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Ballistic heat transport in 1-D nanostructures



KARAZIN UNIVERSITY
CLASSICS AHEAD OF TIME

with scattering centers : - a probabilistic approach -



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Abstract

Within the framework of the theory of random walk [1] and following a Landauer-like formalism [2], we derive an analytical expression for the global transmission coefficient which defines the fraction of the total heat that is transported by ballistic phonons from the hot to the cold reservoirs in the presence of defects, impurities, grain boundaries, interfaces... This transmission coefficient depends only on probabilities p (forward scattering), q (backward scattering), r (absorption) and N , (number of scattering centers), regardless of phonon frequencies and wavelengths [5].

Model for ballistic phonon flux in the presence of scattering centers

Impurities, defects, grain boundaries, interfaces... constituent sites for scattering (called scattering centers SCs).

These sites are modeled as multiple screens at which 3 processes are possible :

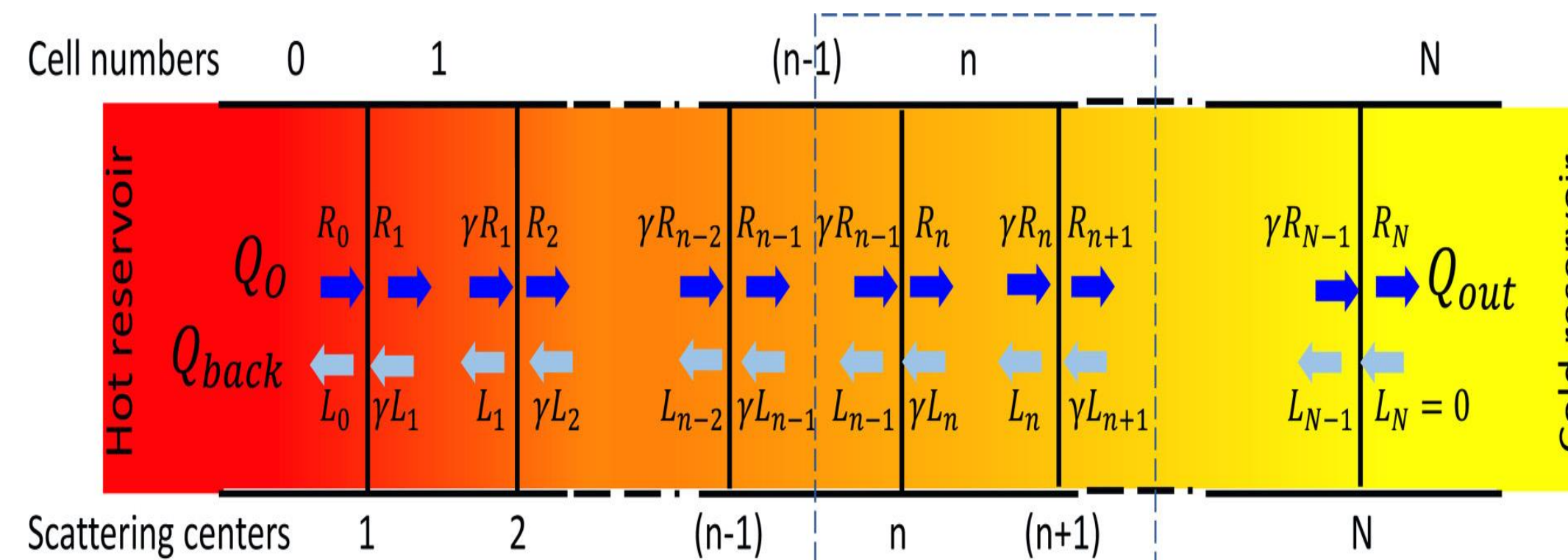
- forward scattering with probability p
- backward scattering with probability q
- absorption with probability r

Screens divide the nanostructure into cells.

Sum of probabilities at a SC : $p + q + r = 1$

Absorption is also permitted within the material with a probability $(1-\gamma) < 1$

Let R_n represent flux flow to the right in n^{th} cell
 L_n represent flux flow to the left in n^{th} cell



Flux flow balance between n^{th} and $(n+1)^{\text{th}}$ cells :

$$\begin{aligned} R_{n+1} &= \gamma p R_n + \gamma q L_{n+1} \\ L_n &= \gamma q R_n + \gamma p L_{n+1} \end{aligned} \quad \text{or} \quad \begin{pmatrix} R_{n+1} \\ L_{n+1} \end{pmatrix} = S \begin{pmatrix} R_n \\ L_n \end{pmatrix}$$

(spatial evolution matrix notation)

Connecting flux and heat flows in N^{th} cell to first cell :

$$\begin{pmatrix} R_N \\ L_N \end{pmatrix} = S^N \begin{pmatrix} R_0 \\ L_0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} Q_{out} \\ 0 \end{pmatrix} = S^N \begin{pmatrix} Q_0 \\ Q_{back} \end{pmatrix}$$

where Q_0 input heat, Q_{out} final out-going heat flux,
 Q_{back} total backward heat flux

Transmission coefficient (probability)

$$P = \frac{Q_{out}}{Q_0} = \frac{1}{(S^N)_{22}}$$

Evolution matrix:

$$S = \frac{1}{p^2} \begin{pmatrix} \gamma(p^2 - q^2) & q \\ -q & 1/\gamma \end{pmatrix}$$

Probability for a phonon to go from hot to cold reservoir :

$$P = \frac{\gamma^2 p (\lambda_+ - \lambda_-)}{\lambda_+^N (1 - p\gamma\lambda_-) - \lambda_-^N (1 - p\gamma\lambda_+)} \quad \star$$

where λ_{\pm} are eigenvalues of matrix S :

$$\begin{aligned} \lambda_{\pm} &= b \pm \sqrt{b^2 - 1} \\ \text{and} \quad b &= \frac{\gamma^2(p^2 - q^2) + 1}{2p\gamma} \end{aligned}$$

Heat flux

Ballistic motion of phonons justifies use of Landauer formalism.

Heat flux per phonon mode

$$Q = Q_{max} P = K_0 \Delta T P = \frac{\Delta T}{R_{\Sigma}}$$

where Q_{max} is the maximum heat flux flow per phonon mode through a 1-D channel and

$$K_0 = \frac{\pi^2 k_B^2 T}{3h} \equiv \text{quantum of thermal conductance [3]}$$

R_{Σ} is the effective thermal resistance

Transmission for limiting cases and Kapitza resistance, R_K

Absence of *absorption* implies $\gamma = 1$ and $r = 0$. Phonons now experience forward and backward scattering and total heat flux is conserved : $Q_0 = Q_{out} + Q_{back}$

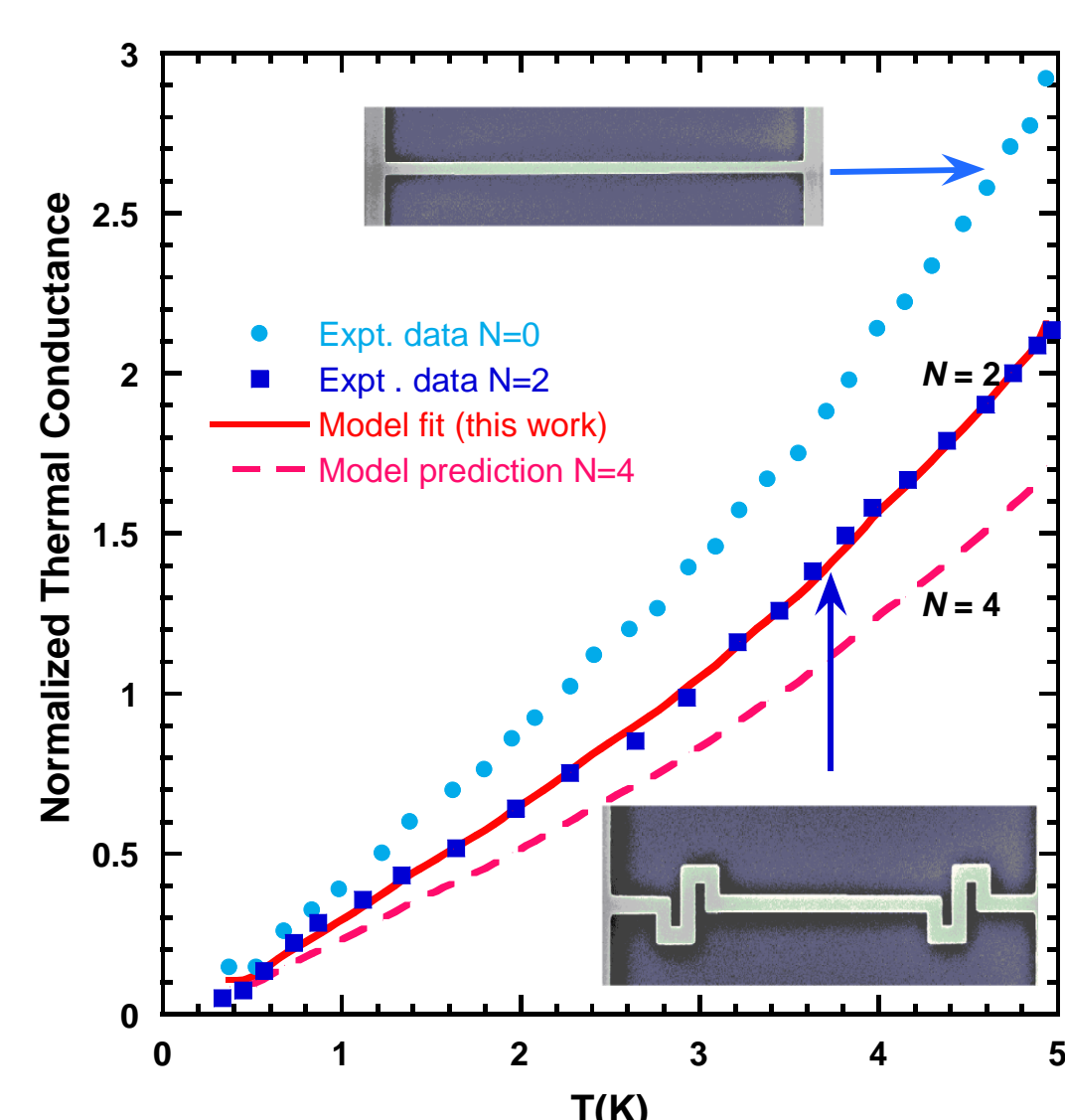
Transmission probability is given by : $P = \frac{p}{p + N(1-p)} \quad \star \quad P = \frac{1}{N+1}$ for $p = q = \frac{1}{2}$
equiprobable scattering

Relationship between P_N and P_{N-1} : $P_N^{-1} = P_{N-1}^{-1} + \frac{1-p}{p}$

For cells of different materials forming a *superlattice*, P is unambiguously related to R_K :

$$R_{\Sigma} = R_{min} + N R_K \quad \text{with} \quad R_{min} = \frac{1}{K_0} \quad (N = 0) \quad \text{and} \quad R_K = \frac{1-p}{p} \frac{3h}{\pi^2 k_B^2 T}$$

Comparison with experiment : Thermal conductance of Si nanowires



Experimental data of thermal conductance of Si nanowires normalized w. r. t. 4 quanta of thermal conductance :
O. Bourgeois *et al.* C. R. Phys. 17, 1154 (2016) Copyright 2016, Elsevier [4]

Dots and squares correspond to data for a straight Si nanowire and for a Si nanowire with S-shaped chicanes (see photos)

Experiments conducted between 0.4K and 5 K : phonon motion is predominantly *ballistic*. S-shaped serpentine plays the role of scattering centers $N = 2$. Dominant phonon thermal wavelength $\lambda \leq$ dimensions of sample 100 nm x 200 nm x 10 nm

Using \star : $\frac{K_{2S-shape}(T)}{K_{straight}(T)} = \frac{p}{2-p}$ Red curve fit is obtained for a UNIQUE value of $p = 0.85$ with $r = 0$.

Conclusion

- An explicit analytical expression for the Landauer-like transmission coefficient is derived for ballistic phonons in the presence of scattering centers
- The transmission coefficient depends only on probabilities of forward/ backward scattering (p and q), absorption γ of phonons and on the number of scattering centers N , regardless of phonon wavelengths and frequencies

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