Quantum transport treatment: the Non-Equilibrium Green's Function (NEGF) formalism

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Modeling Nanomaterials for Energy Transport and Storage
Summer school *MONACOSTE - The 12th of May 2022*

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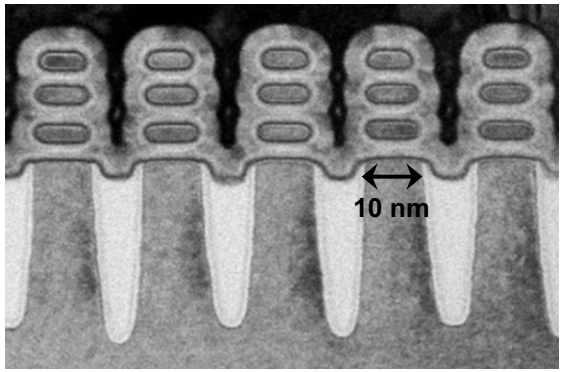
Outline

- Context: partial coherence in nanodevices
- Handwavy introduction to NEGF (electrons)
  - The Dyson equation.
  - The concept of self-energy → description of the contacts
- Inelastic interactions: Self-consistent Born approximation (SCBA)
- SCBA: numerically demanding --> direct approaches (LOA)
- NEGF can also be applied to solve transport of phonons
- Coupling transport of electrons and phonons: energy devices (thermoelectricity, solar cells…)

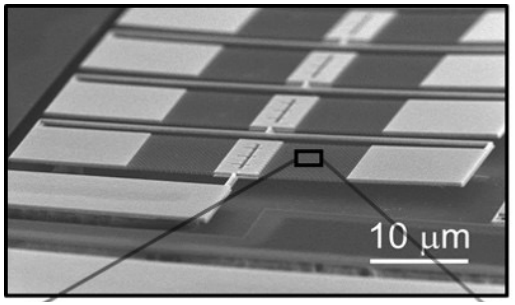
Inside the devices

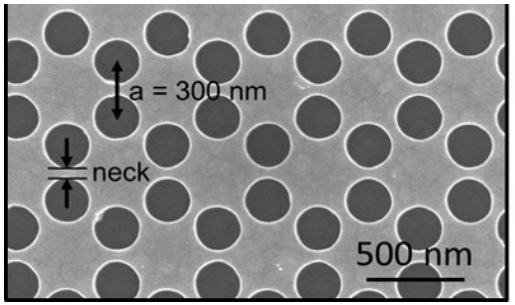
Integrated circuits



5 nm transistors IBM, VLSI 2017

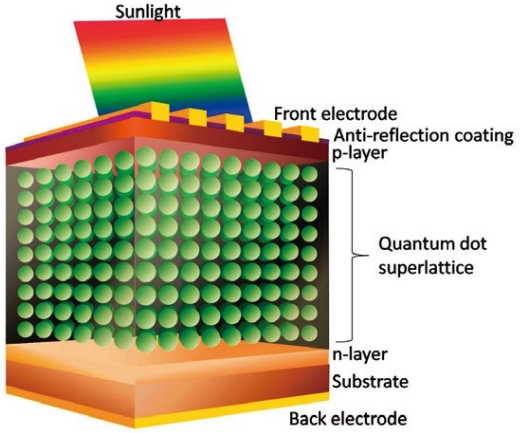
Thermoelectric generators





Nomura Lab, UTokyo, Appl. Phys. Express **13**, 095001 (2020)

3rd generation solar cells



Okada Lab, UTokyo, Nat. Commun. **10**, 43 (2019)

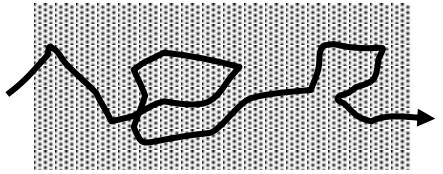
Nanoscale:
Importance of quantum and coherent effects

Electron in nanodevice

Quasi-equilibrium

Large classical device

Diffusion: Impurities, Phonons

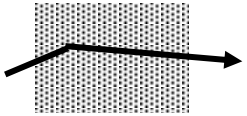


Life is not perfect.

Scattering with phonons, electrons, ...

Partial quantum coherence

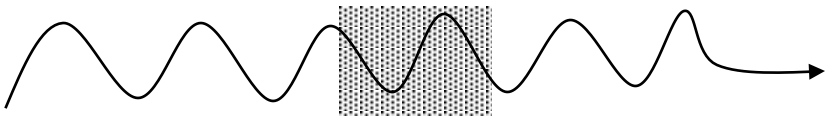
Practical nanodevice



Perfect quantum coherence

$H\psi = E\psi$

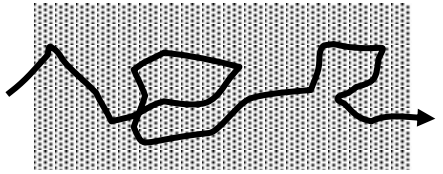
Ideal nanodevice



Electron in nanodevice

Large classical device

Diffusion: Impurities, Phonons



Quasi-equilibrium

Life is not perfect.
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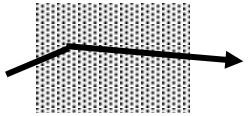
Practical nanodevice



Perfect quantum coherence

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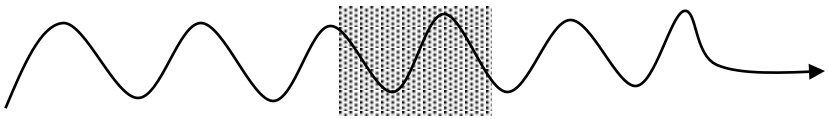
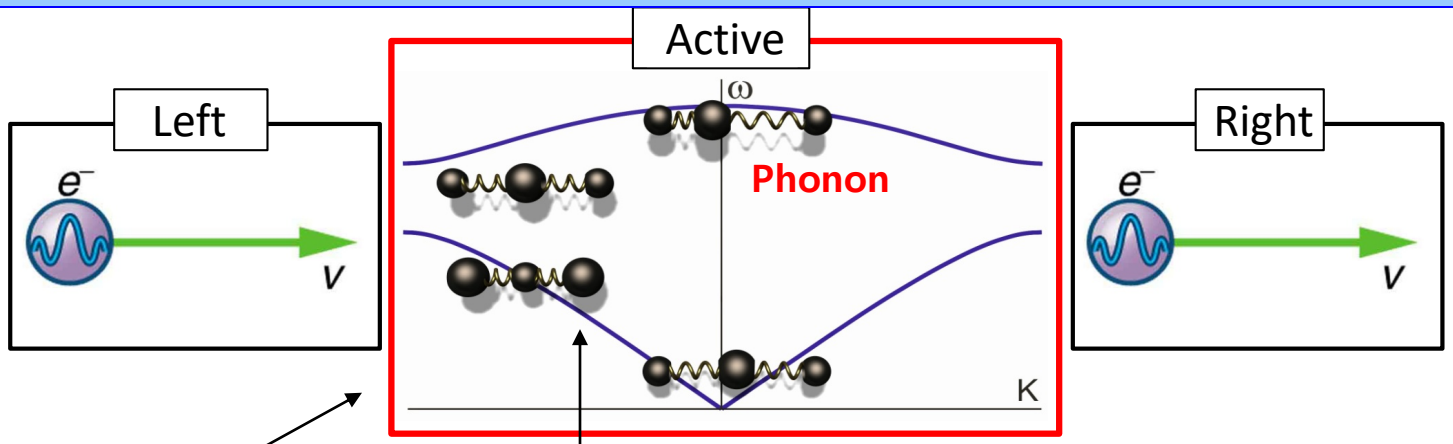
Ideal nanodevice



Modeling Approach – with scattering



Contact-nanodevice interface
Open boundary conditions

Influence of active region properties
(band structure, impurities, defects)

Scattering of electron with
phonons / electrons / photons …
Partial phase coherence

What theoretical tool do we need?

Description of nanodevices

- Electron: Schrodinger's Equation
- Open nanosystem:
  - Coupling with contacts
  - Inelastic interactions
- Where are the energy levels of system?

->Hamiltonian of the nanodevice:

Effective Mass Equation (continuous)

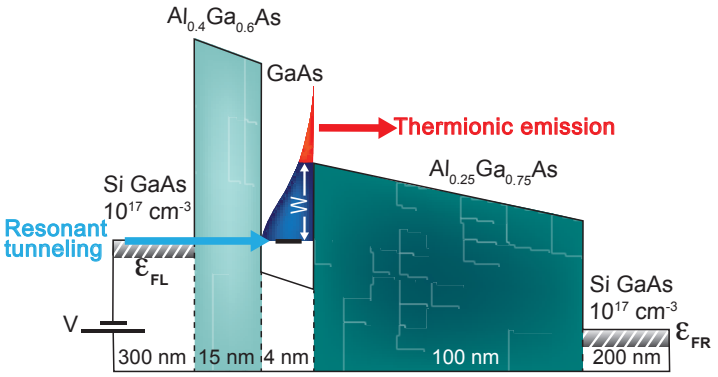
↓

Tight Binding (atomistic empirical)

↓

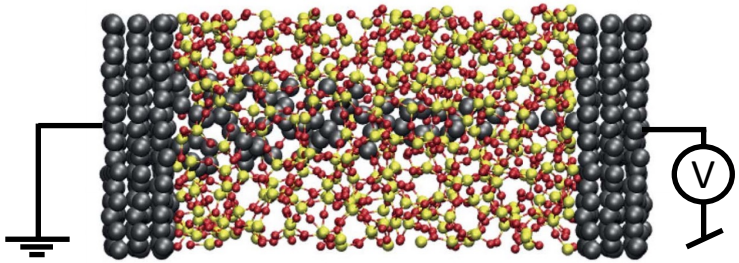
Density Functional Theory (atomistic *ab initio*)

Hetereostructure



LIMMS, Nat. Commun. **10**, 4504 (2019)

CBRAM



ETH, Nanoscale Adv. **2**, 2648 (2020)

Predictive quantum mechanical methods are crucial for disruptive nanodevice design

The Non-Equilibrium Green's Function Formalism (a handwavy introduction)

Where does it come from?

- Time independent Hamiltonian: $H|\Psi\rangle = \varepsilon|\Psi\rangle \Rightarrow (H - \varepsilon I)|\Psi\rangle = 0$

  Eigenvector — Eigenvalue

- Solution if $det(H-\varepsilon I)=0$ for several values of ε.

- For these values of energy $(H-\varepsilon I)^{-1}$ is infinite.

$\Rightarrow$ idea: adding a complex term to avoid the divergence

$\Rightarrow$ This is the retarded Green's function: $$G(\varepsilon) = \lim_{\eta \to 0^+} \frac{1}{\varepsilon I - H + i\eta I}$$

- In the eigenvalue basis, the expression is:

$$G(\varepsilon) = \lim_{\eta \to 0^+} \sum_k \frac{|\Psi_k\rangle\langle\Psi_k|}{\varepsilon - \varepsilon_k + i\eta}$$

ε_k : Eigenvalue associated to the eigenvector $|\Psi_k\rangle$

Where does it come from?

- Physical parameters are "easy" to calculate:

  Example: Density of states at the equilibrium

  ✓ General definition: $N(\varepsilon) = \sum_k \delta(\varepsilon - \varepsilon_k)$

  Delta function

$$Im(TrG(\varepsilon)) = -\sum_k \lim_{\eta \to 0^+} \frac{\eta}{(\varepsilon - \varepsilon_k)^2 + \eta^2}$$

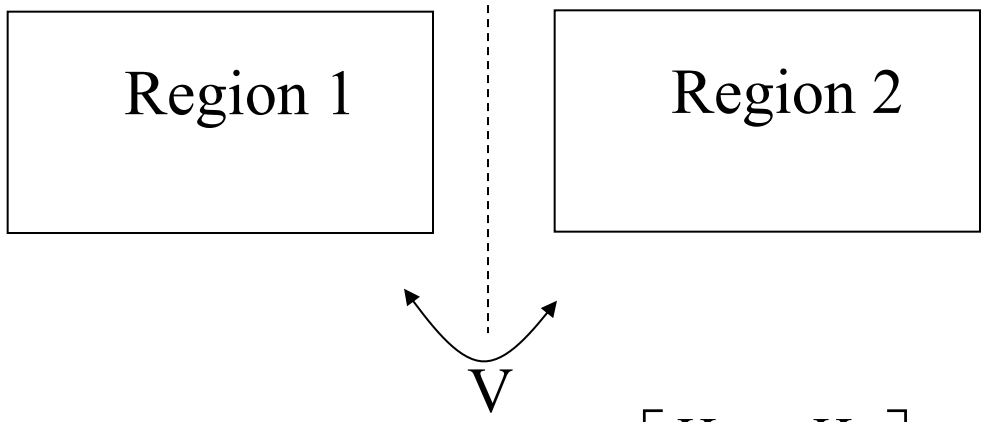
$G(\varepsilon) = \lim_{\eta \to 0^+} \sum_k \frac{|\Psi_k\rangle\langle\Psi_k|}{\varepsilon - \varepsilon_k + i\eta}$ in a matrix expression: $G(\varepsilon) = \begin{bmatrix} \lim_{\eta \to 0^+} \frac{1}{\varepsilon - \varepsilon_1 + i\eta} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lim_{\eta \to 0^+} \frac{1}{\varepsilon - \varepsilon_1 + i\eta} \end{bmatrix}$

And: $\int_{-\infty}^{+\infty} \frac{\eta}{(\varepsilon - \varepsilon_k)^2 + \eta^2} = \left[Arc\tan\left(\frac{\varepsilon - \varepsilon_r}{\eta}\right) \right]_{-\infty}^{+\infty} = \pi$

Therefore: $\lim_{\eta \to 0^+} \frac{\eta}{(\varepsilon - \varepsilon_k)^2 + \eta^2} = \pi\delta(\varepsilon - \varepsilon_k)$

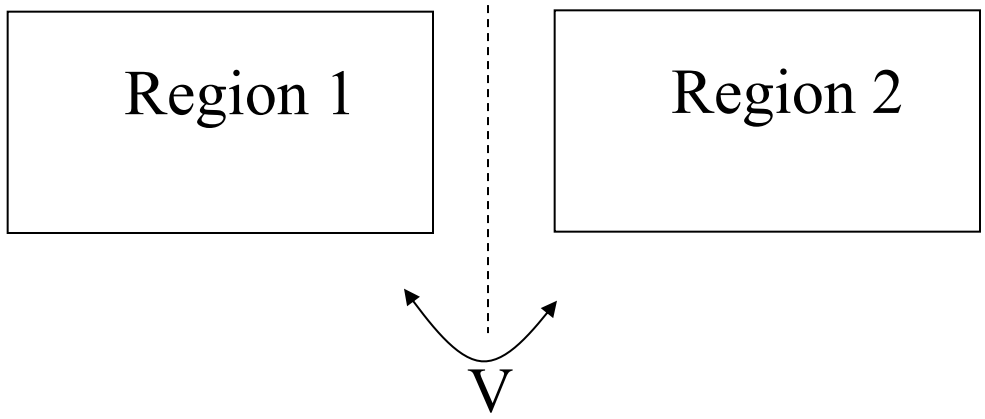
$$\Rightarrow \boxed{N(\varepsilon) = -\frac{1}{\pi} Im(Tr(G(\varepsilon)))}$$ **DOS**

The Dyson equation



- Hamiltonian of the coupled system: $H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}$
- Hamiltonian of the uncoupled system: $H_0 = \begin{bmatrix} H_{11} & 0 \\ 0 & H_{22} \end{bmatrix}$
- Coupling matrix: $V = \begin{bmatrix} 0 & H_{12} \\ H_{21} & 0 \end{bmatrix}$
- We have: $H = H_0 + V$

The Dyson equation



- Let's define: $G_0(\varepsilon) = \lim_{\eta \to 0^+} (\varepsilon I - H_0 + i\eta I)^{-1}$ and $G(\varepsilon) = \lim_{\eta \to 0^+} (\varepsilon I - H + i\eta I)^{-1}$

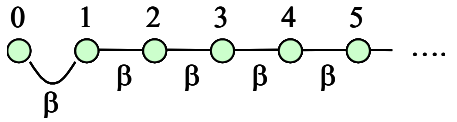
$$\Rightarrow G^{-1}(\varepsilon) = \lim_{\eta \to 0^+} (\varepsilon I - H_0 - V + i\eta I) = G_0^{-1} - V$$

$\Rightarrow$ Dyson equation: $$\boxed{G(\varepsilon) = G_0(\varepsilon) + G_0(\varepsilon) V G(\varepsilon)}$$

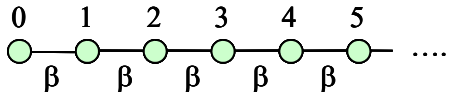
- **Applicable to any type of perturbation V (connection to reservoirs, point defects, inelastic scattering etc…**

Green's function of a semi-infinite reservoir

- Let's consider a semi-infinite linear chain where:



Atom 0 is not coupled ≡ H^0



Atom 0 is not coupled ≡ H

$$V = \begin{bmatrix} 0 & \beta & 0 & \cdots \\ \beta & 0 & \cdots & \cdots \\ 0 & \vdots & \ddots & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

$$H^0 = \begin{array}{c} \begin{matrix} 0 & 1 & 2 & \cdots \end{matrix} \\ \begin{bmatrix} H_{00} & 0 & \cdots & \cdots \\ 0 & H_{11} & \beta & \cdots \\ \vdots & \beta & \ddots & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \end{array} \begin{matrix} 0 \\ 1 \\ 2 \\ \vdots \end{matrix} \Rightarrow g^0 = \begin{bmatrix} g^0_{00} & 0 & \cdots & \cdots \\ 0 & g^0_{11} & \cdots & \cdots \\ \vdots & \vdots & \ddots & \cdots \\ 0 & \vdots & \vdots & \ddots \end{bmatrix}$$

$$H = \begin{array}{c} \begin{matrix} 0 & 1 & 2 & \cdots \end{matrix} \\ \begin{bmatrix} H_{00} & \beta & 0 & \cdots \\ \beta & H_{11} & \beta & \cdots \\ 0 & \beta & \ddots & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \end{array} \begin{matrix} 0 \\ 1 \\ 2 \\ \vdots \end{matrix} \Rightarrow g = \begin{bmatrix} g_{00} & g_{01} & \cdots & \cdots \\ g_{10} & g_{11} & \cdots & \cdots \\ \vdots & \vdots & \ddots & \cdots \\ 0 & \vdots & \vdots & \ddots \end{bmatrix}$$

Dyson equation:

$$g = g^0 + g^0 V g$$

$$g^0_{11} = g_{00}$$

(Recursion method)

Green's function of a semi-infinite reservoir

Green's function of a semi-infinite reservoir

- **From Green's function to wave function**:

By solving the Dyson equation for the semi-infinite linear chain:

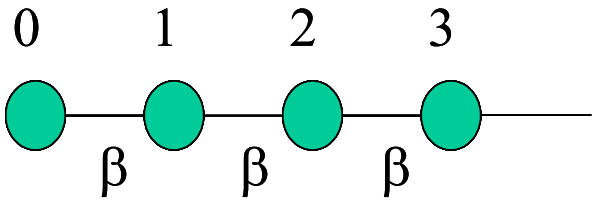
$$g_{00}(\varepsilon) = \frac{1}{2\beta^2}\left(\varepsilon - i\sqrt{4\beta^2 - \varepsilon^2}\right), \quad if \quad |\varepsilon| < 2|\beta|$$

With $\varepsilon = 2\beta\cos(ka)$:

$$\Rightarrow \quad g_{00}(\varepsilon) = \frac{1}{2\beta^2}\left(2\beta\cos(ka) - i2|\beta|\sin(ka)\right)$$

$$\Rightarrow \quad g_{00}(\varepsilon) = \frac{1}{\beta}e^{ika}$$

Equivalent to a plane wave!

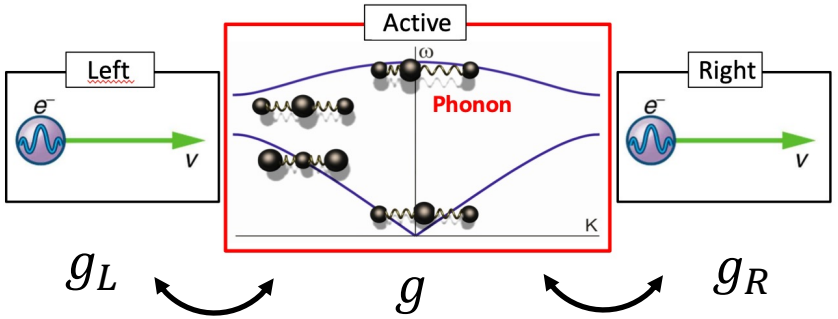


The concept of self-energy

$$G(E) = \left[EI - H - \Sigma_L - \Sigma_R\right]^{-1}$$

Self-energy of the left contact

Self-energy of the right contact



g_L g g_R

V_{LA} V_{AR}

$\Sigma_L = V_{LA}^{\dagger} g_L V_{LA}$ $\Sigma_R = V_{AR} g_R V_{AR}^{\dagger}$

Dyson equation:

$$G = g + g\Sigma_C\, G \qquad \text{with} \qquad \Sigma_C = \Sigma_L + \Sigma_R$$

- **Self-energies of the contacts**: Modification of the Hamiltonian [H] to incorporate the « boundary conditions ». Elegant, but Not necessarily numerically more efficient (Scattering matrix approach).
- Concept of self-energy:
  -> much more general.
  -> can be used to describe all kinds of interactions (e-phonon, e-photon, phonon-phonon).

The NEGF algorithm (ballistic)

1) Retarded Green's function: G. Baym, L. P. Kadanoff, and Keldysh in 1962.

$$G^r = [(E - V)I - H - \Sigma_L^r - \Sigma_R^r]^{-1}$$

2) Lesser and Greater contact self-energies:

$$\Sigma_{L,R}^{<}(E) = -2\mathrm{Im}(\Sigma_{L,R}^r(E)) \times (f_{FD}(E))$$

$$\Sigma_{L,R}^{>}(E) = 2\mathrm{Im}(\Sigma_{L,R}^r(E)) \times (1 - f_{FD}(E))$$

3) Lesser/Greater Green's function: $G^{\lessgtr} = G^r \left(\Sigma_L^{\lessgtr} + \Sigma_R^{\lessgtr}\right) G^{r\dagger}$

4) Carrier density:

$$n_j = -i \int_{-\infty}^{+\infty} G^<(j,j;E)dE$$

$$= \int_{-\infty}^{+\infty} LDOS(j;E) f(E, \mu_j, T_j^e) dE.$$

Out-of-equilibrium local distribution

5) Carrier current:

$$J_{j \to j+1} = \int_{-\infty}^{+\infty} dE \frac{e}{\hbar} \left[H_{j,j+1} G^<(j+1,j;E) - G^<(j,j+1;E) H_{j+1,j}\right]$$

Treatment of inelastic interactions

1) Inelastic scattering self-energy (e-phonon, e-photon):

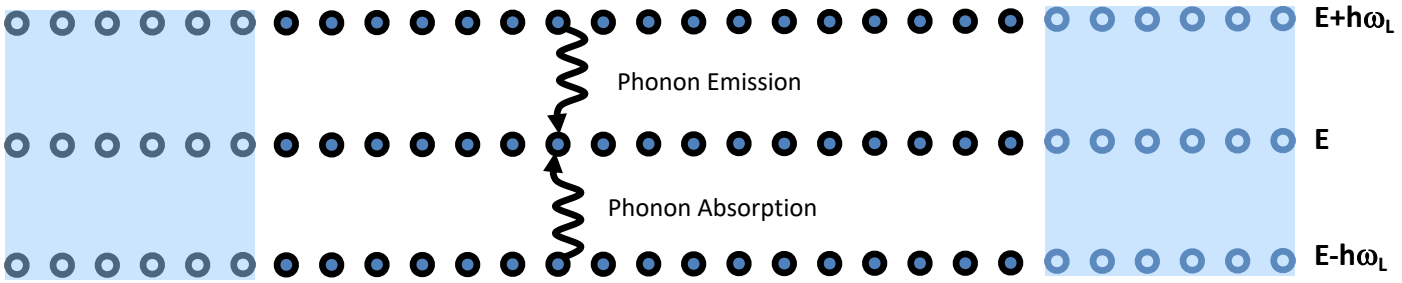
Bose-Einstein

Phonon frequency

$$\Sigma^{\lessgtr}_{inel}(E) = M^2\left[(n_L+1)G^{\lessgtr}(E\pm\hbar\omega_L) + (n_L)G^{\lessgtr}(E\mp\hbar\omega_L)\right]$$

Emission

Absorption



2) New retarded Green's function:

$$G^r = [(E-V)I - H - \Sigma^r_L - \Sigma^r_R - \Sigma^r_{inel}]^{-1} \quad \text{with} \quad \Sigma^r_{inel} = \frac{1}{2}[\Sigma^>_{inel} - \Sigma^<_{inel}]$$

3) New lesser/greater Green's function: $G^{\lessgtr} = G^r\left(\Sigma^{\lessgtr}_L + \Sigma^{\lessgtr}_R + \Sigma^{\lessgtr}_{inel}\right)G^{r\dagger}$

4) Current Calculation: Conserved? Yes → OK **No : self-consistent Born approximation (SCBA)**

$$J_{j\to j+1} = \int_{-\infty}^{+\infty} dE \frac{e}{\hbar}\left[H_{j,j+1}G^<(j+1,j;E) - G^<(j,j+1;E)H_{j+1,j}\right]$$

Self-consistent Born Approximation and beyond…

The self-consistent Born approximation (SCBA)

G. Baym, L. P. Kadanoff, and Keldysh in 1962.

- **Advantage of NEGF**: Any scattering can be included in the formalism *via* ∑ self-energy term.

$$G = \left[EI - H - \Sigma_{L/R} - \Sigma_{e-ph}\right]^{-1}$$

- Self-Consistent Born Approximation (SCBA)

$$G = g_0 + g_0\Sigma[G]G$$

Dyson Equation

g_0: Non-interacting GF (ballistic)
G: Full interacting NEGF
Σ: Interacting self energy

$$G_1 = [g_0^{-1} - \Sigma_1]^{-1}$$

$\bullet$
$\bullet$
$\bullet$

A lot of loops until converged

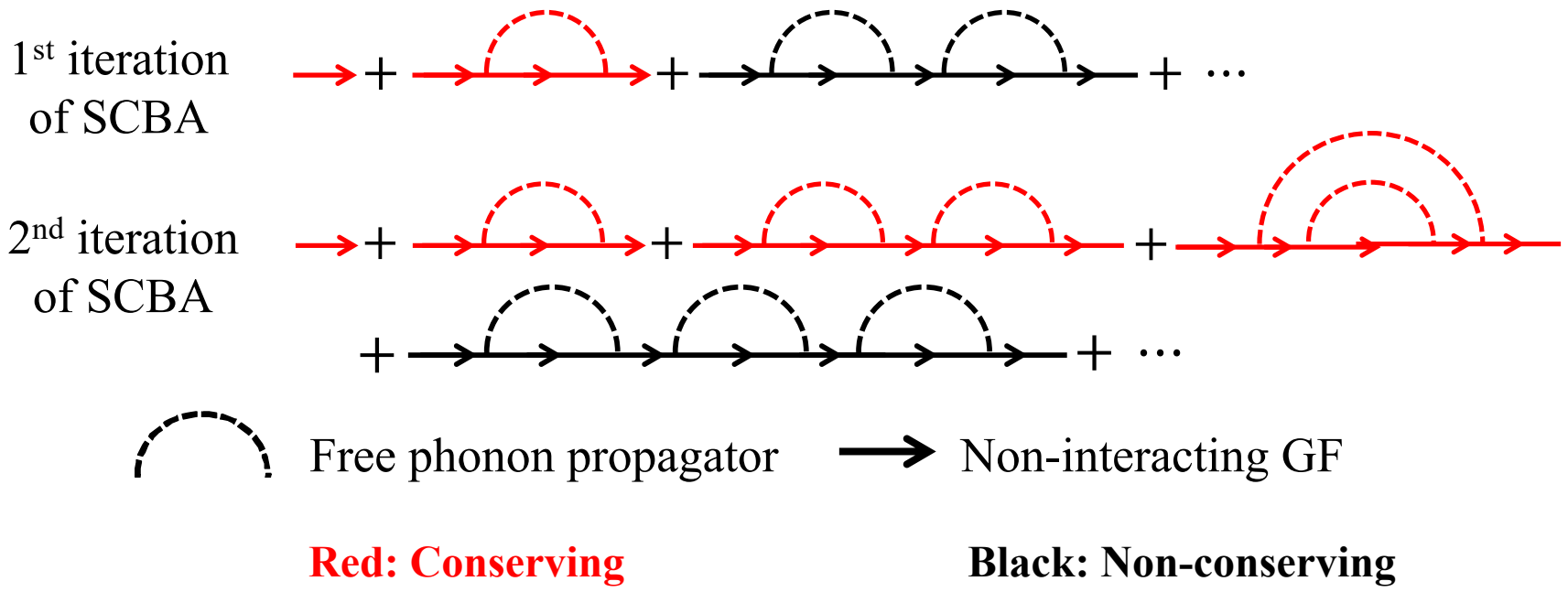
$$G_N = [g_0^{-1} - \Sigma_N]^{-1}$$

$$= \left[g_0^{-1} - \Sigma[G_{N-1}]\right]^{-1}$$

The self-consistent Born approximation (SCBA)

- **SCBA**: Iterating until the conserving diagrams are more dominant than non-conserving diagrams

$$G_n = \left[I - g_0\Sigma[G_{n-1}]\right]^{-1} g_0 = g_0 + g_0\Sigma[G_{n-1}]g_0 + g_0\Sigma[G_{n-1}]g_0\Sigma[G_{n-1}]g_0 + \cdots$$



Self-consistency: Numerically very expensive!

Lowest Order Approximation (LOA)

- Φ-derivable self-energy
  - *"Self-Consistent Approximations in Many-Body System", G. Baym, Phy. Rev.* ***127****, 1391 (1962)*
  - In this paper, G. Baym already mentioned that ***"In the above proofs of the conservation laws we need not have required all the internal lines in Σ to be G(U)'s. They could also have been G_0(U)'s."***

Φ-derivable condition

$$\Sigma[G] = \frac{\delta\Phi[G]}{\delta G}$$

Σ =  $= DG$

Φ $= 1/2$  $= 1/2DGG$

1st iteration of SCBA

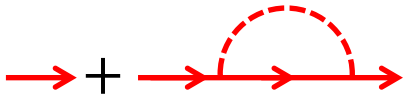
$$G = g_0 + g_0\Sigma[g_0]G$$

$$\Sigma[g_0] \neq \frac{\delta\Phi[G]}{\delta G}$$

Lowest Order Approximation (LOA)

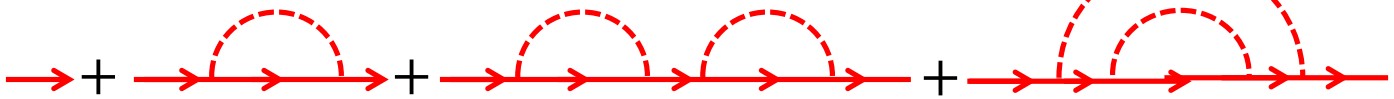
- **LOA**: Collecting only the conserving diagrams for each order
  - M. Paulsson et al. *Phys. Rev. B* **72**, 201101(R) (2005)

1st order LOA



$$g_1 = g_0 + g_0\Sigma[g_0]g_0 = g_0 + \boxed{g_0\Sigma_1\Delta g_0} \Rightarrow \Delta g_1$$

2nd order LOA



$$g_2 = g_1 + \boxed{g_0\Sigma_2\Delta g_0 + g_0\Sigma_1\Delta g_1} \Rightarrow \Delta g_2$$

Retarded(r)/advanced(a) notations suppressed

- Generalization of LOA algorithm

$$g_N = g_{N-1} + g_0 \sum_{n=0}^{N-1} (\Sigma_{N-n}\Delta g_n)$$

H. Mera *et al.*, *Phys. Rev. B* **88**, 075147 (2013).

LOA + Analytic Continuation

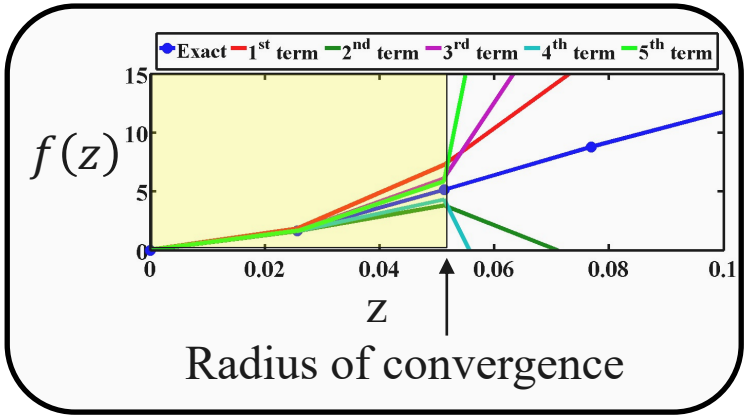
- **LOA series** : Converge or diverge depending on the scattering strength (the value of M)

$$g_0 + \Delta g_1(M) + \Delta g_2(M^2) + \cdots$$

LOA series

$$f(z) = \sum_{i=0}^{\infty} f_i z^i = f_0 + f_1 z + f_2 z^2 + \cdots$$

Power series



- **Pade Approximants** : Analytic function outside the radius of convergence

$$f(z) = f_0 + f_1 z + f_2 z^2 + \cdots + f_{l+m} z^{l+m} = \frac{l_0 + l_1 z + l_2 z^2 + \cdots + l_l z^l}{1 + m_1 z + m_2 z^2 + \cdots + m_m z^m}$$

LOA + Analytic Continuation

- **LOA**: Calculating only the first few orders
- **LOA + Padé approximant**: Simple, fast convergence for strong scattering

$$g_1 = g_0 + \Delta g_1 \Rightarrow I_1 = I_0 + \Delta I_1 \rightarrow I_{0/1}\ \text{(Padé 0/1)}$$

$$g_2 = g_1 + \Delta g_2 \Rightarrow I_2 = I_1 + \Delta I_2 \rightarrow I_{1/1}\ \text{(Padé 1/1)}$$

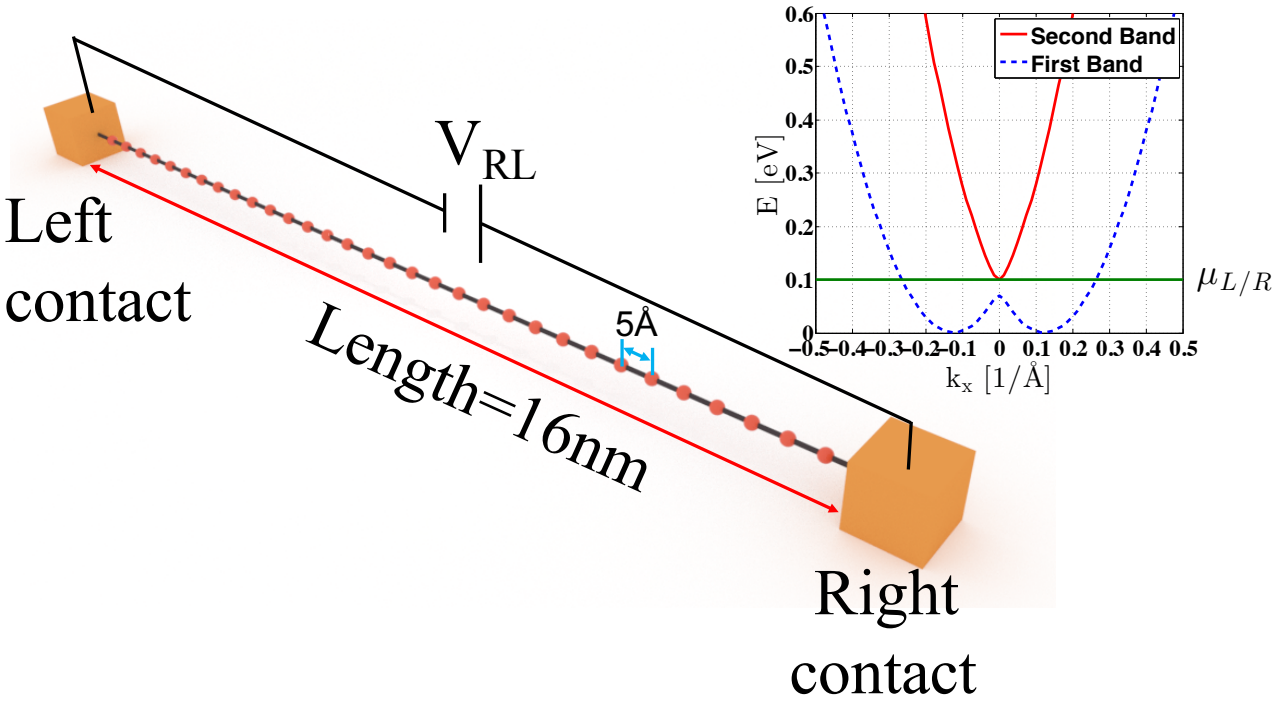
$$g_3 = g_2 + \Delta g_3 \Rightarrow I_3 = I_2 + \Delta I_3 \rightarrow I_{1/2}\ \text{(Padé 1/2)}$$

Padé Table

$$I_{l/m} = \begin{pmatrix} I_0 & I_0 + \Delta I_1 & I_0 + \Delta I_1 + \Delta I_2 \\ \dfrac{I_0}{1 - \Delta I_1/I_0} & \dfrac{I_0 + \Delta I_1 - I_0 \Delta I_2/\Delta I_1}{1 - \Delta I_2/\Delta I_1} & \cdots \\ \dfrac{I_0}{1 - \Delta I_1/I_0 + (\Delta I_1/I_0)^2 - \Delta I_2/I_0} & \vdots & \ddots \end{pmatrix}$$

1D linear chain simulation

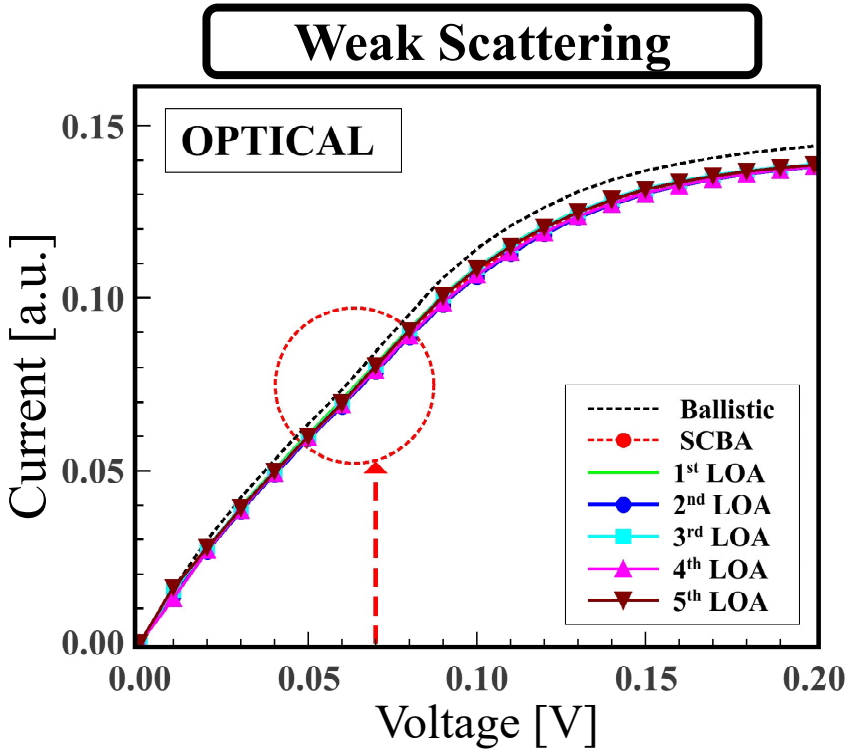
- Simulation Conditions
  - 2 Band **k·p** Hamiltonian – Strong inter-band coupling
  - V_{RL} is an applied bias, considering constant electric field
  - Optical phonon $\hbar\omega$ = 60 [meV], SCBA tolerance ~ 0.1%

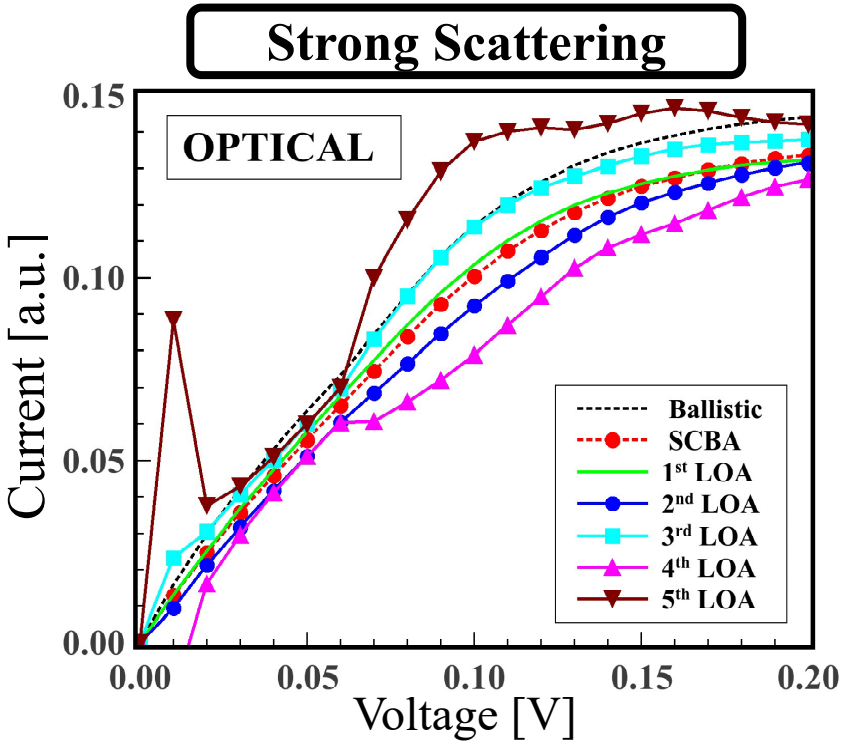


Y. Lee *et al.*, *Phys. Rev. B* **93**, 205411 (2016)

LOA Calculation – LOA current Series

- Optical Phonon Interaction
  - LOA series converge or diverge according to strength of scattering

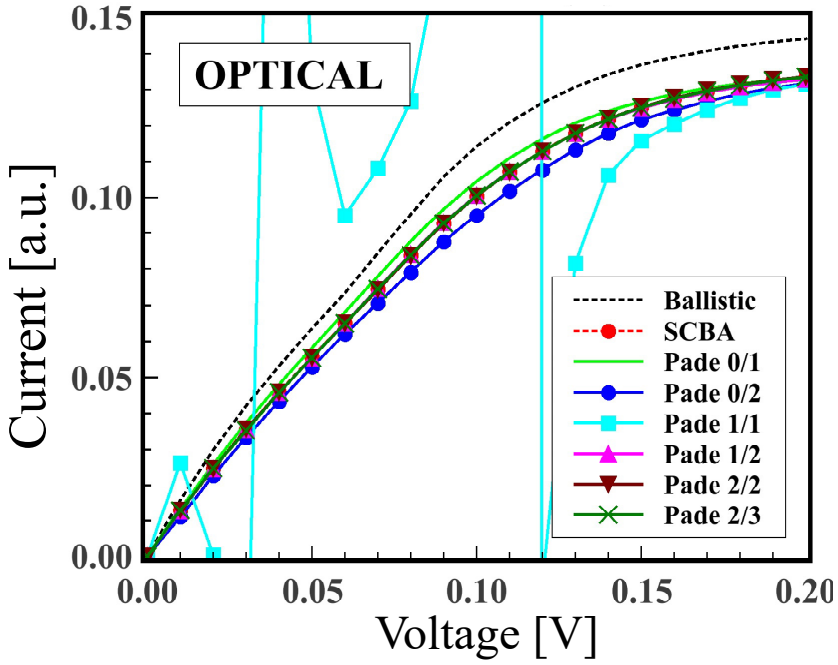




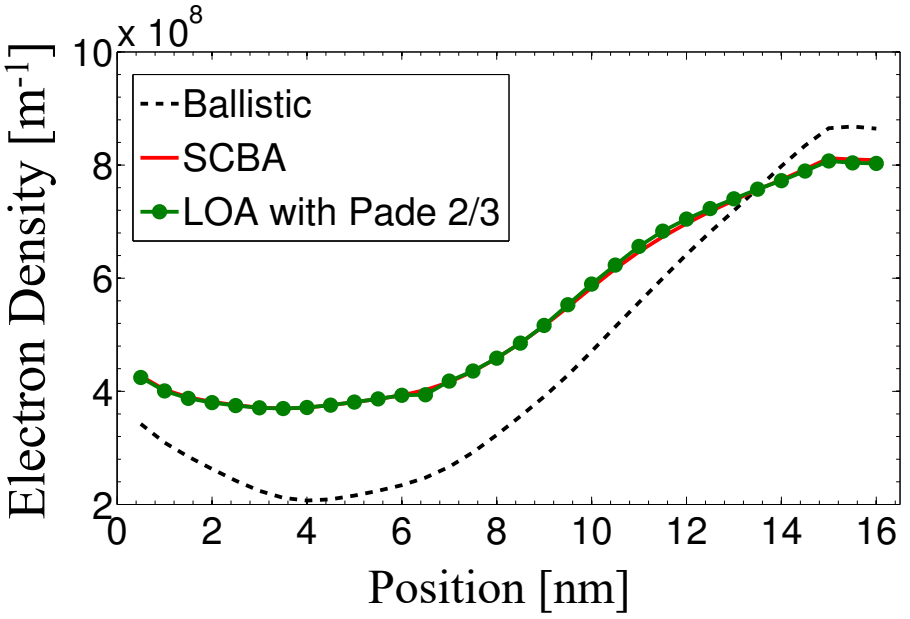
Padé calculation – Current and density

- Optical Phonon Interaction
  - Strong Scattering (Mop = 1×10^{-3} [eV^2])

Current - Voltage

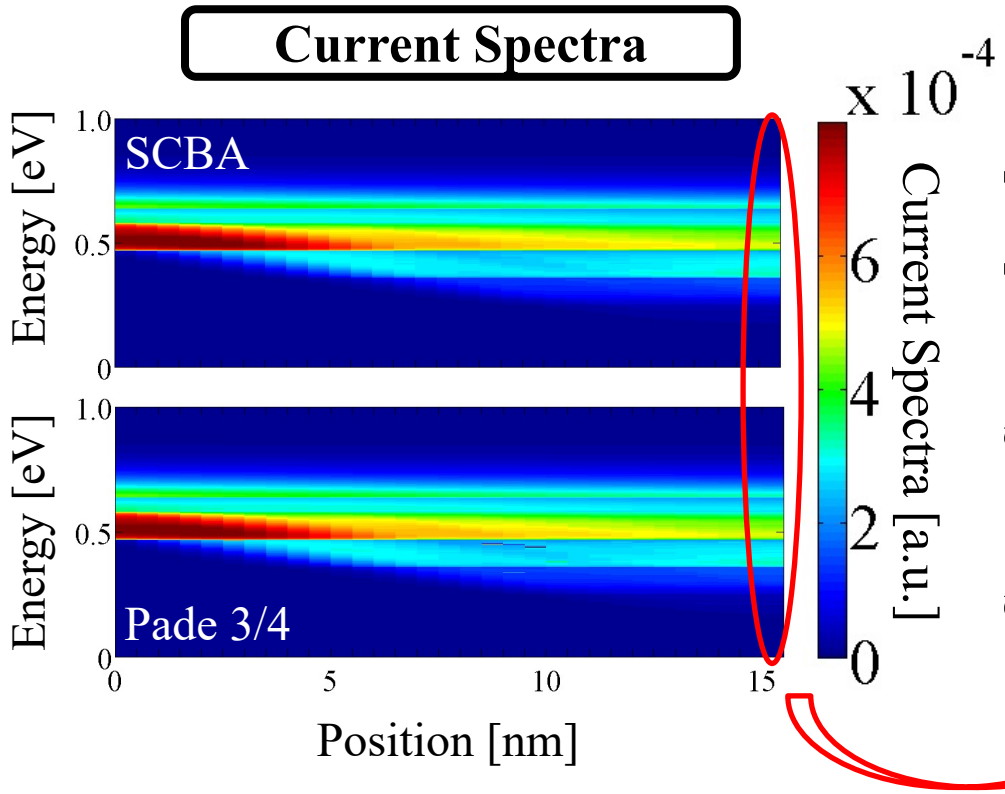


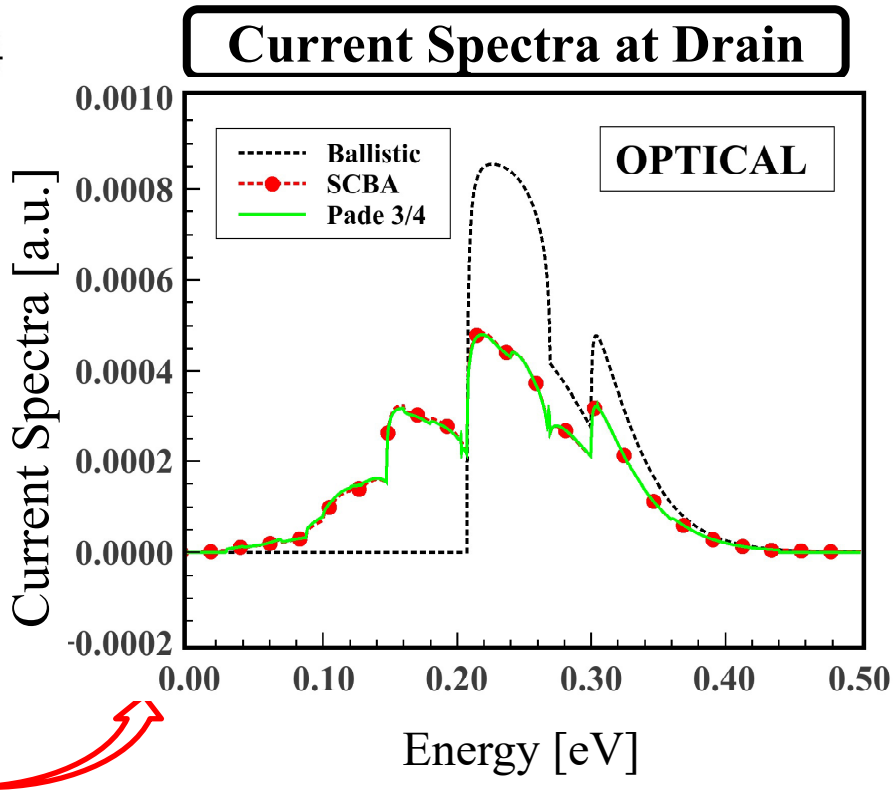
Electron Density



Padé calculation – Current spectra

- Optical Phonon Interaction
  - Strong Scattering (Mop = 1×10^{-3} [eV^2])

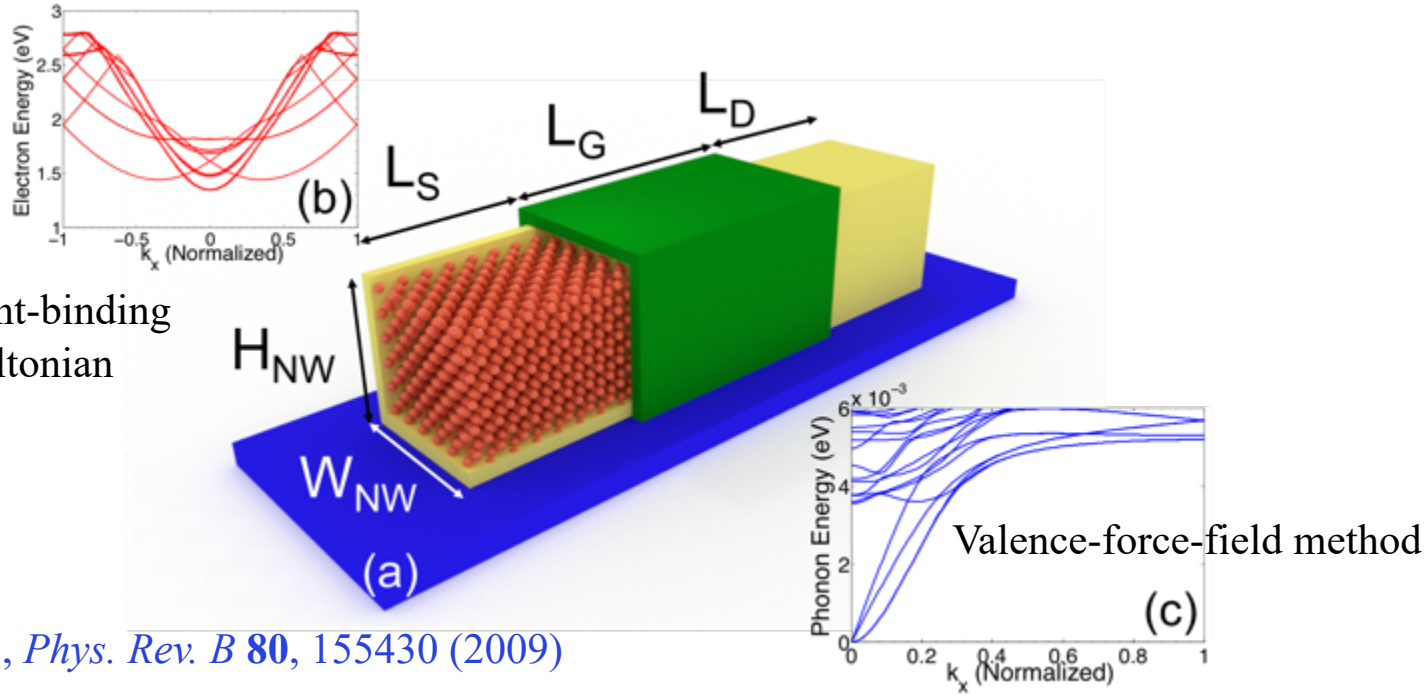




Application to 3D simulations

3D Nanowire Device simulations

- N-type Silicon Square Nanowire by OMEN (ETH Zurich)
  - <100> transport direction, L_S=L_D=9nm, L_G=13nm
  - 3 x 3 nm^2 cross section, Doping in S/D = 10^{20} cm^{-3}



Full-band tight-binding $sp^3d^5s^*$ Hamiltonian

Valence-force-field method

M. Luisier *et al.*, *Phys. Rev. B* **80**, 155430 (2009)

3D Nanowire Device simulations

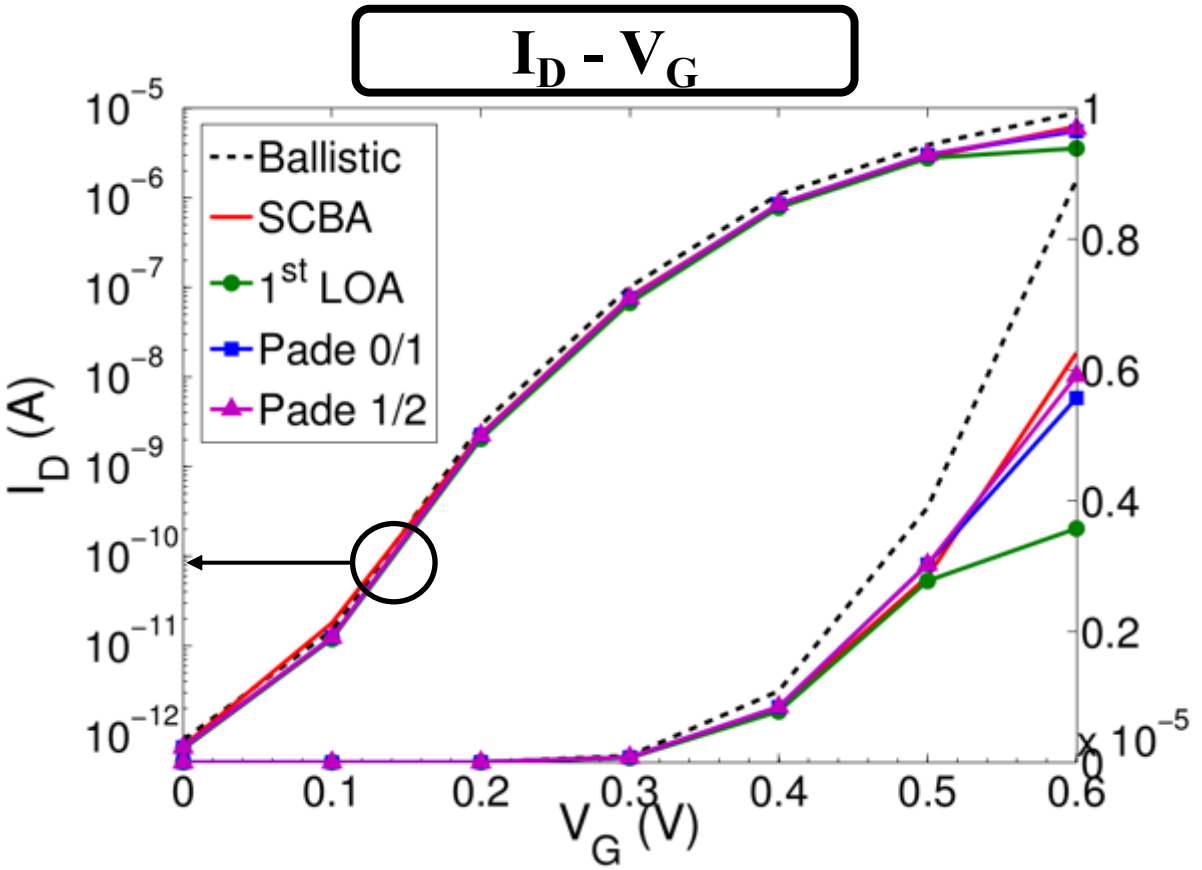
- N-type Silicon Square Nanowire
  - 1st LOA with Padé 0/1: **90% accuracy**, 3rd LOA with Padé 1/2: **95% accuracy**

N^{th} order currents

$$I_{NthLOA} = I_0 + \sum_{n=1}^{N} \Delta I_n$$

$$\Delta I_N = (\lambda_N)^N I_{NthLOA} - \sum_{n=0}^{N-1} (\lambda_N)^{N-n} \Delta I_n$$

$$\Delta I_0 = I_0$$



Y. Lee *et al.*, *Phys. Rev. B* **95**, 201412(R) (2017)

Anharmonic phonon-phonon scattering

Phonon transport based on NEGF

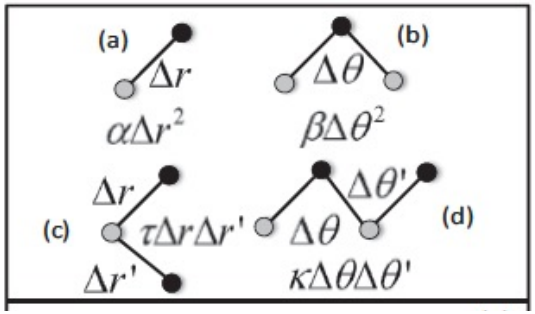
- NEGF for electrons: Schrödinger equation

$$(E\mathbf{I} - \mathbf{H})\overline{\psi} = \bar{0} \quad \Rightarrow \quad \left[G^R(E)\right]$$

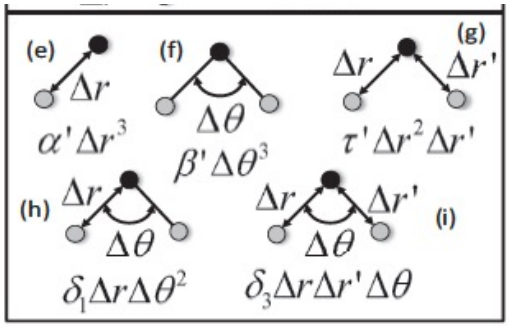
- NEGF for phonons: dynamical equation

$$\omega^2 \mathrm{M} + \Phi_{nm}^{ij} \bar{R} = \bar{O} \qquad \text{with} \qquad \Phi_{nm}^{ij} = \frac{\partial^2 V^{harm}}{\partial R_n^i \, \partial R_m^j}$$

Vibration frequency — Mass of the atoms (matrix) — Dynamical matrix — Displacement of the atoms



Harmonic



Anharmonic

M. Luisier *et al.*, *Phys. Rev. B* **86**, 245407 (2012)

Phonon-phonon interaction self-energy

- Anharmonic phonon NEGF methodology development

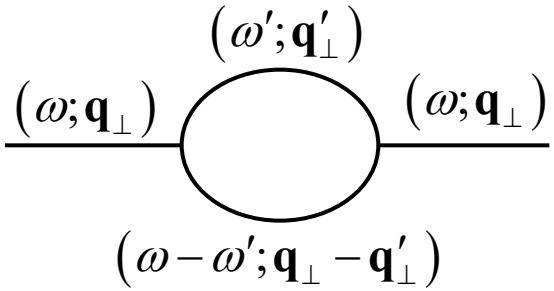
(1) Development of anharmonic NEGF formalism for 3D nanostructures

(2) Parallelized computational framework

(3) DFT (ab initio) input of both 2nd- and 3rd-order FCs

Greater/lesser scattering self energy matrix:

$$\Sigma_{ll'}^{<,>ij}(\omega;\mathbf{q}_\perp)=\frac{i\hbar}{2}\sum_{l_1l_2l_3l_4}\sum_{j_1j_2j_3j_4}\frac{1}{N}\sum_{\mathbf{q}'_\perp}\tilde{\Phi}_{ll_1l_2}^{ij_1j_2}(\mathbf{q}'_\perp,\mathbf{q}_\perp-\mathbf{q}'_\perp)\tilde{\Phi}_{l'l_3l_4}^{jj_3j_4}(\mathbf{q}'_\perp-\mathbf{q}_\perp,-\mathbf{q}'_\perp)$$
$$\times\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}G_{l_1l_4}^{<,>j_1j_4}(\omega';\mathbf{q}'_\perp)G_{l_2l_3}^{<,>j_2j_3}(\omega-\omega';\mathbf{q}_\perp-\mathbf{q}'_\perp)$$

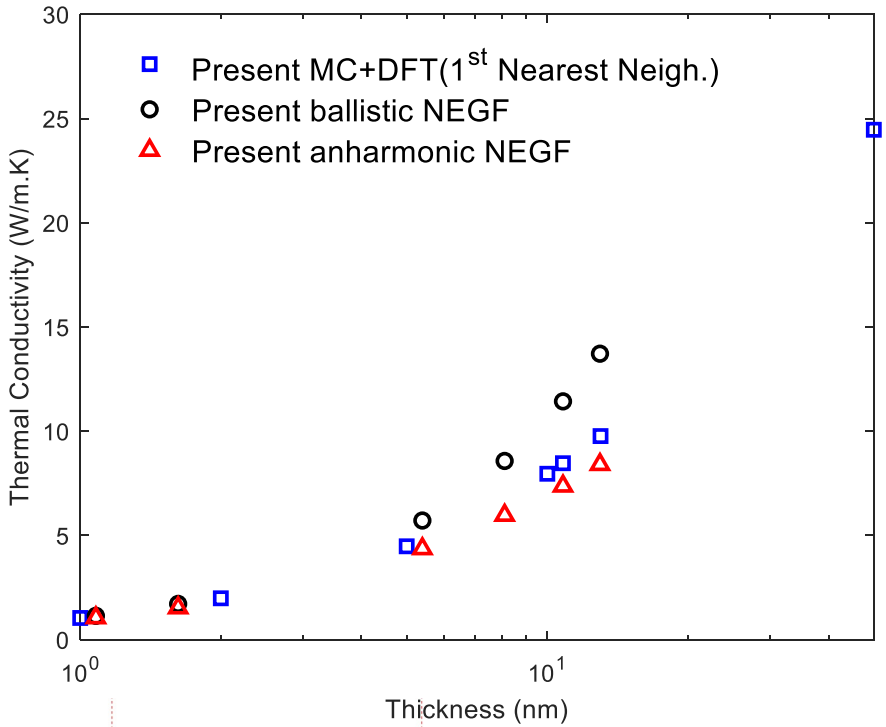


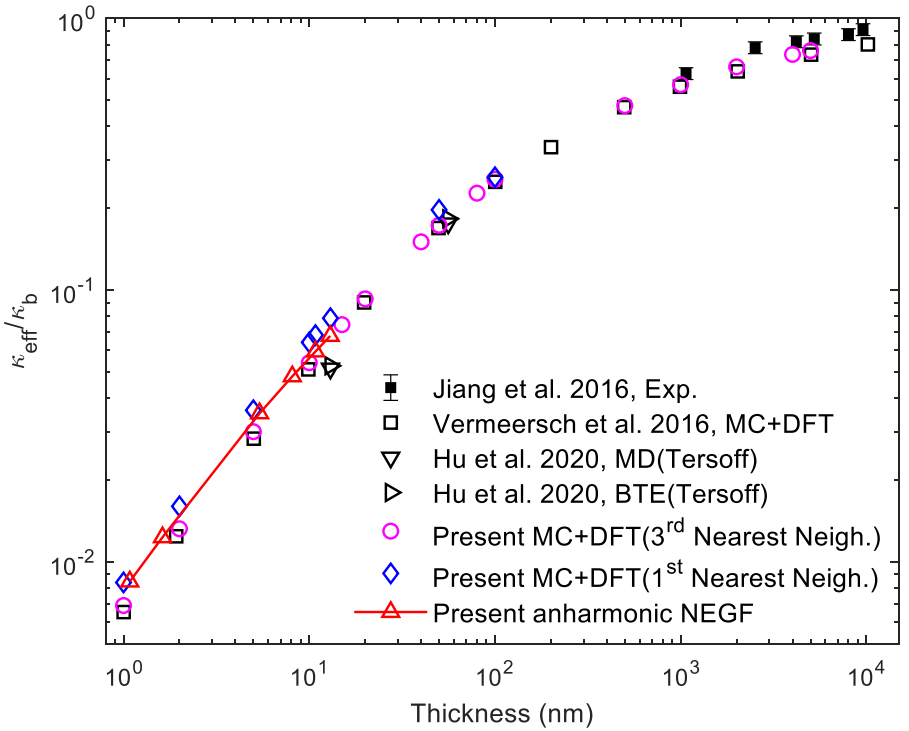
Phonon-phonon interactions: the anharmonic decay of a high-energy phonon (ω) into two lower energy phonons (ω-ω′ and ω′).

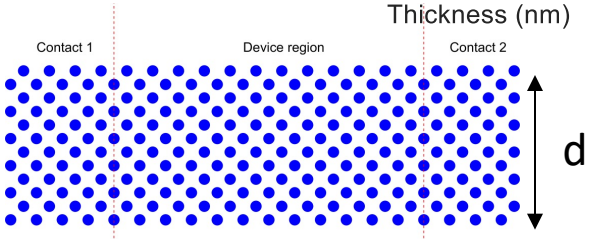
Y. Guo, M. Bescond, Z Zhang, M Luisier, M Nomura, S Volz, *Phys. Rev. B* **102**, 195412 (2020).

Phonon-phonon interaction self-energy

- Validation of the anharmonic phonon NEGF framework



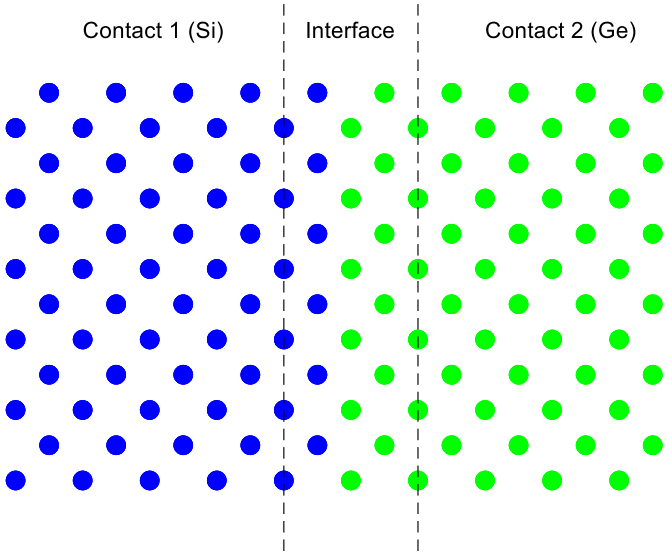




Cross-plane thermal conductivity of Si thin film at 300K

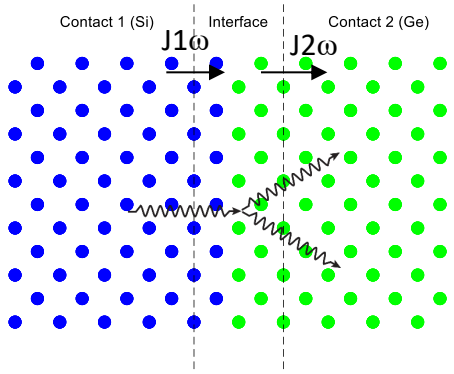
First NEGF code for phonons validated!

"Interfacial heat transport between Si/Ge”

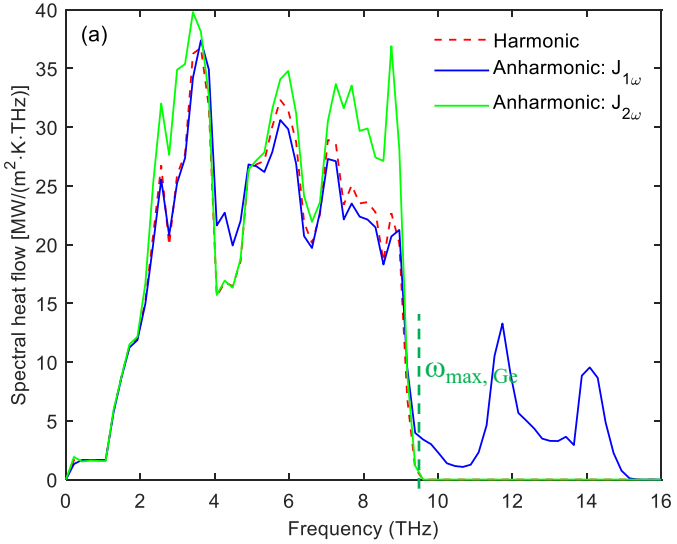


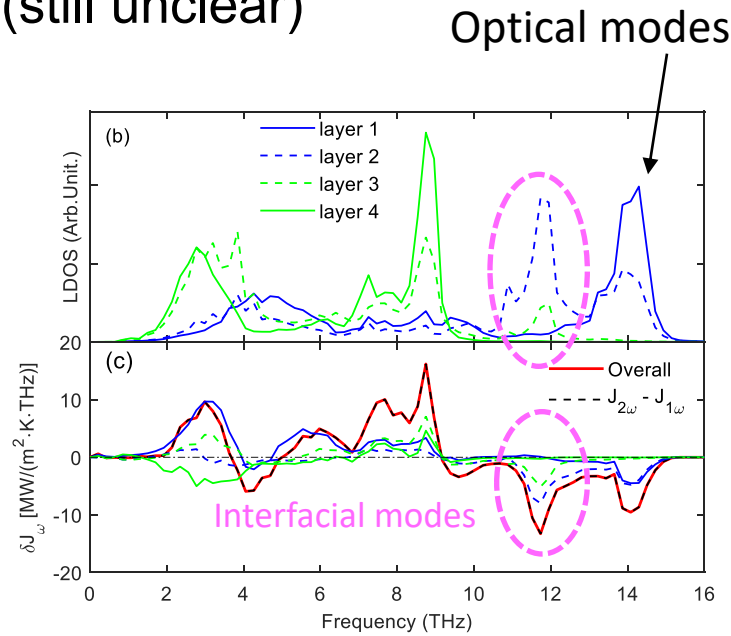
Phonon-phonon interaction self-energy

- Heat transport across smooth Si/Ge interface (still unclear)



Schematic of physical model



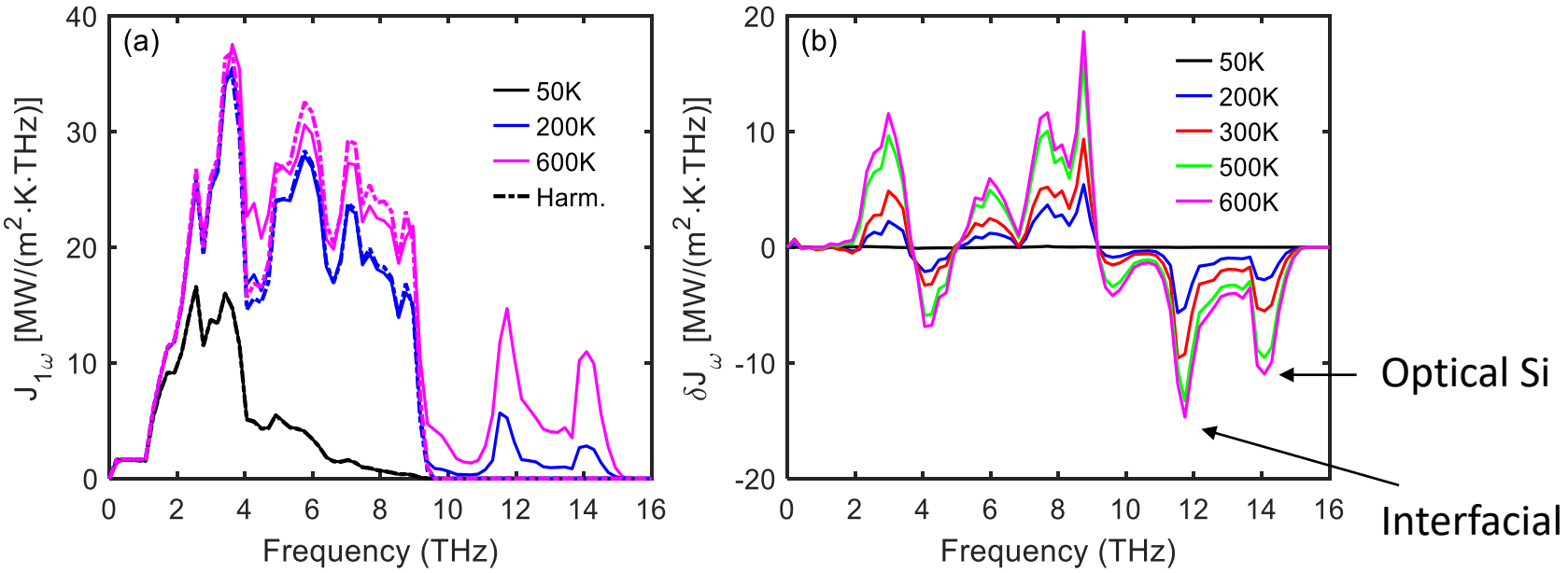


500 K

- An appreciable contribution of heat flux arises from Si phonons beyond the cut-off frequency of Ge phonons.
- Strong phonon annihilation in the intermediate two layers around 12 THz, which corresponds to the interfacial phonon modes.
- Around 14 THz: Decay of the optimal phonon modes in Si.

Y. Guo, Z. Zhang, M. Bescond, S. Xiong, M. Nomura, and S. Volz, *Phys. Rev. B* **103**, 174306 (2021).

Temperature dependence

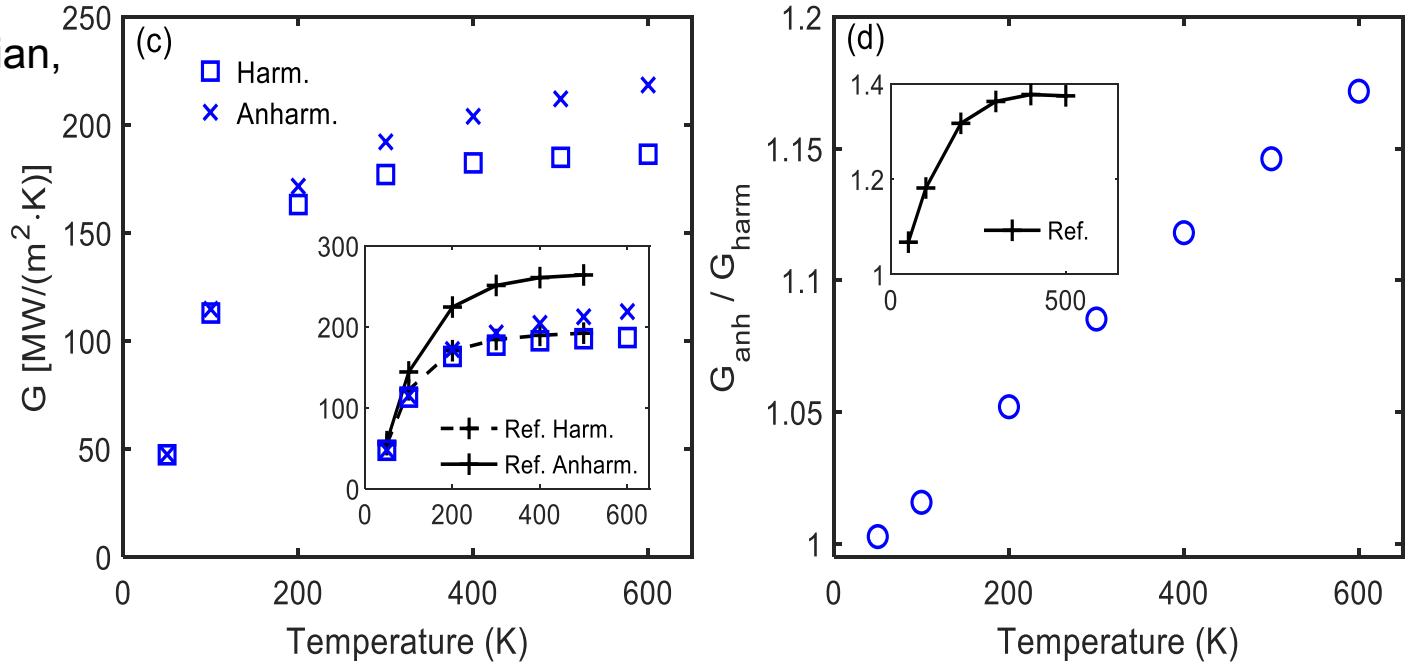


- Low T: anharmonic NEGF result coincides with the harmonic one (weak phonon-phonon scattering).
- Overall spectral energy exchange: amplitude of two dips in the high-frequency range (> 10 THz) gradually rises with temperature: decay of interfacial phonon modes and optical phonon modes.

Y. Guo, Z. Zhang, M. Bescond, S. Xiong, M. Nomura, and S. Volz, *Phys. Rev. B* **103**, 174306 (2021).

Temperature dependence

Ref.: Dai & Tian, PRB, 2020



- Thermal boundary conductance increases with temperature.
- Difference between the anharmonic result and the harmonic one also becomes larger at higher temperature.
- Enhancement of 10% at RT and reaches about 20% at 600 K.
- Appreciably smaller than the results in a very recent study of the same problem (Cornel).

Y. Guo, Z. Zhang, M. Bescond, S. Xiong, M. Nomura, and S. Volz, *Phys. Rev. B* **103**, 174306 (2021).

Energy based devices: Coupling between electron and phonon transport

Heat transport may impact electronic properties and vice-versa: thermoelectricity

Coupling between electron and phonon transport

- Option 1: coupling GFs of electrons and those of phonons.

  --> Self-energy of the electron-phonon coupling:

$$\Sigma^{\lessgtr}_{inel}(E) = M^2 \left[(n_L + 1)G^{\lessgtr}(E \pm \hbar\omega_L) + (n_L)G^{\lessgtr}(E \mp \hbar\omega_L)\right]$$

Replace the Bose-Einstein distribution (equilibrium) by the one of phonon Green's function

- Advantage : Full quantum simulations: physical properties of the both phonons and electrons in a non-equilibrium regime.

- Drawback : numerically very demanding (full band description (phonons=bosons) and the non-local treatment of anharmonic interactions).

➡ Applicable to relatively small systems (few nanometers)

R. Rhyner, M. Luisier, *Physical Review B* **89**, 235311 (2014)

Coupling between electron and phonon transport

- Option 2: coupling GFs of electrons and classical phonon transport.

NEGF equations for electrons

$$G^r = [(E - V)I - H - \Sigma_L^r - \Sigma_R^r - \Sigma_{inel}^r]^{-1}$$

Heat equation

$$-\nabla \cdot (\kappa_{\text{th}} \nabla T_{\text{ac}}) = Q \left[G^{\gtrless}(T_{ac}, T_{op}) \right]$$

$$\Sigma_{inel}^{\lessgtr}(E) = M^2 \left[(n_L + 1) G^{\lessgtr}(E \pm \hbar\omega_L) + (n_L) G^{\lessgtr}(E \mp \hbar\omega_L) \right]$$

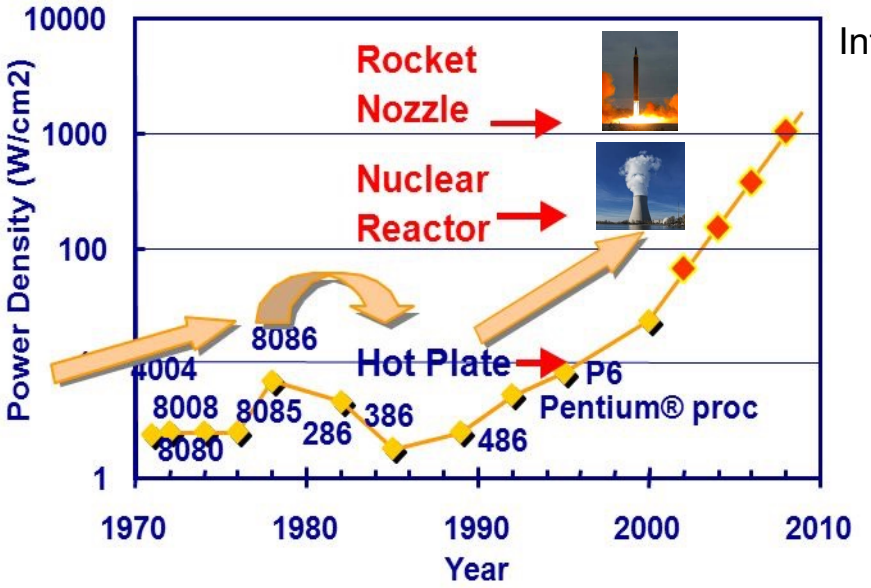
- Advantage : can treat devices of several hundred of nanometers.

- Drawback : only provides the rigorous physical properties of electrons (validity of heat equation at the nanometer scale?)

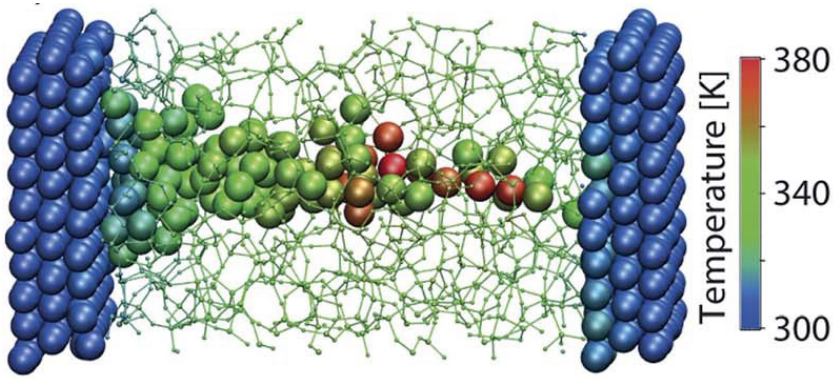
*M. Bescond *et al. J. Phys.: Condens. Matter* **30**, 064005 (2018).
** M. Moussavou *et al."Phys. Rev. Appl.* **10**, 064023 (2018).

Cooling at the nanoscale

- **Self-heating: scientific and industrial issues**



Intel, 2004



CBRAM

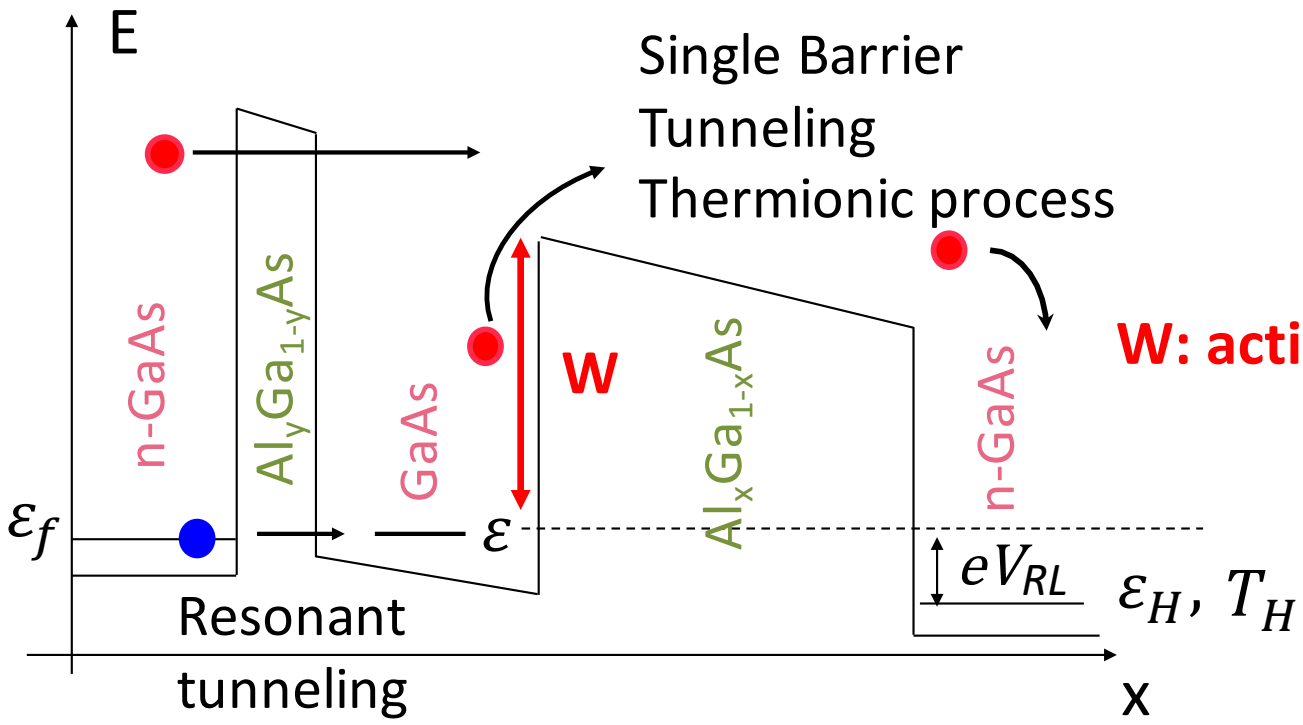
Nanoscale Adv., **2,** 2648 (2020)
Courtesy M. Luisier, ETH Zurich

- Significant reduction of lifetimes and performances.
- "Bulk" refrigeration is extremely power consuming.

Urgent need of local source of cooling

Original thermionic cooling devices

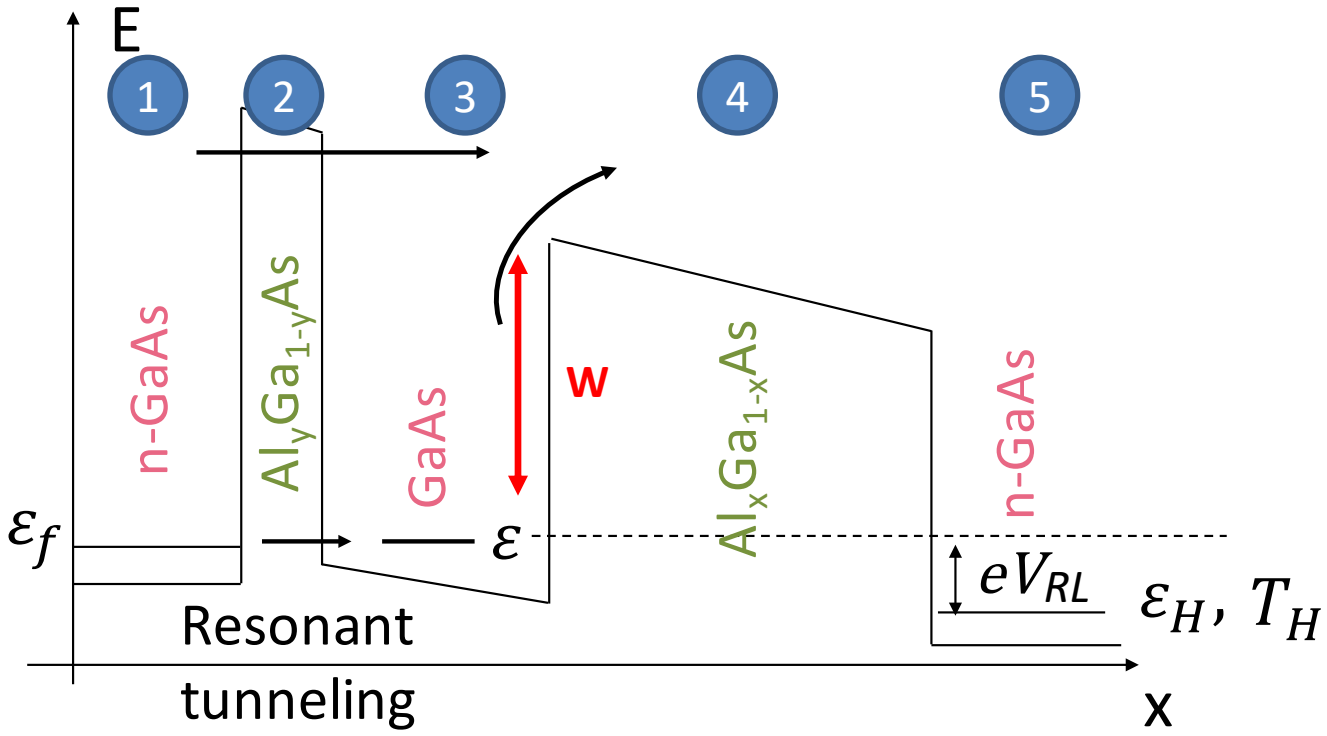
- Coupling localized state and tunneling barrier*:



- Main idea: injecting cold electrons and extracting hot electrons.
- Investigate the concept of local temperature at the nanoscale.

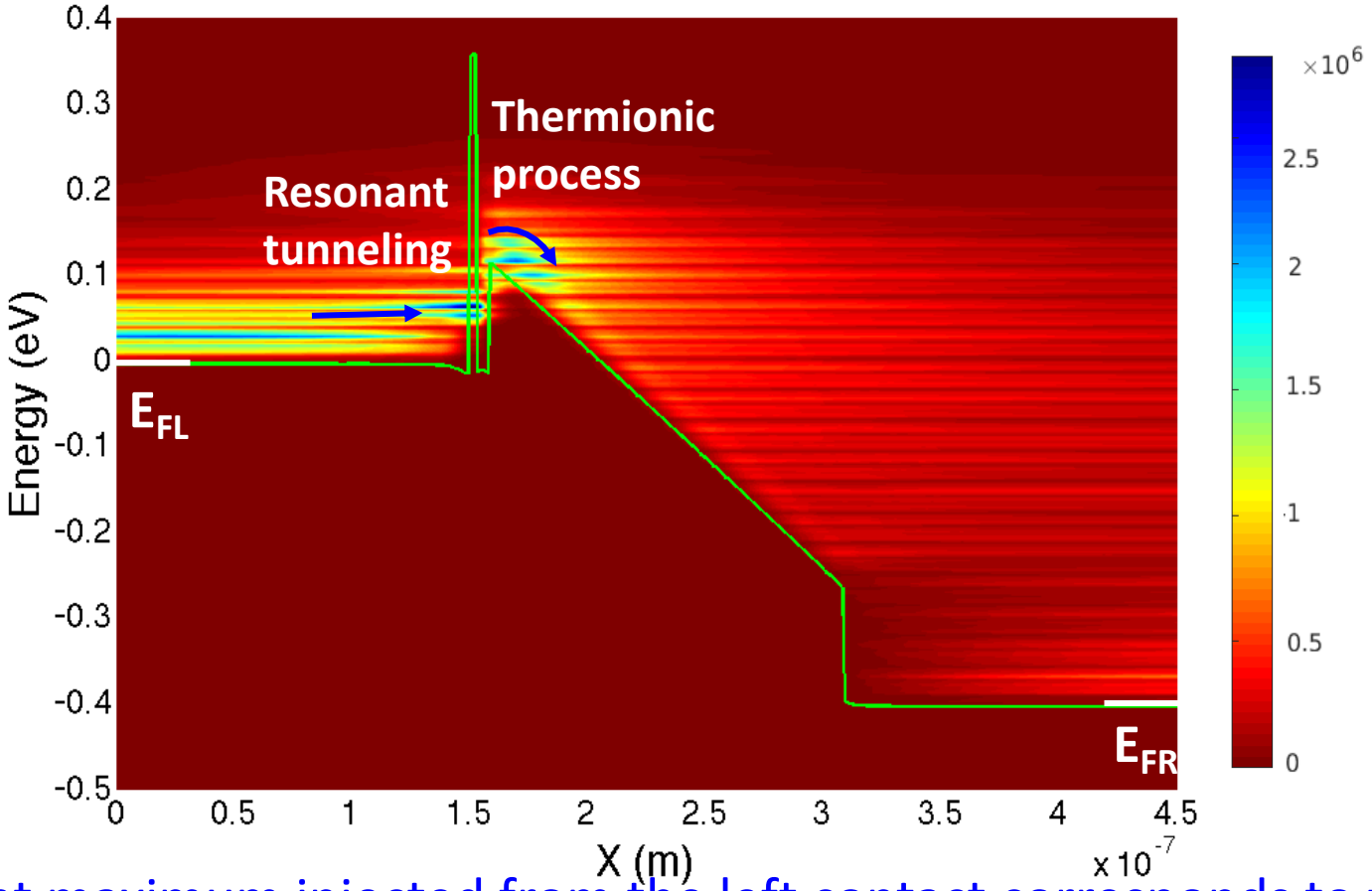
*K. A. Chao, M. Larsson, and A. G. Mal'shukov, *Appl. Phys. Lett.*, **87**, 022103 (2005).

First Structure



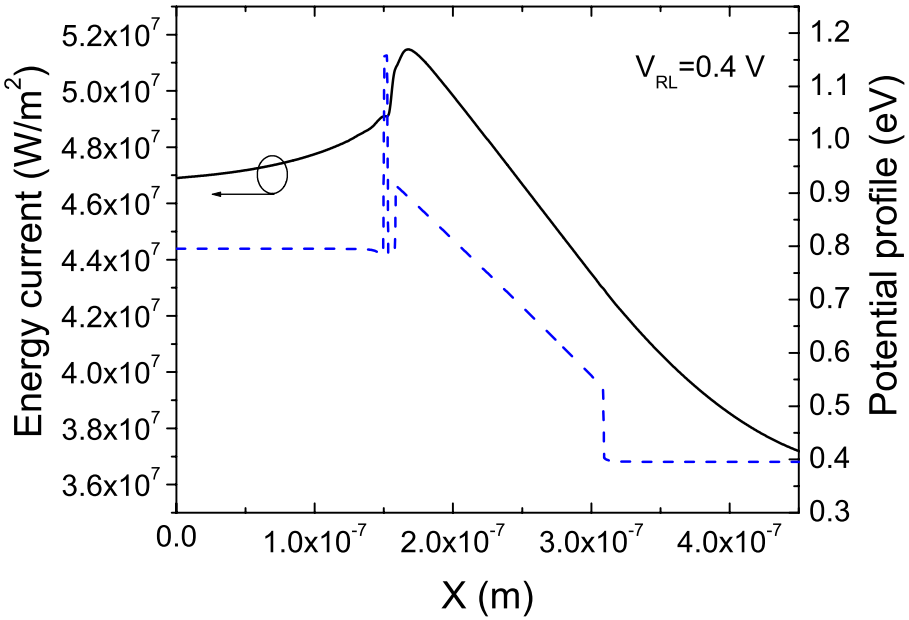
- The device is defined by 5 regions (see figure):
  - 1: n-GaAs – Doping: $N_D=10^{24}$ m^{-3} – L_1=150 nm.
  - 2: $Al_{0.3}Ga_{0.7}As$ – Doping: $N_D=10^{21}$ m^{-3} – L_2=2.3 nm.
  - 3: n-GaAs – Doping: $N_D=10^{21}$ m^{-3} – L_3=5 nm.
  - 4: $Al_{0.12}Ga_{0.88}As$ – Doping: $N_D=10^{21}$ m^{-3} - L_4=150 nm.
  - 5: n-GaAs – Doping: $N_D=10^{24}$ m^{-3} – L_5=150 nm.

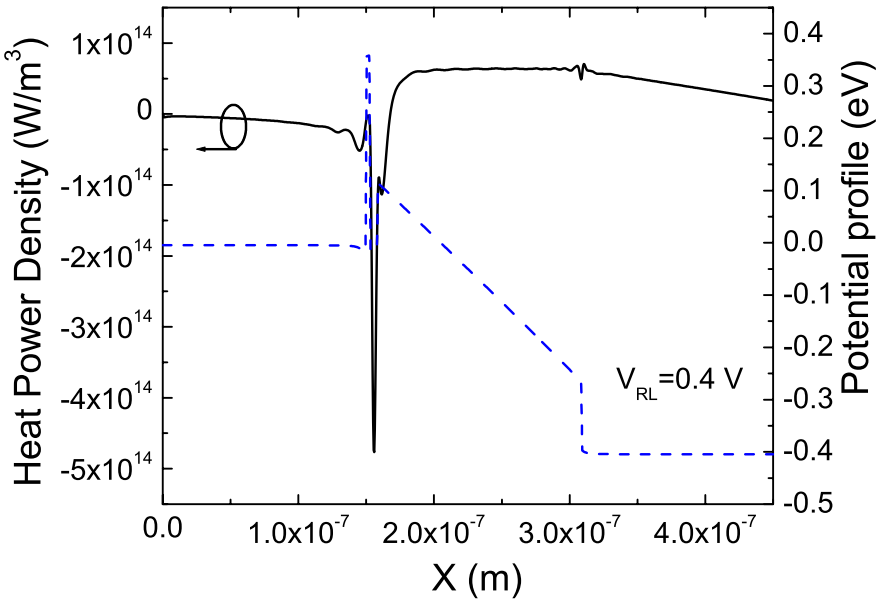
Current spectrum - T=300 K – V_{RL}=0.4 V



- Current maximum injected from the left contact corresponds to the quantum-well state (tunnel injection).
- Current is also important above the $Al_xGa_{1-x}As$ region: thermionic component.

Heat power density Q



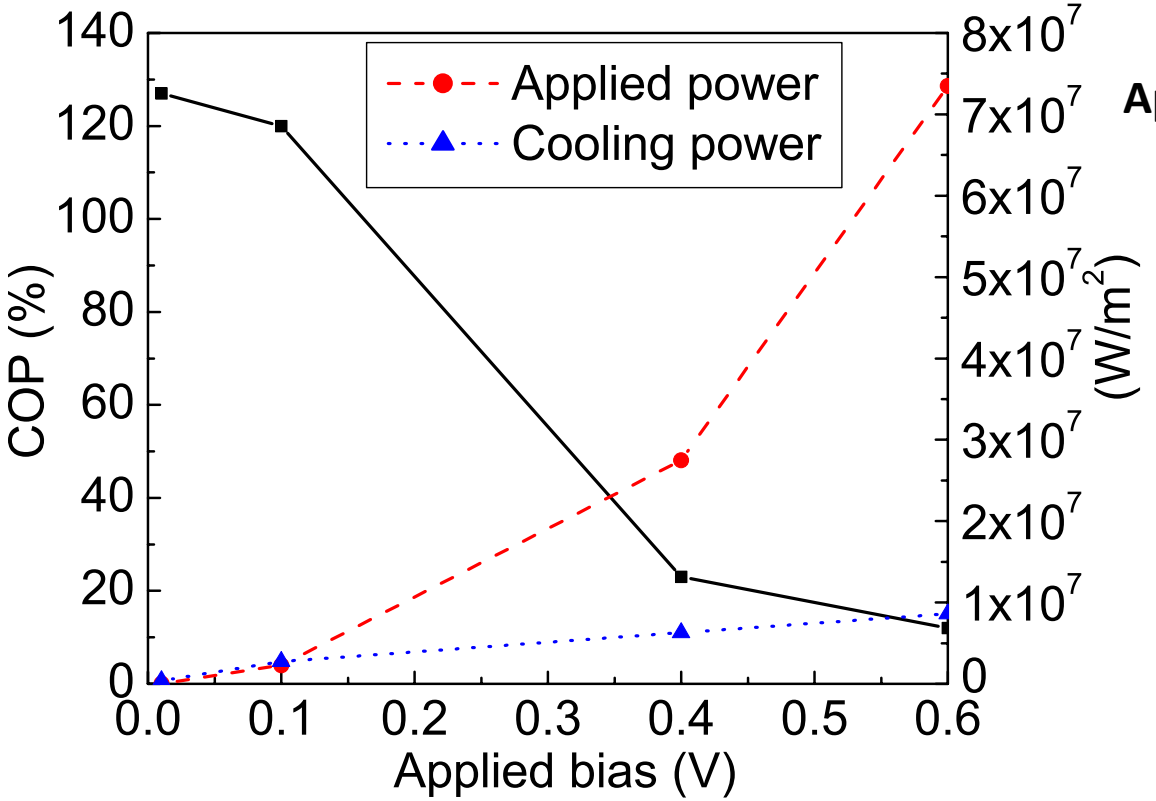


$$I_E(x) = \int_{-\infty}^{+\infty} E.I(x,E)dE \quad \Rightarrow \quad Q(x) = -\nabla_x . I_E(x)$$

Energy current — Carrier current spectrum — Heat power density

- Heat Power Density defines heat power transferred locally to the lattice.
  Q>0 --> Energy transfers to phonon bath – Q<0 --> heat transfers to electrons

Coefficient Of Performance - COP



Applied power=V_{RL}.I

- Cooling power increases with the applied bias, but...
- COP (=Cooling power/Appl. power) presents the opposite feature.
- **COP can be larger then 100% !!**

M. Bescond and K. Hirakawa, *Phys. Rev. Appl.* **14** (6), 064022 (2020).
A. Yangui, M. Bescond, T. Yan, N. Nagai, and K. Hirakawa, *Nature Commun.* **10**, 4504 (2019).

Conclusion

- NEGF formalism provides most of the physical internal (LDOS) and external (current, electron density) properties of the system.
- Initially developed for electronic transport.
- Concept of self-energy: allows to describe many types of inelastic interactions (e-phonon, e-photon).
- Usual technique: Self-consistent Born approximation (SCBA)
- SCBA: numerically demanding --> direct approaches (LOA)
- NEGF can also be applied to solve transport of phonons
- Coupling transport of electrons and phonons: energy devices (thermoelectricity, solar cells…)

→ Future work: e-e interactions, include higher order anharmonic phonon scattering, numerical improvements.

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Now at ETH Zurich

Pr. N. Cavassilas

Dr. F. Michelini

Dr. A.-M. Daré

Pr. M. Lannoo

LIMMS at the University of Tokyo:

Phonon transport

Dr. Y. Guo

Now at the University of Lyon

Dr. Z. Zhang

Pr. S. Volz

Pr. M. Nomura

Refrigeration

Pr. K. Hirakawa

Dr. C. Salhani

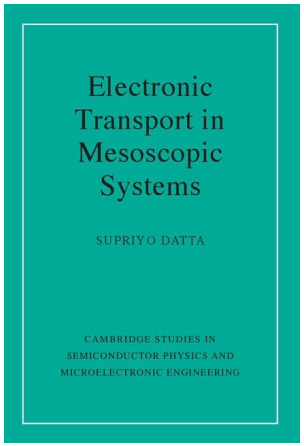
Mr. X. Zhu

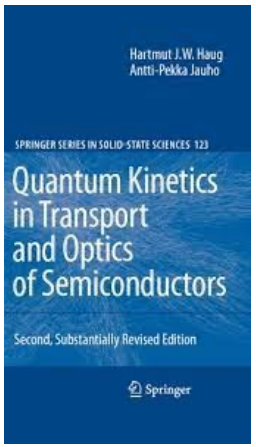
Deeper analysis on NEGF

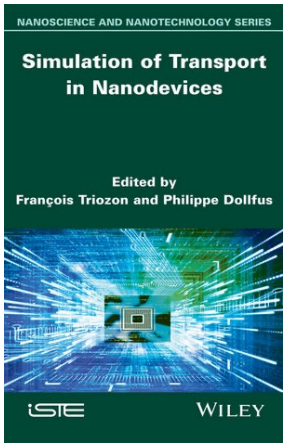
- S. Datta, “Electronic Transport in Mesoscopic Systems”, Cambridge university press.

- H. Haug & Jauho, “Quantum Kinetics in Transport and Optics of Semiconductors”, Springer.

- Book chapter on NEGF : M. Lannoo and M. Bescond Edited by F. Triozon, P. Dollfus, “Simulation of Transport in Nanodevices”, Wiley.







Thank you!

*e-mail: marc.bescond@im2np.fr