Heat transport in hybrid nanosystems using the atomistic Green's functions

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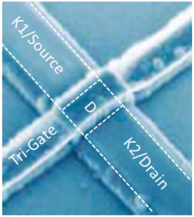
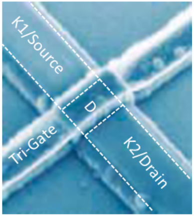
Introduction: hybrid systems and heat transport



- Contact 1/2: open, classical treatable, thermodyn. reservoirs with constant temperatures $T_{1/2}$, diffusiv transport
- Device: ideal nanocrystal structure, quasi-ballistc transport, interface scattering, scattering theory, quantum mechanics

Introduction: transport of phonons



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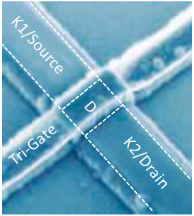

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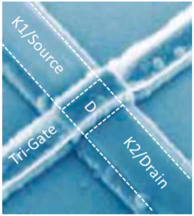

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- So heterogeneous structures and associated interface effects play a central part.
- On this nanometre scale the wave nature of phonons becomes more important.

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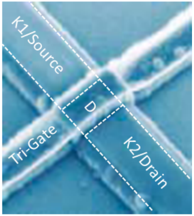

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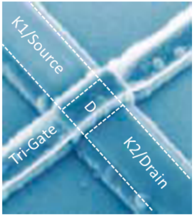

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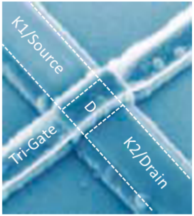
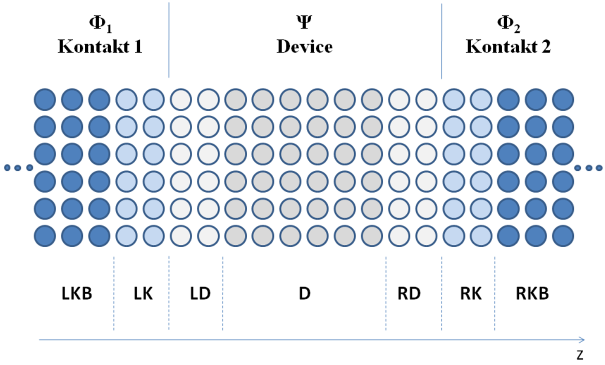


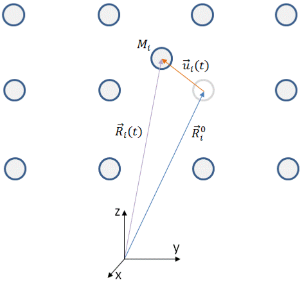
- In this case, the classical approaches are rather not qualified.
- We have quasi ballistic transport with interface scattering.
- This phenomena, we can describe with the method of the atomistic Green's functions (AGF).

Model of a contact-device-contact-structure



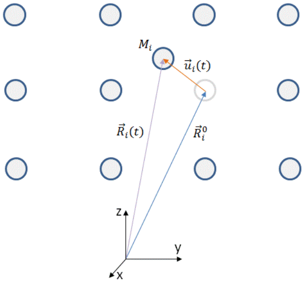
- N-atomic structure divided into diverse substructures.
- d degrees of freedom per atom.

Harmonic Matrix



- The AGF-Formalism is based on a harmonic or dynamic matrix.

Harmonic Matrix



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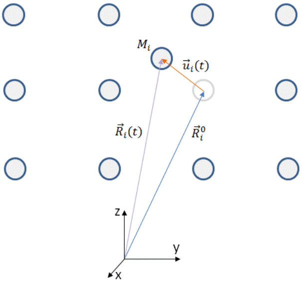

- The AGF-Formalism is based on a harmonic or dynamic matrix.
- We use a harmonic approximation of the crystal potential $U(\underline{R}(t))$.
- For device length less than 20 nm are anharmonic effects at room temperature negligible.

Harmonic matrix

- For the total potential in harmonic approximation we can also write:

$$U(\underline{u}(t)) = \frac{1}{2} \sum_{p,q=1}^{Nd} \left(\frac{\partial^2 U}{\partial R_p \partial R_q} \right)_{\underline{R}^0} u_p(t) u_q(t).$$

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- It is: $U(\underline{R}^0) := 0$ and $\vec{\nabla} U(\underline{R})|_{\underline{R}^0} = 0$.
- We define the harmonic matrix:

$$\Phi_{p,q} := \left(\frac{\partial^2 U}{\partial R_p \partial R_q}\right)_{\underline{R}^0}.$$

Dynamic matrix and the eigenvalue problem

- Equation of motion for every degree of freedom u_i:

$$M_i \frac{d^2}{dt^2} u_i(t) = -\frac{\partial U(\underline{u})}{\partial u_i} = -\sum_{j=1}^{Nd} \Phi_{i,j} u_j(t).$$

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- Here we have the dynamic matrix $[D]$ (real, symmetric and positiv definite) with:

$$[D]_{i,j} = D_{i,j} = \frac{\Phi_{i,j}}{\sqrt{M_i M_j}}.$$

The Green´s function / Green´s matrix

- Consider following equation where $\widehat{L}$ represents a linear operator in matrix notation and S represents a perturbation:

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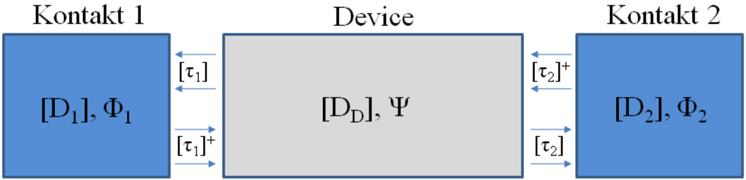
- The last equation provides us a important relation:

$$[G] := [\widehat{L}_\Psi]^{-1} \quad \Leftrightarrow \quad [\widehat{L}_\Psi][G] = [I].$$

The modified eigenvalue problem

- The eigenvalue problem (1) can be written down in a structured and simple modified form:

$$\begin{bmatrix} [(\omega+i0^+)^2E-D_1] & -[\tau_1]^+ & [0] \\ -[\tau_1] & [\omega^2E-D_D] & -[\tau_2] \\ [0] & -[\tau_2]^+ & [(\omega+i0^+)^2E-D_2] \end{bmatrix} \begin{Bmatrix} \Phi_1 \\ \Psi \\ \Phi_2 \end{Bmatrix} = \begin{Bmatrix} S_1^R \\ 0 \\ S_2^R \end{Bmatrix}$$



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- With matrix algebra we get:

$$\boxed{([\omega^2 E - D_D] - [\Sigma_1(\omega)] - [\Sigma_2(\omega)])\Psi(\omega) = S(\omega).} \qquad (2)$$

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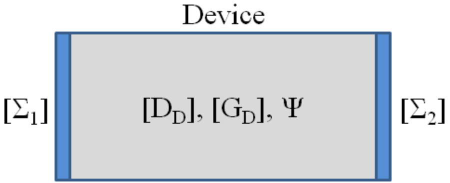
  - $[g_{1/2}(\omega)]=[(\omega+i0^+)^2E-D_1]^{-1}$
  - $S(\omega)=S_1(\omega)+S_2(\omega)=[\tau_1]\Phi_1^R(\omega)+[\tau_2]\Phi_2^R(\omega)$

The closed problem



- The green´s matrix of the device can be defined by equation (2):

$$\boxed{[G_D(\omega)] := [\omega^2 E - D_D - \Sigma_1(\omega) - \Sigma_2(\omega)]^{-1}.}$$

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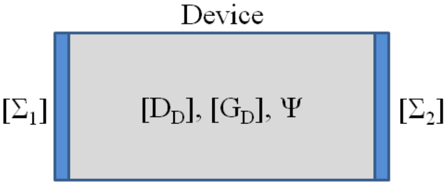

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- $[G_D]$ leads finily to the device solution Ψ with

$$\Psi = [G_D]S.$$

Total current and thermal conductance

- The current in the AGF-Formalism is given in a typical Landauer form:

$$\boxed{J(T_1, T_2) = \int_0^\infty \frac{\hbar\omega}{2\pi} \Xi(\omega)[N(\omega, T_1) - N(\omega, T_2)]d\omega.}$$

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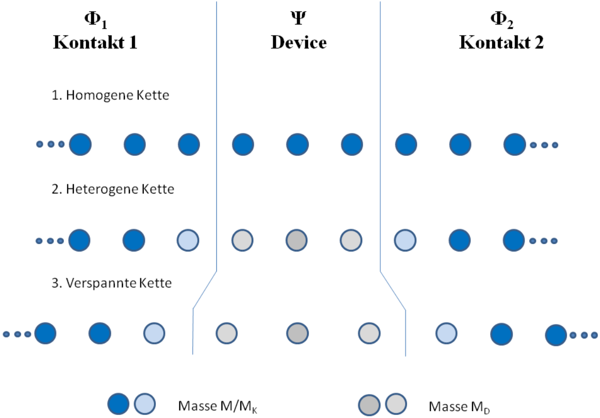
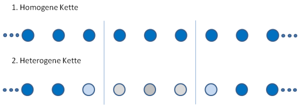
- Finaly the thermal conductance λ is given by:

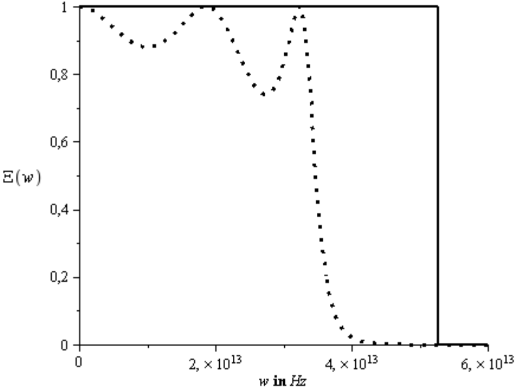
$$\lambda(T_1, T_2) = \frac{J(T_1, T_2)}{\Delta T}, \quad \Delta T = T_1 - T_2.$$

Thermal conductance of the homogeneous chain



Transmission: homogeneous vs heterogeneous chain





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- The thermal conductance λ_h of the homogeneous chain is

$$\lambda_h(T_1, T_2) = \frac{J_h(T_1, T_2)}{\Delta T} = \int_0^{2\omega_0} \frac{\hbar\omega}{2\pi} \frac{[N(\omega, T_1) - N(\omega, T_2)]}{\Delta T} d\omega.$$

Linear Approximation of $[N(\omega, T_1) - N(\omega, T_2)]$

- For $\Delta T \to 0$ we can expand $N(\omega, T_2)$ in a series with

$$
\begin{aligned}
N(\omega, T_2) &= N(\omega, T_1 + \Delta T) = \frac{1}{e^{\frac{\hbar\omega}{k_B(T_1+\Delta T)}} - 1} \\
&\approx N(\omega, T_1) + \frac{\hbar\omega}{k_B T_1^2} \frac{e^{\frac{\hbar\omega}{k_B T_1}}}{\left(e^{\frac{\hbar\omega}{k_B T_1}} - 1\right)^2} \Delta T.
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- In this equation we have replaced T_1 by T.

Parameterization of $\lambda_h(T)$

- Now we define the two dimensionless parameters:

$$\beta := \frac{T}{T_c} \quad \text{with} \quad T_c := \frac{\hbar\omega_0}{k_B} \quad \text{and} \quad x := \frac{\omega}{\omega_0}.$$

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- With this settings, we can write:

$$\lambda_h(\beta) = \frac{1}{2}\lambda_\infty \int_0^2 \frac{x^2 e^{\frac{x}{\beta}}}{\beta^2 \left(e^{\frac{x}{\beta}} - 1\right)^2} dx.$$

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- In this equation is $\lambda_\infty = \frac{k_B \omega_0}{\pi}$ the thermal conductance of a homogeneous chain for $T \to \infty$.

Final formula for the thermal conductance $\lambda_n(\beta)$

- Finally we normalize λ_h by λ_∞ and integrate over x and so we get:

$$\boxed{\lambda_n(\beta) = -\frac{2}{\beta}\left(1 - e^{-\frac{2}{\beta}}\right)^{-1} - \beta \text{dilog}(e^{\frac{2}{\beta}}).}$$

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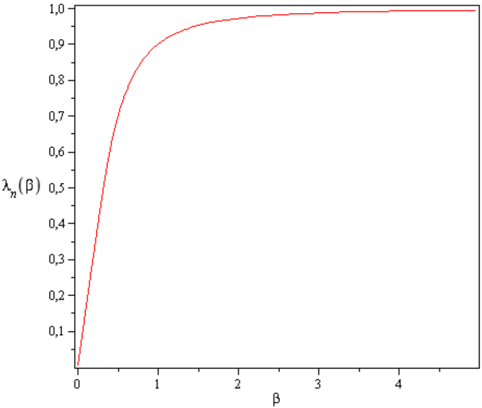
- In this dimensionless equation we have the Dilogarithm Function with the special definition:

$$\mathrm{dilog}(t) := \int_1^t \frac{\ln(s)}{1-s} ds.$$

Graphical representation of $\lambda_n(\beta)$



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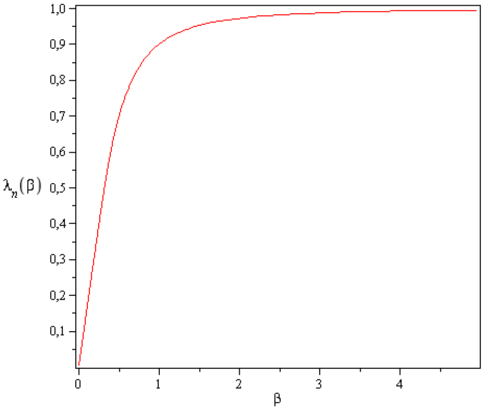

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- The characteristic point of change is given by $\beta = 1$ or $T = T_c$.

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1. For small β we need a asymptotic series expansion and we get:

$$\lambda_n(\beta) \approx \frac{1}{6}\pi^2\beta - (2+\beta)e^{-\frac{2}{\beta}}.$$

Approximations for $\lambda_n(\beta)$

- We have seen that there exist two interesting cases:
  1. $\lambda_n(\beta) \propto \beta$ for small β,
  2. $\lambda_n(\beta) = 1$ for great β.
- Now we want analyze this two cases.

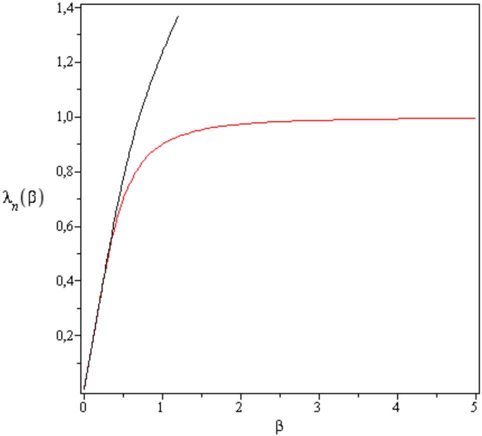
1. For small β we need a asymptotic series expansion and we get:

$$\lambda_n(\beta) \approx \frac{1}{6}\pi^2\beta - (2+\beta)e^{-\frac{2}{\beta}}.$$

2. For great β we need a laurent series expansion and we get:

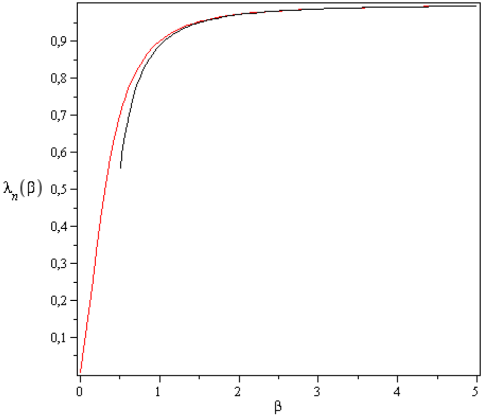
$$\lambda_n(\beta) \approx 1 - \frac{1}{9\beta^2}.$$

Graphical representation of $\lambda_n(\beta)$ for small β



- Black Line: $\lambda_n(\beta) \approx \frac{1}{6}\pi^2\beta - (2+\beta)e^{-\frac{2}{\beta}} = \lambda_0^0(\beta) + \lambda_1^0(\beta)$.

Graphical representation of $\lambda_n(\beta)$ for great β



- Black Line: $\lambda_n(\beta) \approx 1 - \frac{1}{9\beta^2} = \lambda_0^\infty(\beta) + \lambda_1^\infty(\beta)$.

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$$\epsilon_0 = \frac{(2+\beta)e^{-\frac{2}{\beta}}}{\frac{1}{6}\pi^2\beta} \quad \Rightarrow \quad -\frac{2}{\beta}e^{-\frac{2}{\beta}} = e^{-\frac{2}{\beta}} - \frac{1}{6}\epsilon_0\pi^2\beta.$$

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- This special equation is solved by the LambertW function, it is:

$$\beta_0 = -\frac{2}{\mathrm{LambertW}(-\frac{\epsilon_0\pi^2}{6e}) + 1} .$$

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- Silicon with $f = 32N/m$, $M = 4.6e-26kg$ and $\epsilon = \epsilon_0 = \epsilon_\infty = 0.01$:

$$T_c \approx 200K, \quad T_0 = \beta_0 T_c \approx 66K, \quad T_\infty = \beta_\infty T_c \approx 670K.$$