Atomistic Green's Function Method: Introduction

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Based on:

W. Zhang, T.S. Fisher, N. Mingo, "The Atomistic Green's Function Method: An Efficient Simulation Approach for Nanoscale Phonon Transport," *Numerical Heat Transfer: Part B (Fundamentals)*, Vol. 51, No. 3/4, pp. 333-349, 2007.

Overview of Phonon Simulation Tools

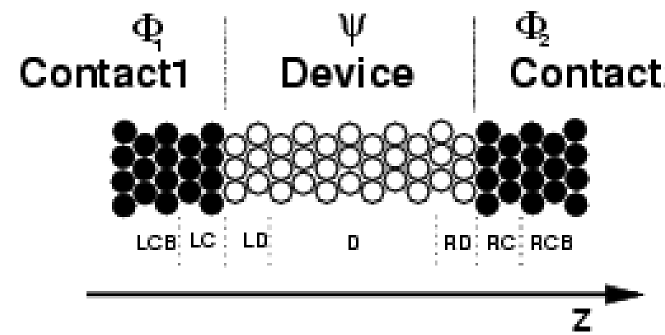
- Boltzmann Transport Equation (BTE)
  - Requires boundary scattering models
  - Requires detailed understanding of phonon scattering and dispersion for rigorous inclusion of phonon physics
- Molecular Dynamics (MD)
  - Computationally expensive
  - Not strictly applicable at low temperatures
  - Handling of boundaries requires great care for links to larger scales and simulation of functional transport processes
- Atomistic Green’s Function (AGF)
  - Efficient handling of boundary and interface scattering
  - Straightforward links to larger scales
  - Inclusion of anharmonic effects is difficult

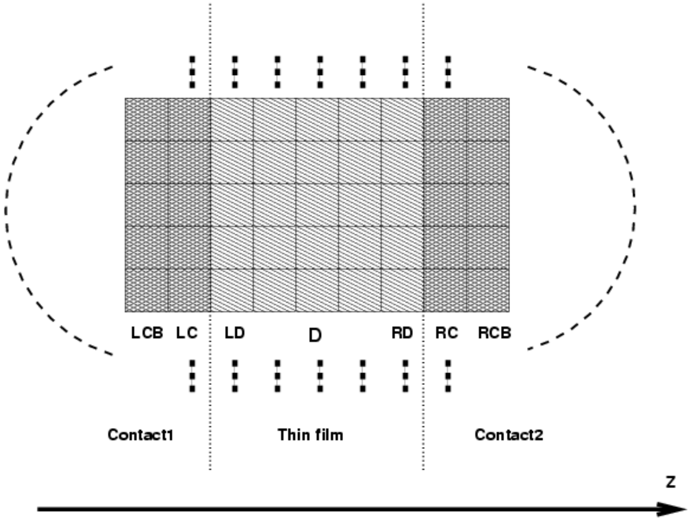
Some Background

- Non-equilibrium Green's function method initially developed to simulate electron ballistic transport (see Datta, 1995)
- Very efficient in the ballistic regime but requires significant effort to implement scattering
- Recently applied to phonon transport (see Mingo, 2003; Zhang et al., 2007a,b)

Atomistic Green's Function

- Includes effects of bulk contacts by expressing their effects mathematically through Green's functions
- Suitable for ballistic transport
  - Nanoscale devices at room temperature, or
  - Low-temperature conditions, or
  - Scattering dominated by boundaries and interfaces
- Required inputs
  - Equilibrium atomic positions
  - Inter-atomic potentials
  - Contact temperatures





Recall Lattice Dynamics

- Equation of motion for a 1D atomic chain

$$m\frac{d^2u_n}{dt^2} = -g\left\{2u_n - u_{n-1} - u_{n+1}\right\}$$

- Plane wave assumption

$$u_n(t) \sim \exp\left\{i\left(Kna - \omega t\right)\right\}$$

- Combine

$$-\omega^2 u_n = -\frac{g}{m}\left\{2u_n - u_{n-1} - u_{n+1}\right\}$$

- Re-arrange and write in matrix form

$$\left[\omega^2\mathbf{I} - \mathbf{H}\right]\mathbf{u} = 0$$

$\mathbf{I}$ is the identity matrix

Harmonic Matrix

- Define the **k** matrix as

$$k_{ij} = -\frac{\partial^2 U^{harm}}{\partial u_i \partial u_j}$$

$$\rightarrow k_{nn} = -2g$$

$$k_{n,n+1} = k_{n,n-1} = g$$

Here, *g* is the spring constant

- Then, define the harmonic matrix **H** as

$$H_{ij} = \frac{1}{\sqrt{M_i M_j}} k_{ij}, \quad \text{no index summation}$$

Harmonic Matrix

$$\mathbf{H} = \begin{bmatrix} -2f & f & \\ f & -2f & f \\ & f & -2f \end{bmatrix}$$

f is spring constant divided by atomic mass

1. **H** is not the same dynamical matrix used to determine the dispersion curve (that matrix is the Fourier transform of **H**).
2. **H** is symmetric.
3. Sum of all elements in any row or sum of all elements in any column is zero, except in the first and last row/column.

Green's Functions

- In general, systems of equations can be written in operator form

$$\mathbf{L}[\mathbf{u}] = \left[\omega^2\mathbf{I} - \mathbf{H}\right]\mathbf{u} = 0$$

- *Green's functions* are often used in such situations to determine general solutions of (usually) linear operators

Green’s Functions, cont’d

- The Green’s function **g** is the solution that results from the addition of a perturbation to the problem

$$\mathbf{L}[\mathbf{g}] = \delta$$

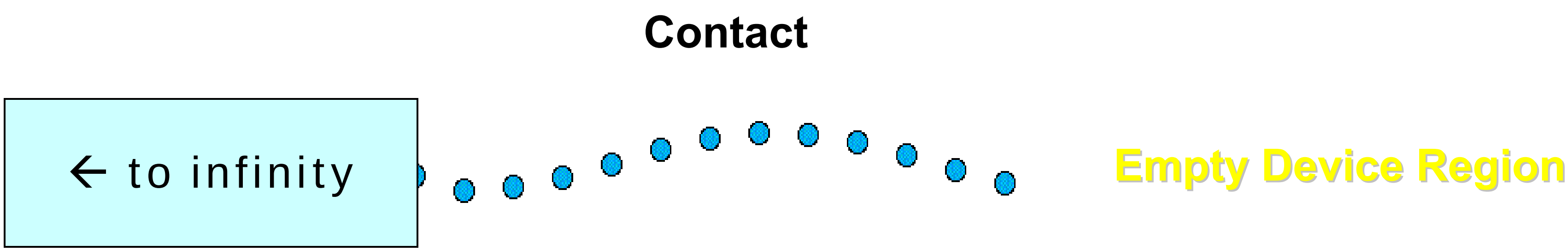
- In the present (matrix) problem, the *uncoupled Green’s function* becomes

$$\mathbf{g} = \left[\left(\omega^2 + \delta i \right) \mathbf{I} - \mathbf{H} \right]^{-1}$$

  - Where δ is called the broadening constant, and *i* is the unitary imaginary number

Uncoupled Contacts

- In our context, Green's functions first appear in the two contact regions
- Imagine first that each contact is unconnected to the 'device' but extends to infinity in the other direction



Uncoupled Contact Green's Functions

- Now, we form the *uncoupled* Green's functions for each contact (**g_1** and **g_2**)

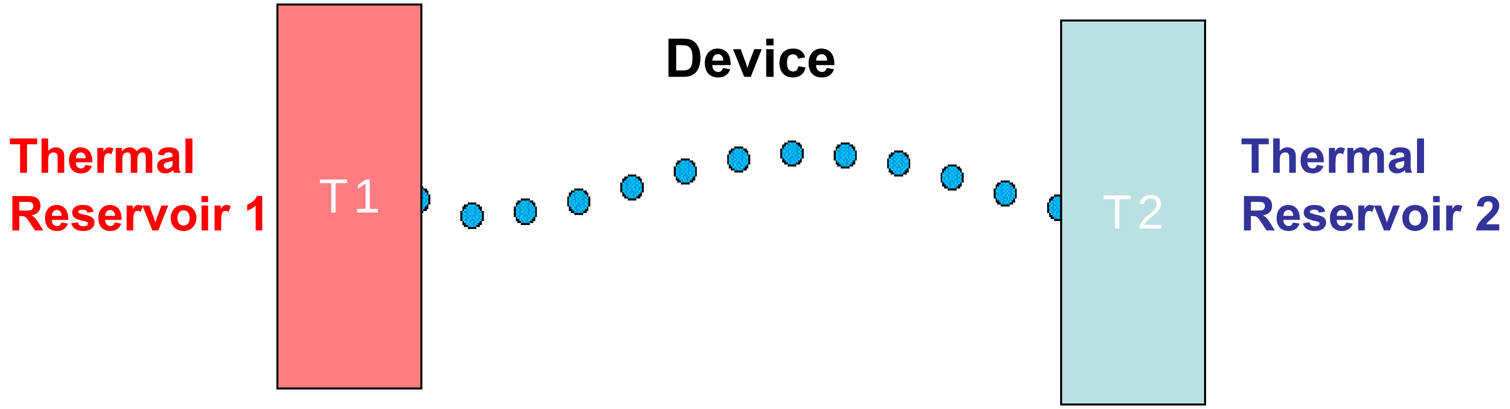
$$\mathbf{g}_1 = \lim_{\delta \to 0} [(\omega^2 + \delta i)\mathbf{I} - \mathbf{H}_1]^{-1}$$

$$\mathbf{g}_2 = \lim_{\delta \to 0} [(\omega^2 + \delta i)\mathbf{I} - \mathbf{H}_2]^{-1}$$

- Where the **H_i**'s are the harmonic matrices for each contact

Toward Realistic Problems

- So far, we have not made much progress in solving real problems
- To solve most practical problems, we need to incorporate different materials and interfaces



Assembling the System

- We now need to *couple* the two contacts with the device
- Our overall matrix equation becomes

Harmonic matrix for contact 1

Harmonic matrix for the device

Uncoupled displacement of contact 1

Effects of device on contact displacements

$$\begin{bmatrix} \omega^2 \mathbf{I} - \mathbf{H}_1 & -\tau_1^\dagger & 0 \\ -\tau_1 & \omega^2 \mathbf{I} - \mathbf{H}_d & -\tau_2 \\ 0 & -\tau_2^\dagger & \omega^2 \mathbf{I} - \mathbf{H}_2 \end{bmatrix} \begin{Bmatrix} \Phi_1^R + \chi_1 \\ \psi \\ \Phi_2^R + \chi_2 \end{Bmatrix} = 0$$

Device displacement

Harmonic matrix for contact 2

Uncoupled displacement of contact 2

The Device Green's Function

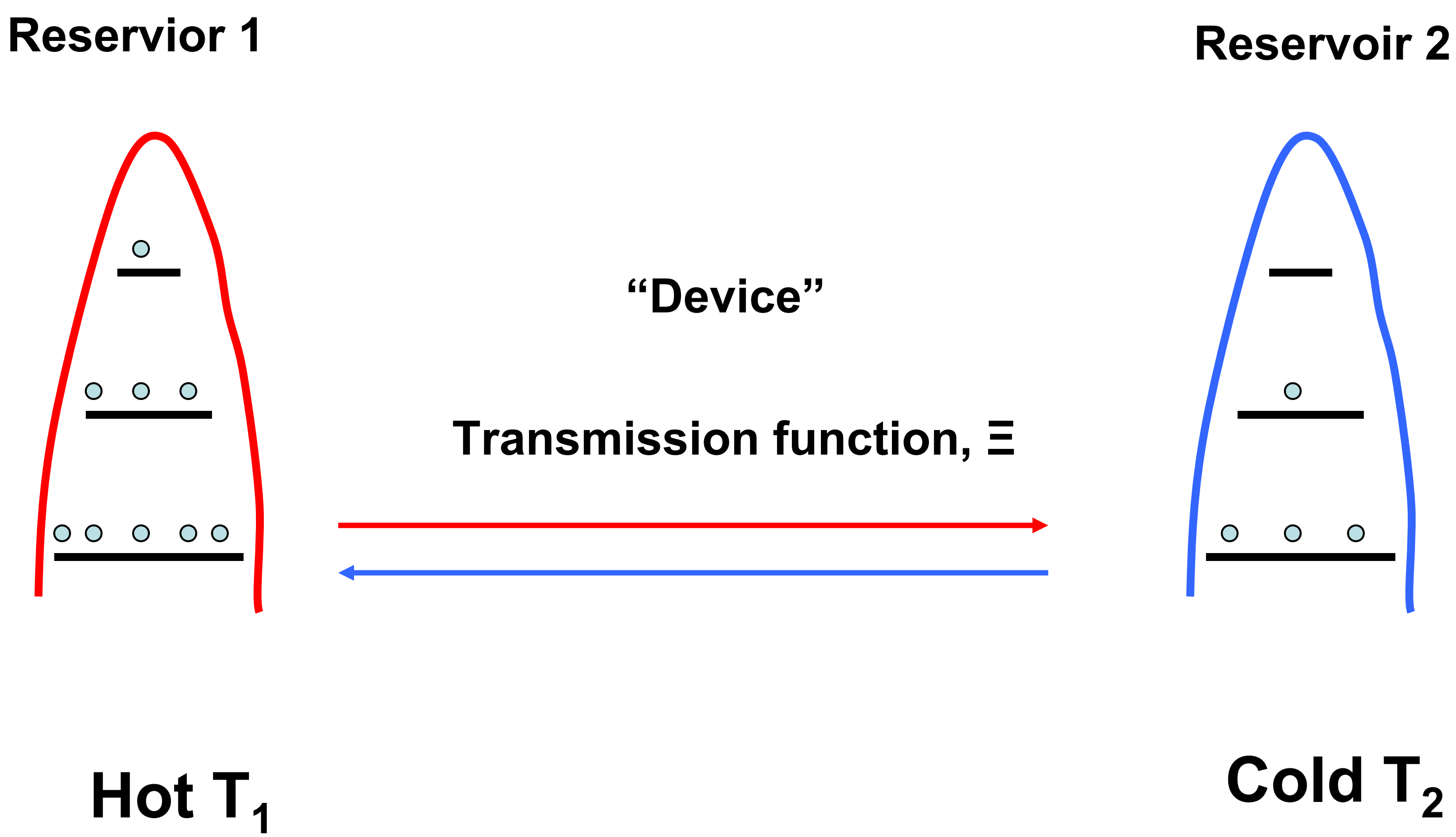
- The device Green's function **G** can now be expressed as

$$\mathbf{G} = \left[\omega^2 \mathbf{I} - \mathbf{H_d} - \underbrace{\tau_1 \mathbf{g}_1 \tau_1^T}_{\boldsymbol{\Sigma}_1} - \underbrace{\tau_2 \mathbf{g}_2 \tau_2^T}_{\boldsymbol{\Sigma}_2} \right]^{-1}$$

superscript "*T*" = conjugate transpose

  - Note that this Green's function does not explicitly contain a δ perturbation
  - The so-called self-energy matrices (Σ_1, Σ_2) that involve uncoupled Green's functions (**g**'s) associated with contacts (i.e., boundaries) serve essentially as perturbations
  - τ matrices handle connections between different system elements (materials, interfaces)
- Very efficient in the ballistic regime but requires significant effort to implement scattering

Toward Transport through a Device between Two Contacts



Relation between Transmission and Green's Functions

- Some definitions of convenience

$$\mathbf{A}_j = i\left[\mathbf{g}_j - \mathbf{g}_j^{\,T}\right]$$

$$\mathbf{\Gamma}_j = \tau_j \mathbf{A}_j \tau_j^{\,T}$$

- The transmission function

$$\Xi(\omega) = Trace\left[\mathbf{\Gamma}_1 \mathbf{G} \mathbf{\Gamma}_2 \mathbf{G}^T\right] = Trace\left[\mathbf{\Gamma}_2 \mathbf{G} \mathbf{\Gamma}_1 \mathbf{G}^T\right]$$

From $\mathbf{g}_1$ and τ_1

Device Green's function

From $\mathbf{g}_2$ and τ_2