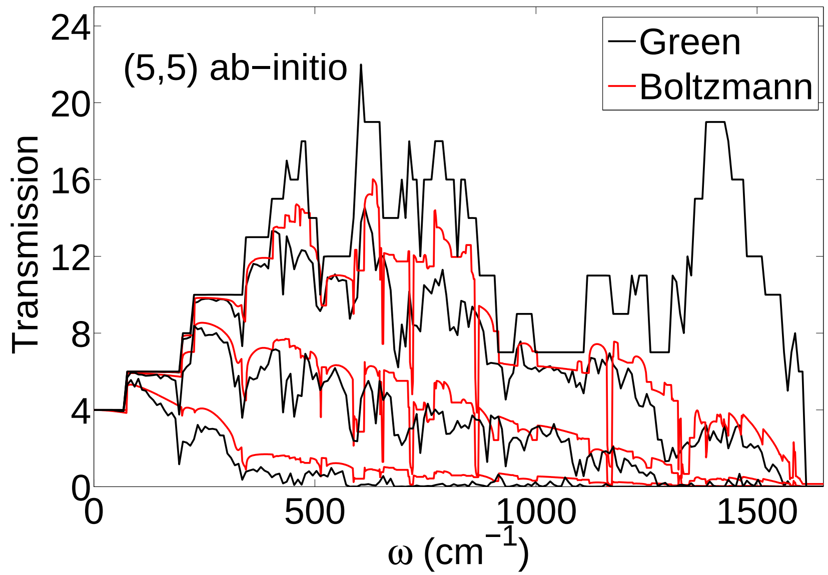




- Hamiltonian $H = \sum_j \frac{p_j^2}{2} + \frac{1}{2}k(q_{j+1} - q_j)^2$ and $T(\omega) = \mathbf{1}_{[0,\omega_{\max}]}(\omega)$
- Isotopic disorder: replacing with probability $0 < c < 1$ the mass of a particle by $1 + \delta$
- It can be shown[a] that $\mathcal{T}_L(\omega) \simeq \exp\left(-\frac{\mathrm{Var}(m)}{\langle m \rangle^2} L\omega^2\right)$, which motivates the scaling of the thermal current $J \sim L^{-1/2}$

[a] Matsuda/Ishi'70, Rubin/Greer'70, O'Connor/Lebowitz'74, Dhar'01

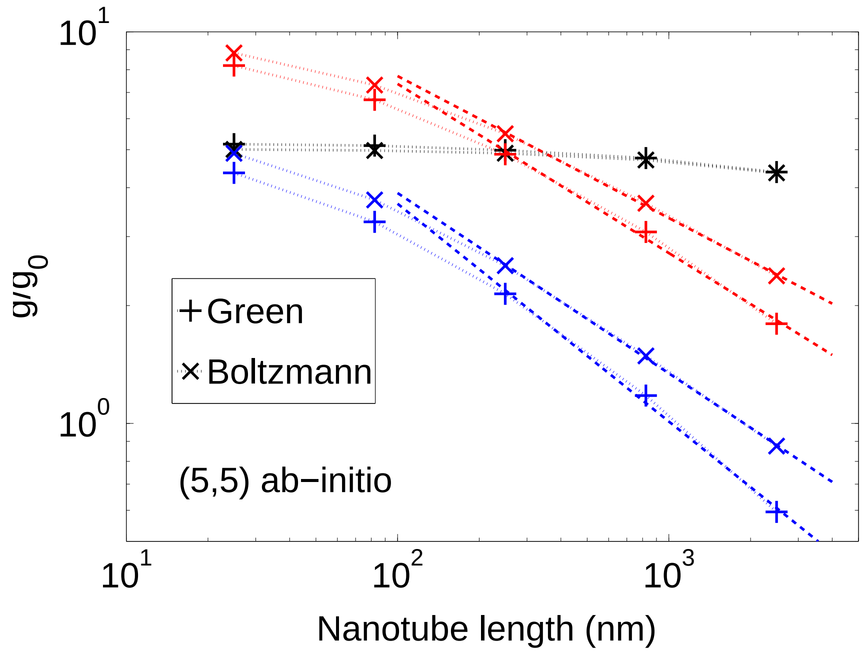


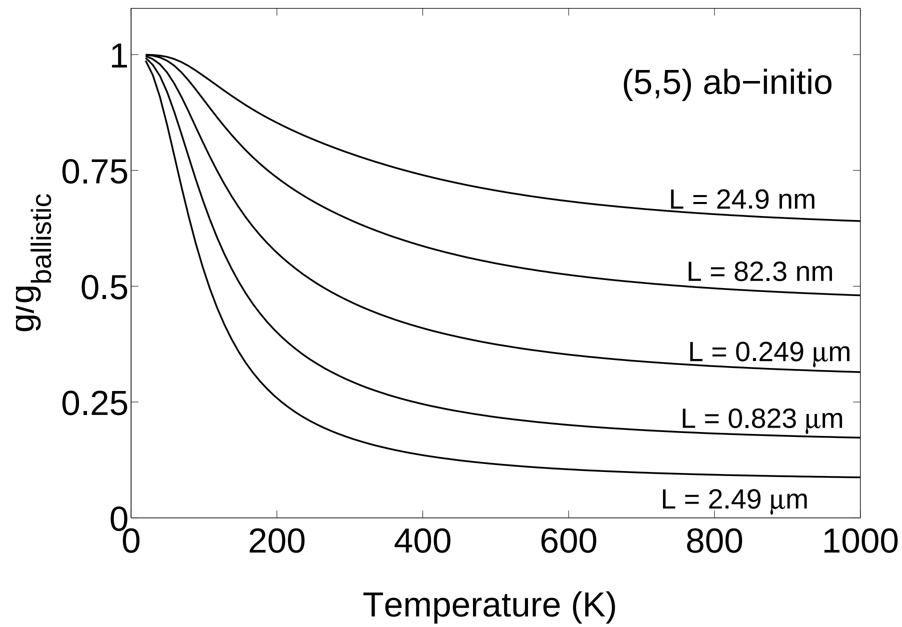


- (5,5) armchair nanotube (metallic properties), isotopic disorder does not change the electronic properties
- Four acoustic modes since the flexural mode (starting with a k^2 dispersion law) is doubly degenerate
- Isotopic disorder: replacing ^{12}C by ^{13}C at random (50% proportion), for tubes of lengths $L = 25$ nm, $L = 249$ nm and $L = 2.49$ μm
- Phonon engineering possible[a]

[a] Stoltz/Lazzeri/Mauri 2009, Stoltz/Mingo/Mauri 2009

Reduction in thermal conductance





- Left: Variation of the normalized conductance for temperatures $T = 50$ K (black curves), $T = 300$ K (red curves), $T = 1000$ K (blue curves). Estimated scalings of the thermal current: $J \sim L^{-\alpha}$ with $\alpha = 0.43$ at $T = 300$ K and $\alpha = 0.55$ at $T = 1000$ K.
- Right: reduction compared to ballistic current