Quantum phonon transport in nanostructures thermalized by local Langevin heat baths

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Motivation

- **Nanostructuring** can be used to create materials with tailor-made thermal properties
- **Phonon transport** is typically not fully ballistic due to, e.g., phonon-phonon interactions
- Processes creating and annihilating phonons can be mimicked by **stochastic heat baths** [1]
- Self-consistent heat bath model is applicable both in the **ballistic and diffusive regimes** of phonon transport and is suitable for systems containing **thousands of atoms** [2]

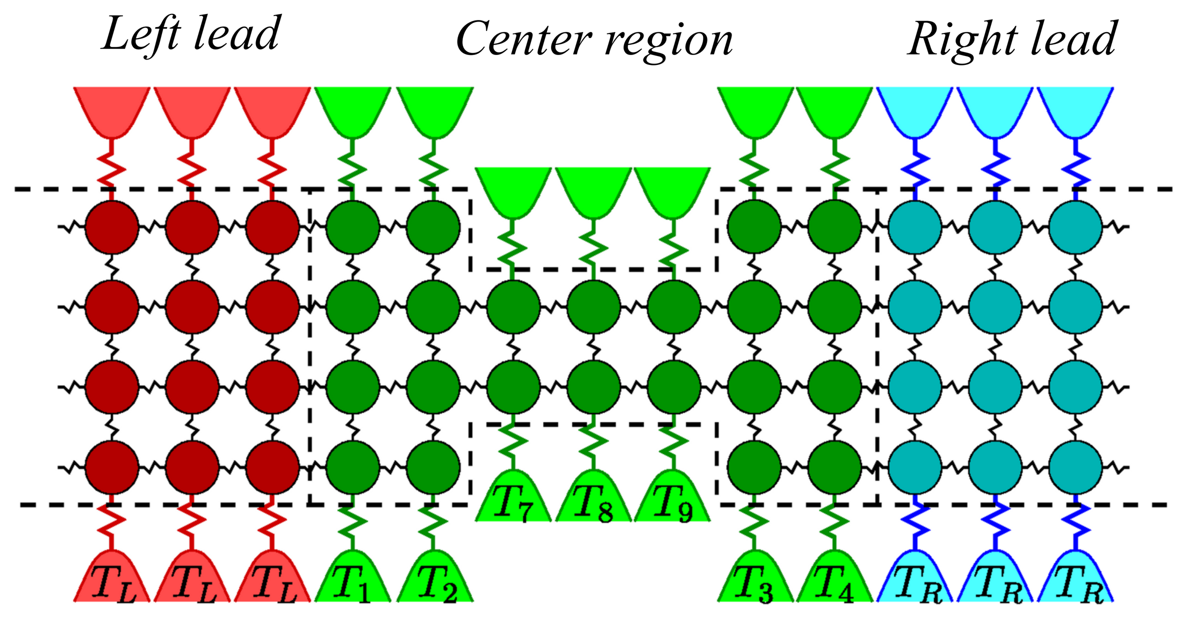
Self-consistent heat bath model

Consider a setup divided to the left lead, center region and the right lead.

Couple **all atoms** to Langevin heat baths, which

- create phonons by thermal **fluctuations**
- absorb phonons by **dissipation**

In the leads, bath temperatures are fixed.
In the center region, **bath temperatures are determined** from $\langle Q_i \rangle = 0$ (zero net energy exchange).



(heat baths shown only for atoms at the edges)

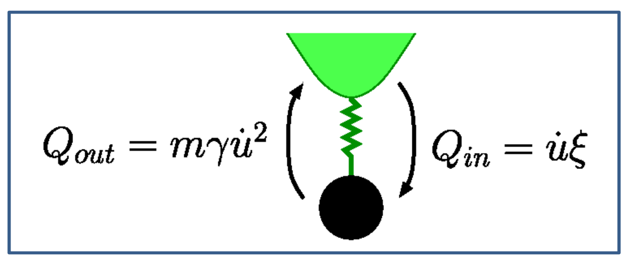
FDT and heat current

Fluctuation-dissipation theorem (FDT) [3] fixes the noise covariance:

$$\langle \hat{\xi}_I(\omega)\hat{\xi}_I(\omega')^T \rangle = 2\pi\delta(\omega+\omega')\Gamma^I(\omega)[f_B(\omega,T_I)+1]$$

Bath coupling function — Bath temperature

Heat current is power: force times velocity



Thermal average of heat current flowing to bath I:

$$\langle Q_I \rangle = \int \frac{d\omega}{2\pi}\omega \sum_J \mathcal{T}_{IJ}(\omega)[f_B(\omega,T_J)-f_B(\omega,T_I)]$$

Phonon transmission function

Solve the non-linear set of equations $\langle Q_i \rangle = 0$ for the bath temperatures in the center region
⇨ **self-consistent bath temperature profile**

Equations of motion and solution

$$m\ddot{\mathbf{u}}_I = -\mathbf{K}_I\mathbf{u}_I - \sum_{J\neq I}\mathbf{V}_{IJ}\mathbf{u}_J + \xi_I - m\gamma_I\dot{\mathbf{u}}_I$$

Atomic displacement in region I=(L,C,R) — Spring constant matrix — Coupling matrix to region J — Langevin **noise and friction**, coupled by **fluctuation-dissipation** relation

Solution in the center region:

$$\hat{\mathbf{u}}_C(\omega) = -\mathbf{G}(\omega)[\hat{\xi}_C(\omega) + \hat{\eta}_L(\omega) + \hat{\eta}_R(\omega)]$$

Fluctuations from local baths and left and right leads

Center region Green's function:

$$\mathbf{G}(\omega) = [m\omega^2 - \mathbf{K}_I + im\gamma_C\omega - \Sigma_L(\omega) - \Sigma_R(\omega)]^{-1}$$

Dissipation from local baths and left and right leads

Fluctuations and dissipation by the leads (I=L,R):

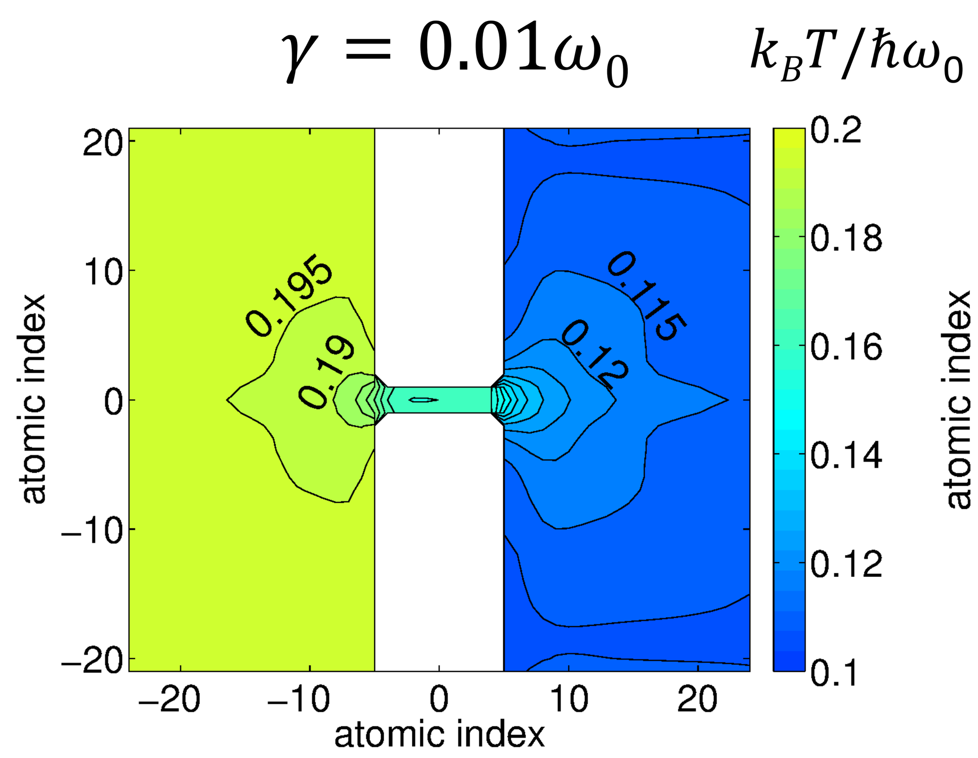
$$\hat{\eta}_I(\omega) = \mathbf{V}_{CI}\mathbf{g}_I(\omega)\hat{\xi}_I(\omega) \qquad \Sigma_I(\omega) = \mathbf{V}_{CI}\mathbf{g}_I(\omega)\mathbf{V}_{IC}$$

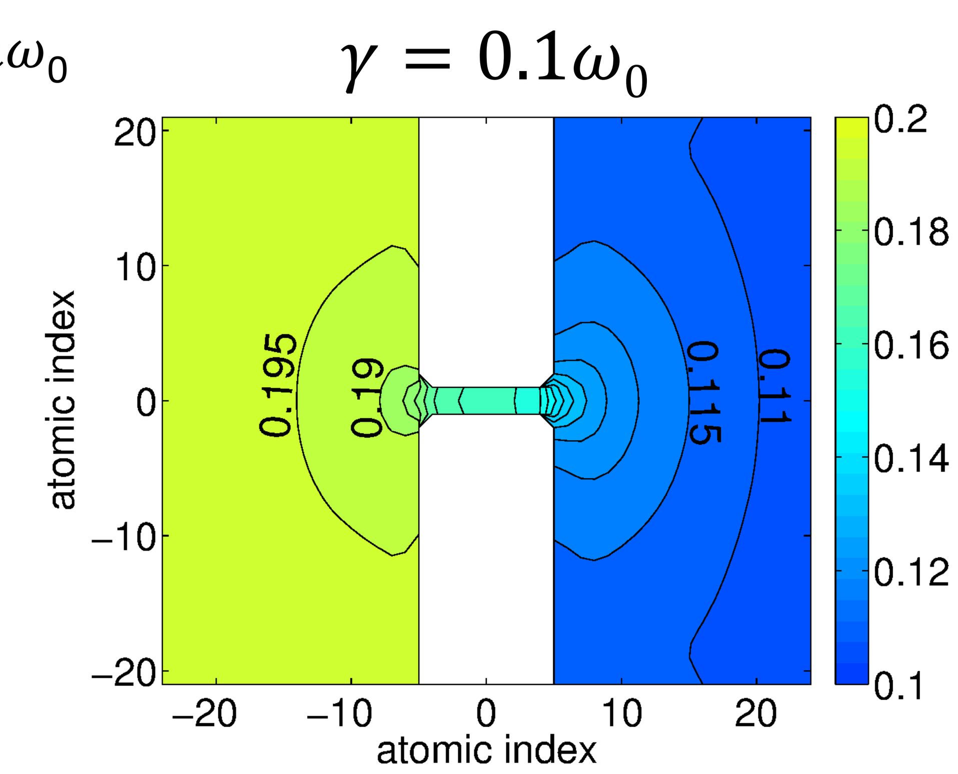
Constriction in 2D

Model: 2D square lattice with nearest neighbor spring interactions

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{\langle j,i \rangle} \frac{1}{2}m\omega_0^2(u_i-u_j)^2$$

$T_L = 0.2, T_R = 0.1$ (in units of $\hbar\omega_0/k_B$)

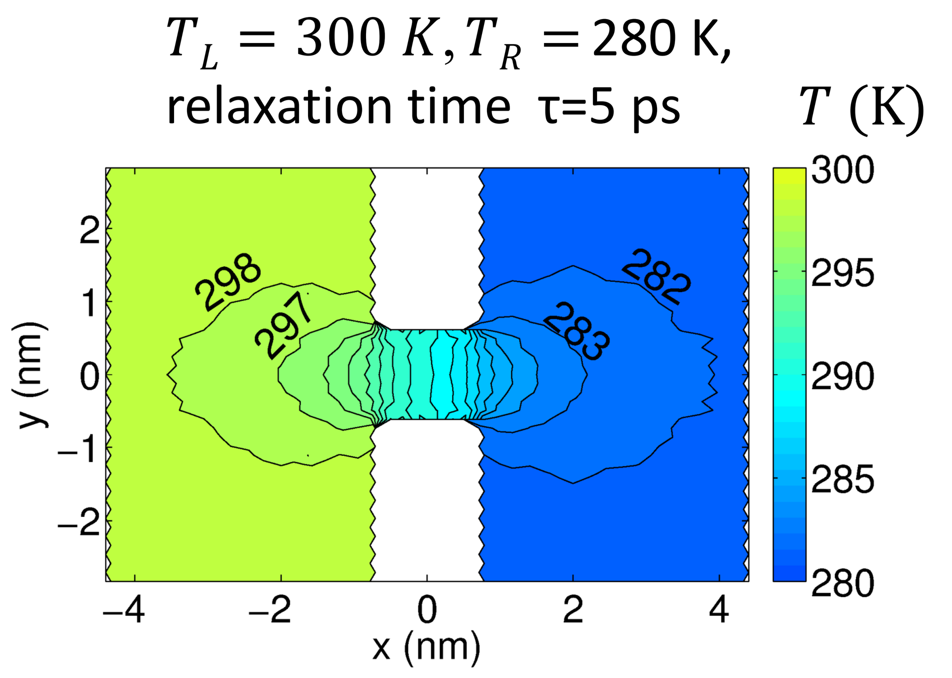


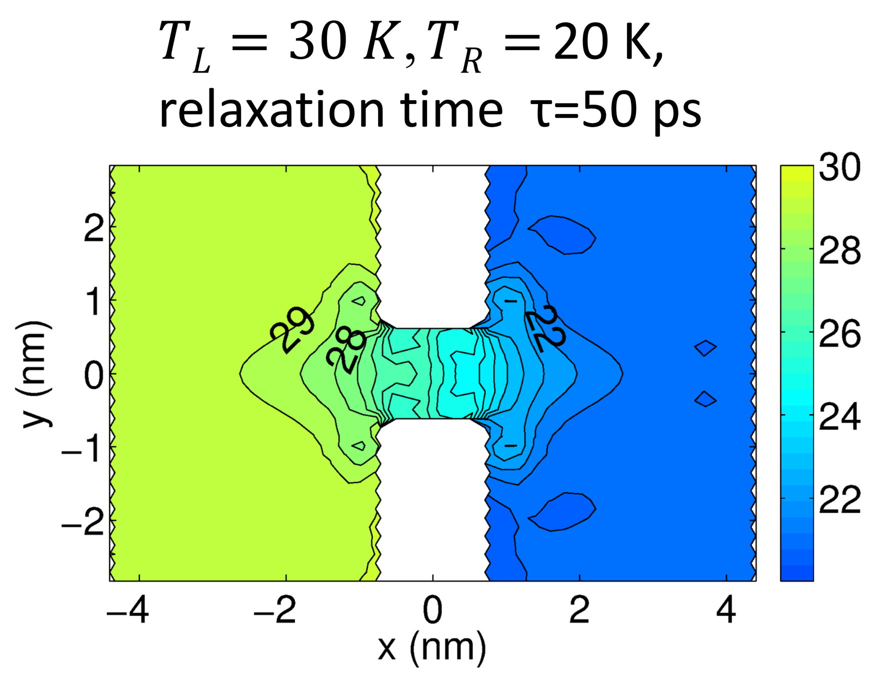


Bath friction constant γ is the **phonon relaxation rate** (ballistic vs. diffusive transport).

Constriction in graphene

C-C interactions modeled with 4th-nearest neighbor spring constant model (L. Wirtz and A. Rubio, Solid. State Comm, 2004). Acoustic phonon relaxation time is τ=5 ps at room temperature (N. Bonini, J. Garg, and N. Marzari, Nano Lett., 2012).





Summary

- Langevin heat baths **create and annihilate phonons**
- Bath coupling constant determines the **phonon relaxation** rate
- In polar materials, heat baths also create **photons** [4]

⇨ **fluctuational electrodynamics**
⇨ unified treatment of phonon-photon heat transfer in nanoscale?

References

[1] M. Bolsterli, M. Rich, and W. M. Visscher, Phys. Rev. A **1**, 1086 (1970).
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[4] F. S. S. Rosa, D. A. R. Dalvit, and P. W. Milonni, Phys. Rev. A **81**, 033812 (2010).

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