Implementación de simuladores realistas de dispositivos DG-MOSFET a nanoescala en plataformas de altas prestaciones

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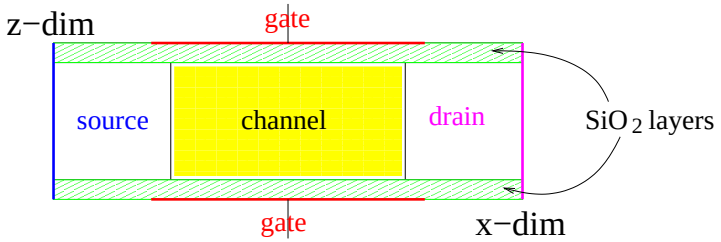
Outline

Outline

Geometry

We afford the simulation of a nanoscaled MOSFET.



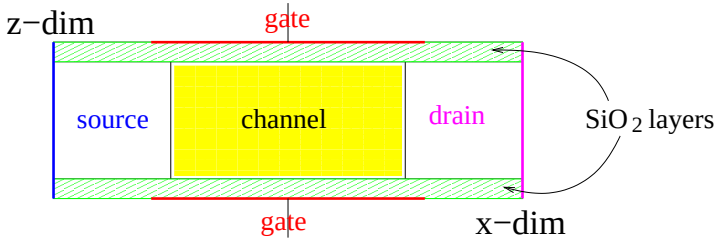
About the scaling

In 1971, the Intel 4004 processor had 1000 transistors, whose channel length was 10000 nm. In 1974, the Intel 8008 processor had 6-7 thousand. In 2003 the Intel Pentium IV had 50 million. Nowadays processors may have 400 million transistors, whose channel is 28 nm long.

Why is it important?

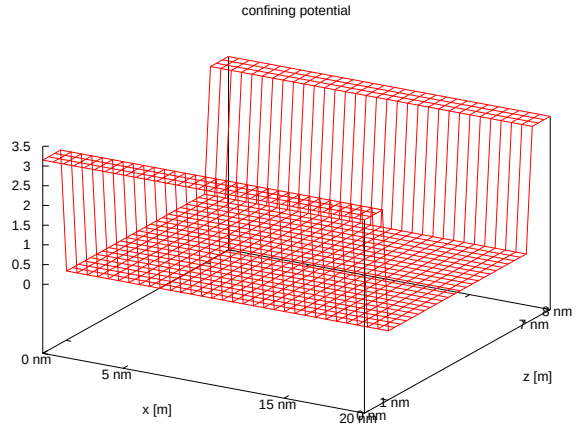
Smaller MOSFETs allow for the construction of smaller devices with better performances; moreover, they allow silicon and energy saving, due to the lower source-drain potential drop needed to switch on or off the transistor.

Geometry



The role of the insulating layers

Electrons are trapped inside a potential well of width 6 nm (comparable to the Debye length) and of depth 3.15 V along the z-dimension.



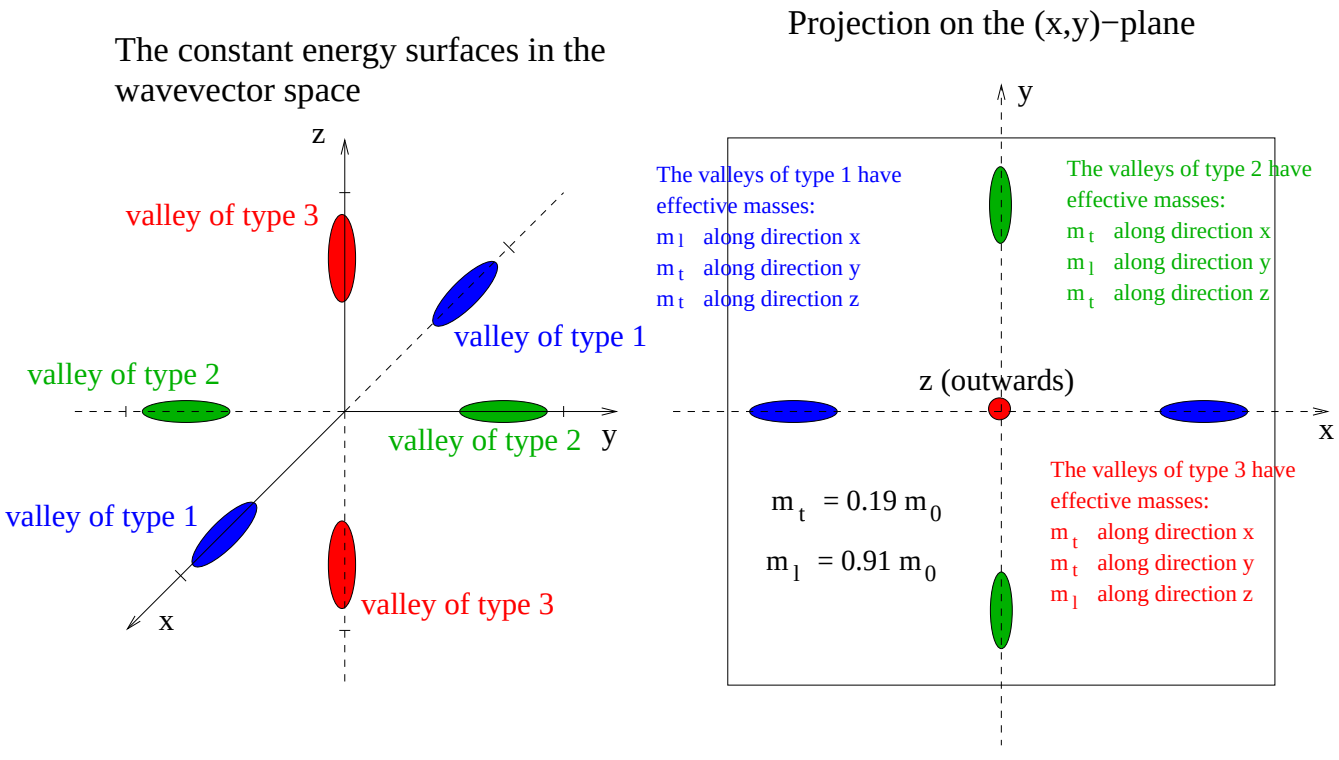
This leads to quantization of energy.

Outline

Band structure

The three valleys

The Si band structure presents six minima in the first Brillouin zone:



The axes of the ellipsoids are disposed along the *x*, *y* and *z* axes of the reciprocal lattice. The three minima have the same value, therefore there is no gap.

Band structure

Non-parabolicity

The band structure around the three minima can be expanded following the Kane non-parabolic approximation (ν indexes the valley):

$$\epsilon_\nu^{kin}(k_x, k_y) = \frac{\hbar^2}{1 + \sqrt{1 + 2\tilde{\alpha}_\nu \hbar^2 \left(\frac{k_x^2}{m_e m_{x,\nu}} + \frac{k_y^2}{m_e m_{y,\nu}} \right)}} \left(\frac{k_x^2}{m_e m_{x,\nu}} + \frac{k_y^2}{m_e m_{y,\nu}} \right),$$

where $m_{x,\nu}$ and $m_{y,\nu}$ are the effective masses along the unconfined dimensions and the $\tilde{\alpha}_\nu$ are the Kane dispersion factors.

z-direction

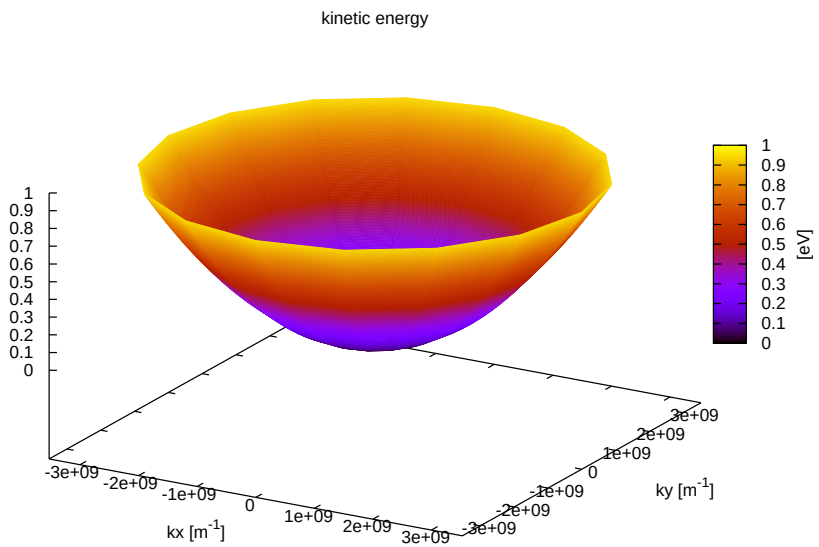
The band structure does not depend on z as the carriers are not free to move along that direction.

Electron population

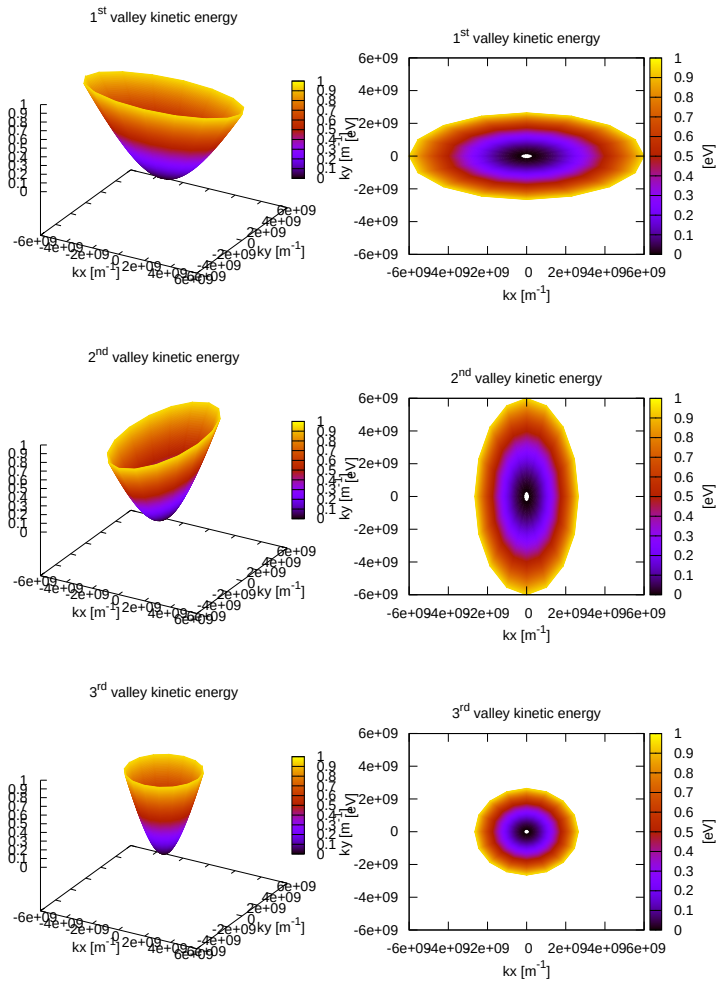
The total amount of carriers is split into independent populations, one for each valley. We shall index them $\nu = 1, 2, 3$.

Band structure

One-valley approximation vs. three-valley approximation



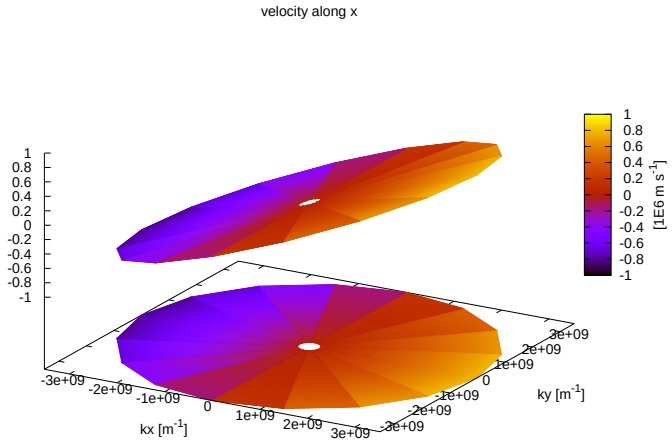
(a) ϵ^{kin} with $\tilde{\alpha} = 0$

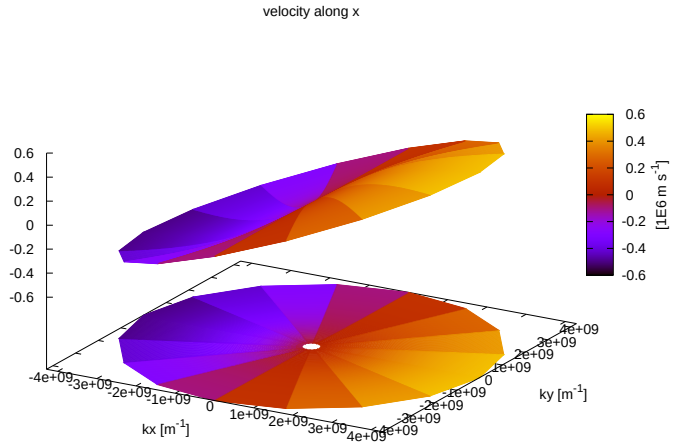


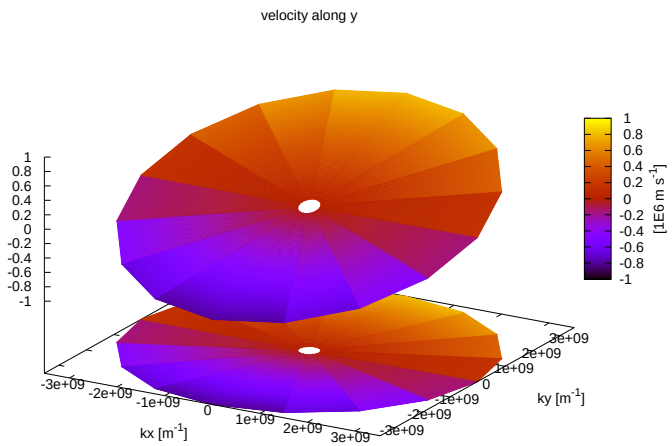
(b) ϵ_ν^{kin} with $\tilde{\alpha}_\nu = 0$

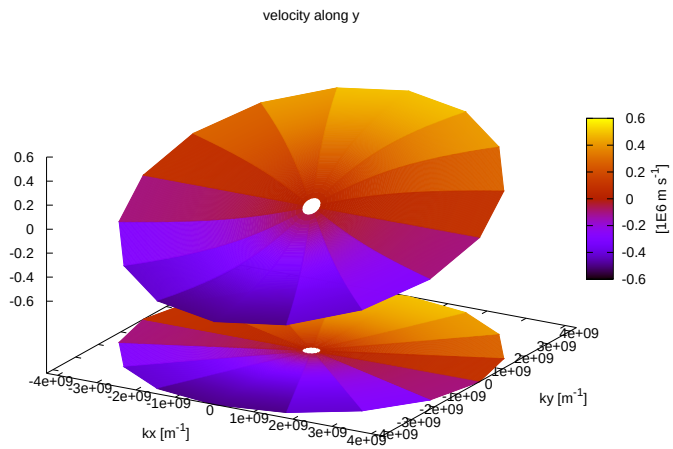
Band structure

Parabolic vs. non-parabolic







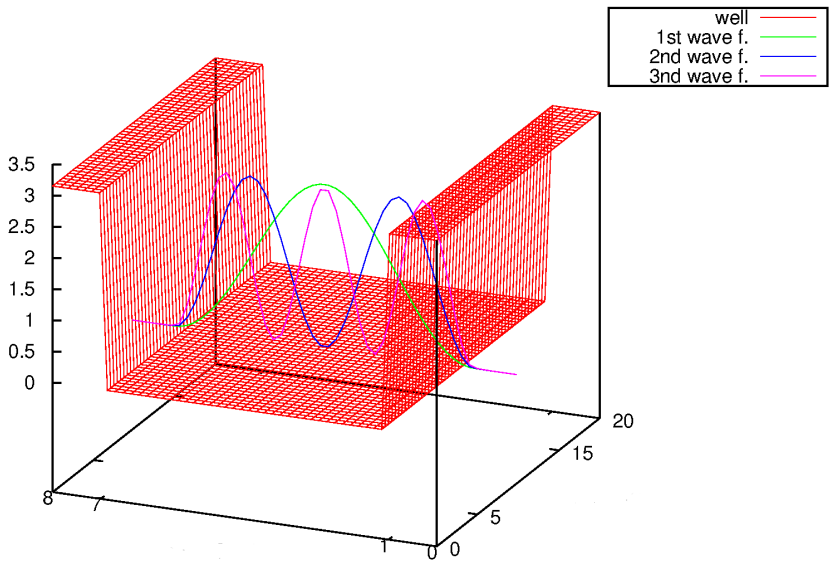


(c) v_x and v_y with $\tilde{\alpha} = 0$

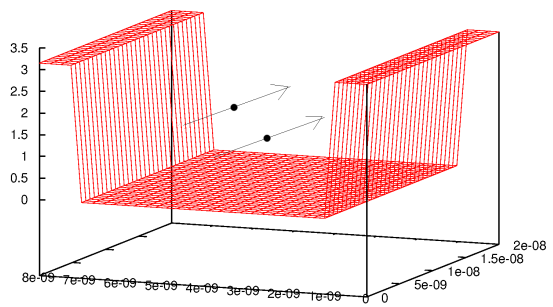
(d) v_x and v_y with $\tilde{\alpha} = 0.5$

Dimensional coupling

Justified because z-dim. is quasi-static with respect to x-dim.



(e) z-dimension: waves



(f) x-dimension: particles

The confinement

Description of the confinement

A set of 1D Schrödinger eigenvalue problems describe the electrons along z.

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_{z,\nu}}\frac{d\chi_{\nu,p}[V]}{dz}\right] - q\left(V + V_c\right)\chi_{\nu,p}[V] = \epsilon_{\nu,p}[V]\chi_{\nu,p}[V]$$

Subbands

The eigenvalues $\{\epsilon_{\nu,p}\}_{p=1}^{\infty}$ represent the energy levels, called *subbands* in physics.

Wave functions

The eigenvectors $\{\chi_{\nu,p}(\cdot)\}_{p=1}^{\infty}$ are called *wave functions* in physics.

Electron population

The subbands decompose the electron population of the ν^{th} valley into independent populations. The densities are indexed on the pair (ν, p).

The unconfined dimension

BTE

The Boltzmann Transport Equation (one for each pair (ν, p)) reads

$$\frac{\partial f_{\nu,p}}{\partial t} + \frac{1}{\hbar}\nabla_k \epsilon_\nu^{kin} \cdot \nabla_x f_{\nu,p} - \frac{1}{\hbar}\nabla_x \epsilon_{\nu,p} \cdot \nabla_k f_{\nu,p} = \mathcal{Q}_{\nu,p}[f], \qquad f_{\nu,p}(t=0) = \rho_{\nu,p}^{eq} M_\nu .$$

The collision operator

Electrons are scattered by the vibration of the crystal lattice, described as phonons:

$$\mathcal{Q}_{\nu,p}[f] = \sum_s \sum_{\nu',p'} \int_{\mathbb{R}^2} \left[S^s_{(\nu',p',k')\to(\nu,p,k)} f_{\nu',p'}(k') - S^s_{(\nu,p,k)\to(\nu',p',k')} f_{\nu,p}(k) \right] dk' .$$

The electrostatic potential

Electrons are driven by the applied bias:

$$-\mathrm{div}_{x,z}\left[\varepsilon_R \nabla_{x,z} V\right] = -\frac{q}{\varepsilon_0}\left(N - N_D\right).$$

Eigenstates, mixed states and classical states.

The classical states are the magnitudes which only depend on the unconfined dimension x, while mixed states depend on both x and z.

Eigenstates

The subbands and the wave functions $\{\epsilon_{\nu,p}(x), \chi_{\nu,p}(x,\cdot)\}_{p=1}^{\infty}$ are eigenstates; they depend on x only as a parameter.

Mixed states

The electrostatic potential $V(x,z)$ and the volume density $N(x,z) = 2\sum_{\nu=1}^{3}\sum_{p=1}^{\infty}\int_{\mathbb{R}^2} f_{\nu,p}(t,x,k)dk\,|\chi_{\nu,p}(x,z)|^2$ are mixed states.

Classical states

The pdf's $\{f_{\nu,p}(t,x,k_x,k_y)\}_{\nu,p}$ are classical states, therefore the surface density

$$\rho(x) = 2\sum_{\nu=1}^{3}\sum_{p=1}^{\infty}\int_{\mathbb{R}^2} f_{\nu,p}(t,x,k)dk$$

is a classical state too, and in general most of the macroscopic magnitudes.

The model

BTE

The Boltzmann Transport Equation (one for each subband and for each valley) reads

$$\frac{\partial f_{\nu,p}}{\partial t} + \frac{1}{\hbar}\nabla_k \epsilon_\nu^{kin} \cdot \nabla_x f_{\nu,p} - \frac{1}{\hbar}\nabla_x \epsilon_{\nu,p} \cdot \nabla_k f_{\nu,p} = \mathcal{Q}_{\nu,p}[f], \qquad f_{\nu,p}(t=0) = \rho_{\nu,p}^{eq} M_\nu .$$

Schrödinger-Poisson block

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_{z,\nu}}\frac{d\chi_{\nu,p}[V]}{dz}\right] - q\left(V + V_c\right)\chi_{\nu,p}[V] = \epsilon_{\nu,p}[V]\chi_{\nu,p}[V]$$

$$-\mathrm{div}_{x,z}\left[\varepsilon_R \nabla_{x,z} V\right] = -\frac{q}{\varepsilon_0}\left(2\sum_{\nu,p}\rho_{\nu,p}\left|\chi_{\nu,p}[V]\right|^2 - N_D\right)$$

These equations cannot be decoupled because we need the eigenfunctions to compute the potential (in the expression of the total density), and we need the potential to compute the eigenfunctions.

The model

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The Boltzmann Transport Equation (one for each subband and for each valley) reads

$$\frac{\partial f_{\nu,p}}{\partial t} + \frac{1}{\hbar}\nabla_k \epsilon_\nu^{kin} \cdot \nabla_x f_{\nu,p} - \frac{1}{\hbar}\nabla_x \epsilon_{\nu,p} \cdot \nabla_k f_{\nu,p} = \mathcal{Q}_{\nu,p}[f], \qquad f_{\nu,p}(t=0) = \rho_{\nu,p}^{eq} M_\nu .$$

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The model

The collision operator

The collision operator takes into account the phonon scattering mechanism. It reads

$$\mathcal{Q}_{\nu,p}[f] = \sum_{s} \sum_{\nu',p'} \int_{\mathbb{R}^2} \left[S^{s}_{(\nu',p',k') \to (\nu,p,k)} f_{\nu',p'}(k') - S^{s}_{(\nu,p,k) \to (\nu',p',k')} f_{\nu,p}(k) \right] dk'.$$

Structure of the S^s

The missing dimension of the wave-vector $k \in \mathbb{R}^2$, instead of $k \in \mathbb{R}^3$, is replaced by an overlap integral $W_{(\nu,p),(\nu',p')}$:

$$S^{s}_{(\nu,p,k) \to (\nu',p',k')} = C_{\nu \to \nu'} \frac{1}{W_{(\nu,p),(\nu',p')}} \delta \left(\epsilon^{tot}_{\nu',p'}(k') - \epsilon^{tot}_{\nu,p}(k) \pm \text{some energy} \right)$$

$$\frac{1}{W_{(\nu,p),(\nu',p')}} = \int_0^{l_z} |\chi_{\nu,p}|^2 |\chi_{\nu',p'}|^2 dz, \qquad [W] = m.$$

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$$\frac{1}{W_{(\nu,p),(\nu',p')}} = \int_0^{l_z} |\chi_{\nu,p}|^2 |\chi_{\nu',p'}|^2 dz, \qquad [W] = m.$$

Initial condition

Strategy

We want to initialize the system under the following constraints:

- let the potential in the corners float to the proper non-zero value;
- fulfill electrical neutrality at the source contact (symmetrically for the drain contact):

$$\int_0^{L_z} N_D(0,z) = \int_0^{L_z} N(0,z);$$

- have a thermodynamical equilibrium for the system, i.e. a distribution which is a zero for both the BTE and the scattering operator.

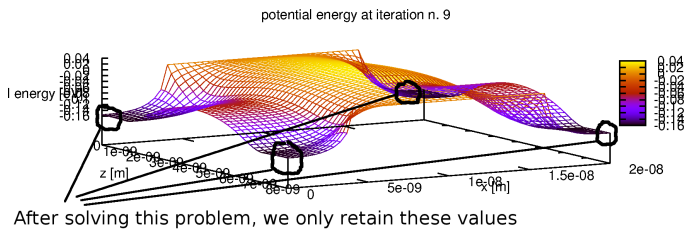
Initial condition

Step 1: the potential in the corners

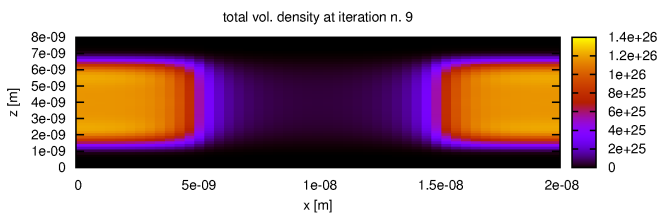
Solve Schrödinger-Poisson for the following density:

$$N[V] = \frac{2}{\pi}\frac{m_e \kappa_B T_L}{\hbar^2} \sum_{\nu,p} \sqrt{m_{x,\nu} m_{y,\nu}} \log\left(1 + e^{-\frac{\epsilon_{\nu,p}[V](x) - \epsilon_F}{\kappa_B T_L}}\right) |\chi_{\nu,p}[V](x,z)|^2$$

with homogeneous Neumann boundary conditions everywhere except at gate contacts. We retain the potential in the corners: $V_{gap} = V(0,0)$ (same value in the other three points).



After solving this problem, we only retain these values



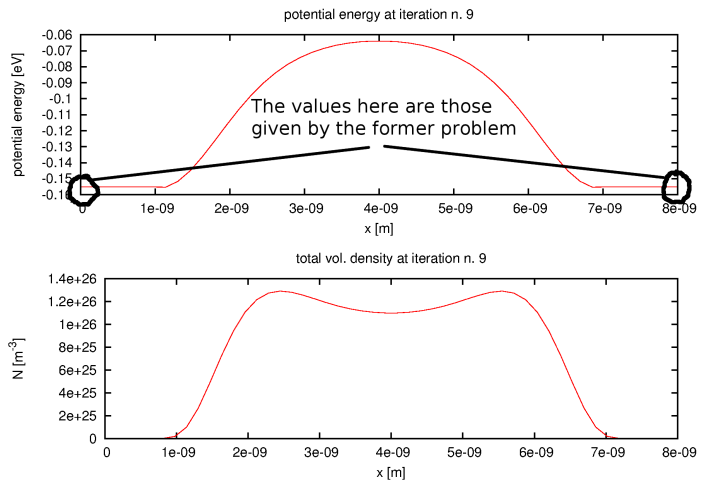
Initial condition

Step 2: the profile at the contacts

Solve a 1D Schrödinger-Poisson problem for the following density:

$$N[V] = \frac{\int_0^{L_z} N_D(0,z)dz}{\sum_{\nu',p'} \sqrt{m_{x,\nu} m_{y,\nu}} e^{-\frac{\epsilon_{\nu,p}[V](0)}{\kappa_B T_L}}} \sum_{\nu,p} \sqrt{m_{x,\nu} m_{y,\nu}} e^{-\frac{\epsilon_{\nu,p}[V](0)}{\kappa_B T_L}} \left|\chi_{\nu,p}[V](0,z)\right|^2$$

with homogeneous Neumann boundary conditions at $z = 0$ and $z = L_z$. Moreover, impose $V(0,0) = V_{gap}$. We retain the profile of V at the contacts: $V_{border}(z) = V(0,z)$.



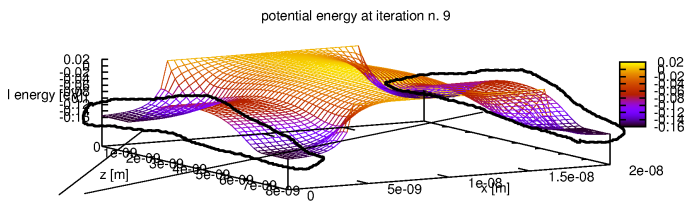
Initial condition

Step 3: the thermodynamical equilibrium

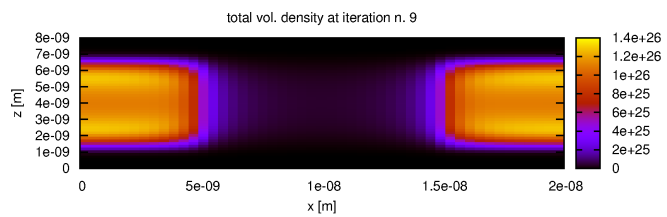
Solve Schrödinger-Poisson problem for the following density:

$$N[V] = \frac{\int_0^{L_z} N_D(0,z)dz}{\sum_{\nu',p'} \sqrt{m_{x,\nu}m_{y,\nu}}e^{-\frac{\epsilon_{\nu,p}[V_{border}]}{\kappa_B T_L}}} \sum_{\nu,p} \sqrt{m_{x,\nu}m_{y,\nu}}e^{-\frac{\epsilon_{\nu,p}[V](x)}{\kappa_B T_L}} \left|\chi_{\nu,p}[V](x,z)\right|^2$$

with Dirichlet conditions at the four metallic contacts and gates, homogeneous Neumann elsewhere. Now the surface densities are of the form $\rho^{eq}_{\nu,p} = Ce^{-\frac{\epsilon_{\nu,p}(x)}{\kappa_B T_L}}$ and are, therefore, a zero for both Boltzmann and the scattering operator.



These profiles come from the solution of the 1D problem



Outline

The Newton scheme

The functional

Solving the Schrödinger-Poisson block

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_{z,\nu}}\frac{d\chi_{\nu,p}[V]}{dz}\right]-q\left(V+V_c\right)\chi_{\nu,p}[V]=\epsilon_{\nu,p}[V]\chi_{\nu,p}[V]$$

$$-\mathrm{div}\left[\varepsilon_R\nabla V\right]=-\frac{q}{\varepsilon_0}\left(N[V]-N_D\right)$$

is equivalt to minimizing, under the constraints of the Schrödinger equation, the functional $P[V]$

$$P[V]=-\mathrm{div}\left(\varepsilon_R\nabla V\right)+\frac{q}{\varepsilon_0}\left(N[V]-N_D\right),$$

The scheme

which is achieved by means of a Newton-Raphson iterative scheme

$$dP(V^{old},V^{new}-V^{old})=-P[V^{old}].$$

The Newton scheme

The functional

Solving the Schrödinger-Poisson block

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$$dP(V^{old},V^{new}-V^{old})=-P[V^{old}].$$

The iterations

Derivatives

The Gâteaux-derivatives of the eigenproperties are needed:

$$
\begin{aligned}
d\epsilon_{\nu,p}(V,U) &= -q\int U(\zeta)|\chi_{\nu,p}[V](\zeta)|^2 d\zeta \\
d\chi_{\nu,p}(V,U) &= -q\sum_{p'\neq p}\frac{\int U(\zeta)\chi_{\nu,p}[V](\zeta)\chi_{\nu,p'}[V](\zeta)d\zeta}{\epsilon_{\nu,p}[V]-\epsilon_{\nu,p'}[V]}\chi_{\nu,p'}[V](z).
\end{aligned}
$$

Iterations

After computing the Gâteaux-derivative of the density and developping calculations, we are led to a Poisson-like equation

$$
\begin{aligned}
&-\mathrm{div}\,(\varepsilon_R\nabla V^{new}) + \int_0^{l_z}\mathcal{A}[V^{old}](z,\zeta)V^{new}(\zeta)d\zeta \\
&= -\frac{q}{\varepsilon_0}\left(N[V^{old}]-N_D\right) + \int_0^{l_z}\mathcal{A}[V^{old}](z,\zeta)V^{old}(\zeta)d\zeta,
\end{aligned}
$$

where $\mathcal{A}[V]$ is essentially the Gâteaux-derivative of the functional $P[V]$.

The iterations

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where $\mathcal{A}[V]$ is essentially the Gâteaux-derivative of the functional $P[V]$.

Comparison Newton-Raphson vs. Gummel

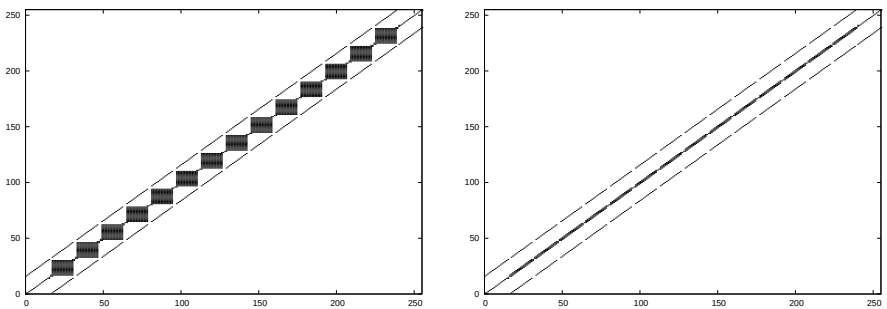
Gummel

$$-\mathrm{div}\left(\varepsilon_R \nabla V^{new}\right) + \frac{q}{\varepsilon_0} N \frac{q}{k_B T_L} V^{new} = -\frac{q}{\varepsilon_0}\left(N - N_D\right) + \frac{q}{\varepsilon_0} N \frac{q}{k_B T_L} V^{old}$$

Newton-Raphson

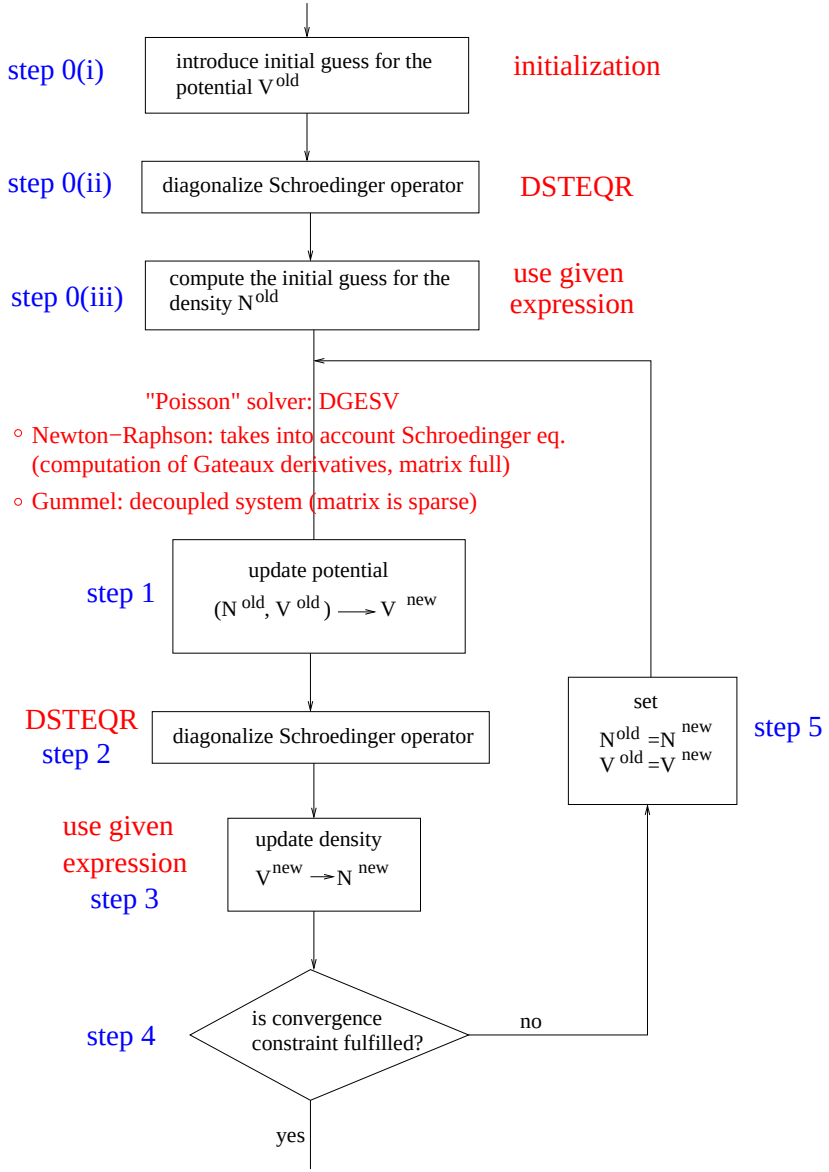
$$-\mathrm{div}\left(\varepsilon_R \nabla V^{new}\right) + \int_0^{l_z} \mathcal{A}(z,\zeta) V^{new}(\zeta) d\zeta = -\frac{q}{\varepsilon_0}\left(N - N_D\right) + \int_0^{l_z} \mathcal{A}(z,\zeta) V^{old}(\zeta) d\zeta$$

Comparison



(g) Newton-Raphson (h) Gummel

Framework


step 0(i)
introduce initial guess for the potential V^{old}
initialization
step 0(ii)
diagonalize Schroedinger operator
DSTEQR
step 0(iii)
compute the initial guess for the density N^{old}
use given expression
"Poisson" solver: DGESV
Newton−Raphson: takes into account Schroedinger eq. (computation of Gateaux derivatives, matrix full)
Gummel: decoupled system (matrix is sparse)
step 1
update potential
$(N^{old}, V^{old}) \longrightarrow V^{new}$
DSTEQR
step 2
diagonalize Schroedinger operator
use given expression
step 3
update density
$V^{new} \longrightarrow N^{new}$
step 4
is convergence constraint fulfilled?
no
yes
set
$N^{old} = N^{new}$
$V^{old} = V^{new}$
step 5

Outline

Numerical methods

We need to solve the Schrödinger eigenvalue problem and Poisson equations.

The Schrödinger equation

Equation

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_{z,\nu}}\frac{d\chi_{\nu,p}}{dz}\right]-q\left(V+V_c\right)\chi_{\nu,p}=\epsilon_{\nu,p}\chi_{\nu,p}$$

is discretized by alternate finite differences for the derivatives then the symmetric matrix is diagonalized by a LAPACK routine called DSTEQR.

The Poisson equation

We need to solve equations like

$$-\mathrm{div}\left[\varepsilon_R\nabla V\right]+\int_0^{l_z}\mathcal{A}(z,\zeta)V(\zeta)d\zeta=\mathcal{B}(z).$$

The derivatives are discretized by finite differences in alternate directions, the integral is computed via trapezoid rule and the linear system (banded) is solved by means of a LAPACK routine called ?GBSV.

Numerical methods

We need to solve the Schrödinger eigenvalue problem and Poisson equations.

The Schrödinger equation

Equation

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_{z,\nu}}\frac{d\chi_{\nu,p}}{dz}\right]-q\left(V+V_c\right)\chi_{\nu,p}=\epsilon_{\nu,p}\chi_{\nu,p}$$

is discretized by alternate finite differences for the derivatives then the symmetric matrix is diagonalized by a LAPACK routine called DSTEQR.

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Outline

Adimensionalization of the wave-vector space

The wave-vector space is adimensionalized by a change of variables into ellipsoidal variables, in order to better integrate the scattering operator and to have a simple expression for the kinetic energy and related magnitudes.

Ellipsoidal coordinated

The wave-vector for the ν^{th} valley reads:

$$(\tilde{k}_x, \tilde{k}_y) = \frac{\sqrt{m_e \kappa_B T_L}}{\hbar} \sqrt{2w(1+\alpha_\nu w)} \left(\sqrt{m_{x,\nu}} \cos(\phi), \sqrt{m_{y,\nu}} \sin(\phi) \right).$$

The Jacobian

The magnitude $s_\nu(w)$ represents the dimensionless Jacobian of the change of variables in the wave-vector space:

$$s_\nu(w) = \left| \det \frac{\partial (k_x, k_y)}{\partial (w, \phi)} \right| = \sqrt{m_{x,\nu} m_{y,\nu}} (1 + 2\alpha_\nu w).$$

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BTE in ellipsoidal coordinates

Let the flux coefficients

$$
\begin{aligned}
a^1_\nu(w,\phi) &= \frac{\sqrt{2w(1+\alpha_\nu w)}\cos(\phi)}{\sqrt{m_{x,\nu}}}\frac{1}{1+2\alpha_\nu w} \\
a^2_{\nu,p}(x,w,\phi) &= -\frac{\partial \epsilon_{\nu,p}}{\partial x}(x)\frac{1}{1+2\alpha_\nu w}\frac{\sqrt{2w(1+\alpha_\nu w)}\cos(\phi)}{\sqrt{m_{x,\nu}}} \\
a^3_{\nu,p}(x,w,\phi) &= \frac{\partial \epsilon_{\nu,p}}{\partial x}(x)\frac{\sin(\phi)}{\sqrt{m_{x,\nu}}\sqrt{2w(1+\alpha_\nu w)}}.
\end{aligned}
$$

Conservation-law form

$$
\frac{\partial \Phi_{\nu,p}}{\partial t} + \frac{\partial}{\partial x}\left[a^1_\nu \Phi_{\nu,p}\right] + \frac{\partial}{\partial w}\left[a^2_{\nu,p}\Phi_{\nu,p}\right] + \frac{\partial}{\partial \phi}\left[a^3_{\nu,p}\Phi_{\nu,p}\right] = \mathcal{Q}_{\nu,p}[\Phi]s(w)
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$$

Runge-Kutta time integration

We use a Runge-Kutta time discretization.

Runge-Kutta

We advance in time by the third order Total Variation Diminishing Runge-Kutta scheme: if the evolution equation reads

$$H_{\nu,p}(\Phi) := -\frac{\partial}{\partial x}\left[a^1_\nu \Phi_{\nu,p}\right] - \frac{\partial}{\partial w}\left[a^2_{\nu,p}\Phi_{\nu,p}\right] - \frac{\partial}{\partial \phi}\left[a^3_{\nu,p}\Phi_{\nu,p}\right] + \mathcal{Q}_{\nu,p}[\Phi]s(w)$$

(no explicit time-dependency), then

1. $\Phi^{(1)}_{\nu,p} = \Delta t H_{\nu,p}(\Phi^n)$
2. $\Phi^{(2)}_{\nu,p} = \frac{3}{4}\Phi^n_{\nu,p} + \frac{1}{4}\Phi^{(1)}_{\nu,p} + \frac{1}{4}\Delta t H_{\nu,p}(\Phi^{(1)})$
3. $\Phi^{n+1} = \frac{1}{3}\Phi^n_{\nu,p} + \frac{2}{3}\Phi^{(2)}_{\nu,p} + \frac{2}{3}H_{\nu,p}(\Phi^{(2)})$

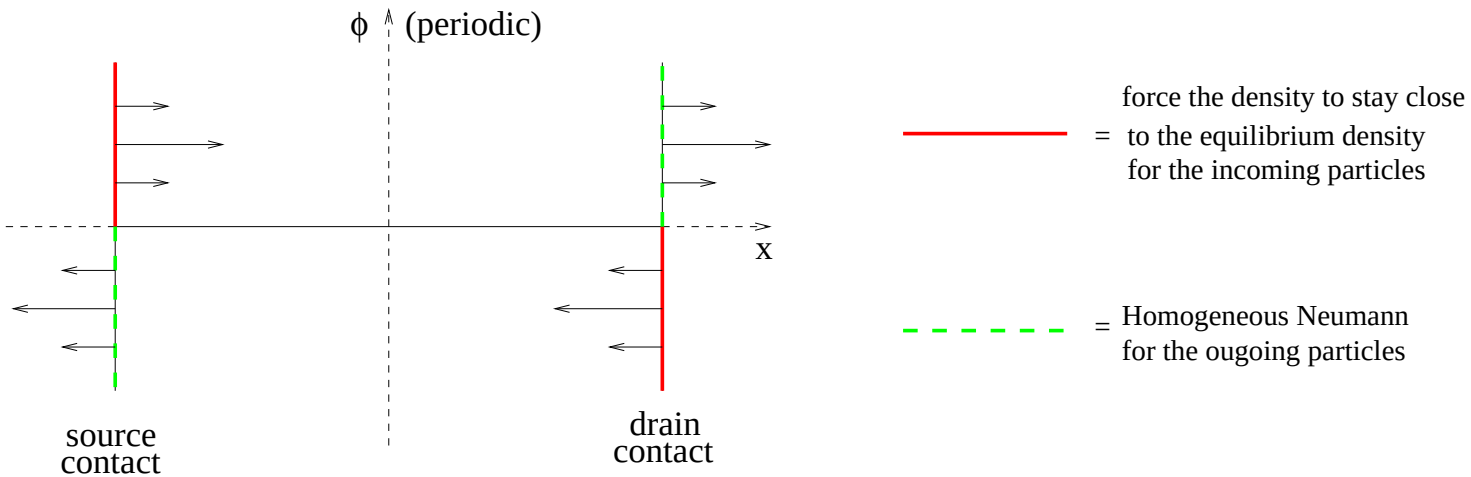
Boundary conditions for the BTE

x-derivative

We use inflow/outflow b.c.: for the incoming particles

$$f_{\nu,p}(t,-x,w,\phi) = \frac{\rho^{eq}_{\nu,p}(0)}{\rho_{\nu,p}(0)} f_{\nu,p}(t,0,w,\phi),$$

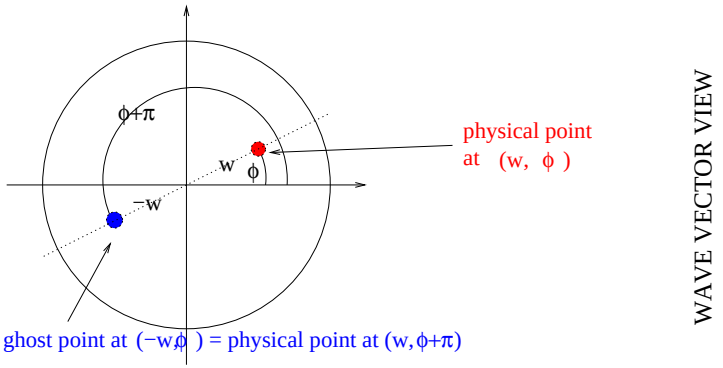
so as to have $\int_{\mathbb{R}^2} f_{\nu,p}(t,0,k)dk = \rho^{eq}_{\nu,p}$, thus filfilling the electrical neutrality constraint. For the outgoing particles, just use homogeneous Neumann b.c.

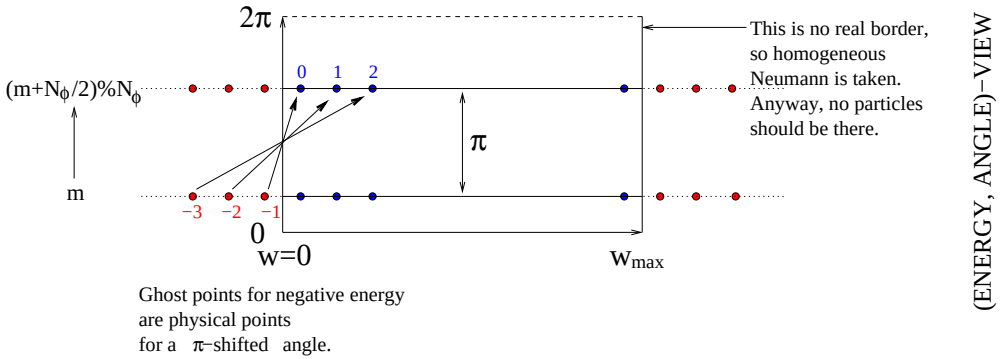


Boundary conditions for the BTE

w-derivative

$w = 0$ is no real boundary; ghost points at $(-w, \phi)$ are physical points at $(w, \phi + \pi)$. At $w = w_{max}$ there should be no particles, for properly chosen meshes: just use homogeneous Neumann b.c.

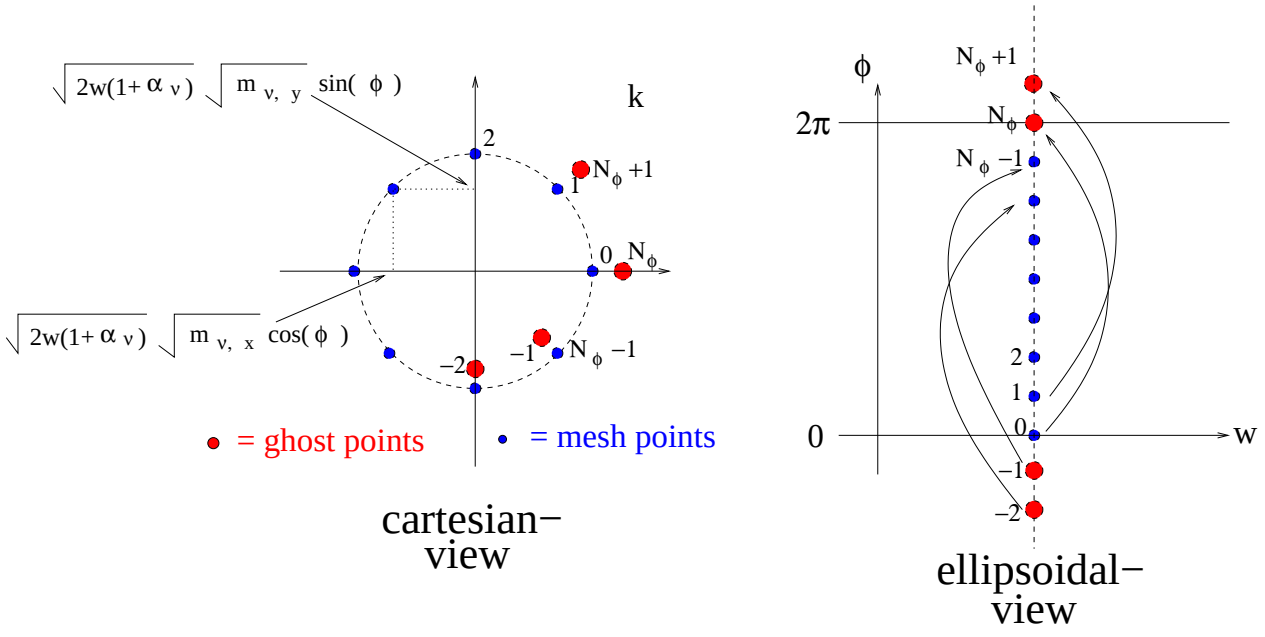




Boundary conditions for the BTE

ϕ-derivative

As ϕ represents an angle, periodicity conditions are taken.



Integrating the scattering operator

Elastic phenomena

$$\begin{aligned}\mathcal{Q}_{\nu,p}[\Phi]s_\nu(w) &= C_1^{\mathcal{Q}} \sum_{p'} \frac{1}{W_{(\nu,p'),(\nu,p)}} \mathbb{I}_{\{\Gamma_0 \geq 0\}} \\ &\times \left[s_\nu(w) \int_{\phi'=0}^{2\pi} \Phi_{\nu,p'}\left(\Gamma_0, \phi'\right) d\phi' - 2\pi \Phi_{\nu,p} s_\nu\left(\Gamma_0\right) \right]\end{aligned}$$

Energy gap

When electrons change their state from (ν, p) to (ν', p'), energy jumps appear:

$$\Gamma_0(x, w) = \epsilon^{tot}_{\nu,p}(x, w) - \epsilon_{\nu',p'}(x).$$

Remark, nevertheless, that they do not exchange energies with the phonons (elastic interaction).

Integrating the scattering operator

Here go the formulae for the integration of the collisional operator in the ellipsoidal dimensionless variables.

Inelastic phenomena

$$
\begin{aligned}
& \mathcal{Q}_{\nu,p}[\Phi] s_\nu(w) \\
= \quad & C^{\mathcal{Q}} s_\nu(w) \sum_{\nu',p'} \frac{\gamma_{\nu'\to\nu} N_{\nu'\to\nu}}{W_{(\nu',p'),(\nu,p)}} \mathbb{I}_{\{\Gamma_- \geq 0\}} \int_{\phi'=0}^{2\pi} \Phi_{\nu',p'}\left(\Gamma'_-, \phi'\right) d\phi' \\
+ \quad & C^{\mathcal{Q}} s_\nu(w) \sum_{\nu',p'} \frac{\gamma_{\nu'\to\nu}\left(N_{\nu'\to\nu}+1\right)}{W_{(\nu',p'),(\nu,p)}} \mathbb{I}_{\{\Gamma_+ \geq 0\}} \int_{\phi'=0}^{2\pi} \Phi_{\nu',p'}\left(\Gamma_+, \phi'\right) d\phi' \\
- \quad & C^{\mathcal{Q}} 2\pi \Phi_{\nu,p}(w,\phi) \sum_{\nu',p'} \frac{\gamma_{\nu\to\nu'} N_{\nu\to\nu'}}{W_{(\nu,p),(\nu',p')}} \mathbb{I}_{\{\Gamma_+ \geq 0\}} s_{\nu'}\left(\Gamma_+\right) \\
- \quad & C^{\mathcal{Q}} 2\pi \Phi_{\nu,p}(w,\phi) \sum_{\nu',p'} \frac{\gamma_{\nu\to\nu'}\left(N_{\nu\to\nu'}+1\right)}{W_{(\nu,p),(\nu',p')}} \mathbb{I}_{\{\Gamma_- \geq 0\}} s_{\nu'}\left(\Gamma_-\right)
\end{aligned}
$$

Integrating the scattering operator

Energy gaps

When electrons change their state from (ν, p) to (ν', p'), energy jumps appear:

$$\Gamma_{\pm}(x, w) = \epsilon^{tot}_{\nu,p}(x, w) - \epsilon_{\nu',p'}(x) \pm \frac{\hbar\omega}{\kappa_B T_L}$$

Remark that, for inelastic interactions, they exchange energies $\hbar\omega$ with the phonons.

Occupation numbers

The occupation numbers read

$$N_{\nu\to\nu'} = \frac{\sqrt{\frac{m_{x,\nu} m_{y,\nu}}{m_{x,\nu'} m_{y,\nu'}}} \frac{1+2\alpha_\nu}{1+2\alpha_{\nu'}} e^{\frac{\hbar\omega}{\kappa_B T_L}} + 1}{\left(e^{\frac{\hbar\omega}{\kappa_B T_L}} + 1\right)\left(e^{\frac{\hbar\omega}{\kappa_B T_L}} - 1\right)},$$

for intra-valley phenomena ($\gamma_{\nu\to\nu'} = 0$ for $\nu' \neq \nu$), reduce to the well-known

$$N = \frac{1}{e^{\frac{\hbar\omega}{\kappa_B T_L}} - 1}.$$

Outline

Parallelization of the transport/collision integration

The Runge-Kutta scheme

The scheme to advance in time

$$H_{\nu,p}(\Phi) = -\frac{\partial}{\partial x}\left[a^1_{\nu}\Phi_{\nu,p}\right] - \frac{\partial}{\partial w}\left[a^2_{\nu,p}\Phi_{\nu,p}\right] - \frac{\partial}{\partial \phi}\left[a^3_{\nu,p}\Phi_{\nu,p}\right] + \mathcal{Q}_{\nu,p}[\Phi]s(w)$$

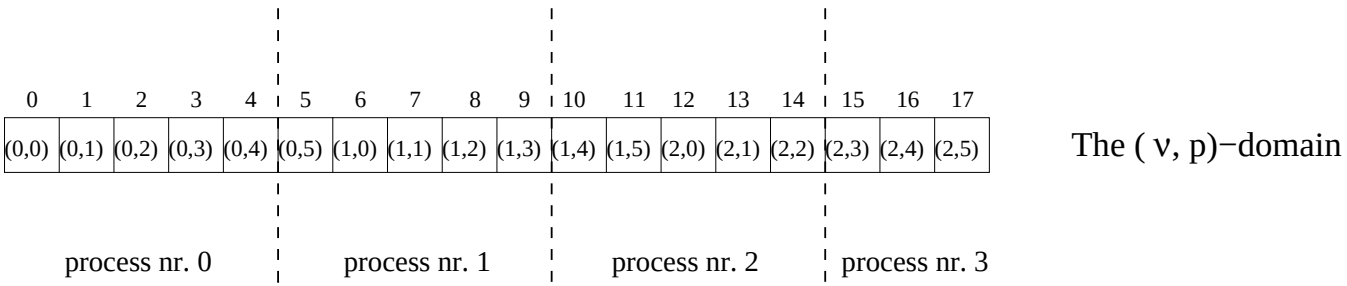
$$\begin{aligned}
\Phi^{(1)}_{\nu,p} &= \Delta t H_{\nu,p}(\Phi^n) \\
\Phi^{(2)}_{\nu,p} &= \frac{3}{4}\Phi^n_{\nu,p} + \frac{1}{4}\Phi^{(1)}_{\nu,p} + \frac{1}{4}\Delta t H_{\nu,p}(\Phi^{(1)}) \\
\Phi^{n+1}_{\nu,p} &= \frac{1}{3}\Phi^n_{\nu,p} + \frac{2}{3}\Phi^{(2)}_{\nu,p} + \frac{2}{3}H_{\nu,p}(\Phi^{(2)})
\end{aligned}$$

is very local in the (ν, p)-space: only the integration of the scattering operator $\mathcal{Q}_{\nu,p}[\Phi]s(w)$ requires information from other valleys and subbands.

Parallelization of the transport/collision integration

1D block decomposition in the (ν, p)-space

We consider (ν, p) as just one dimension and use MPI to exchange data following a 1D block distribution:



The information is gathered after each Runge-Kutta stage.

Parallelization of the Schrödinger diagonalization

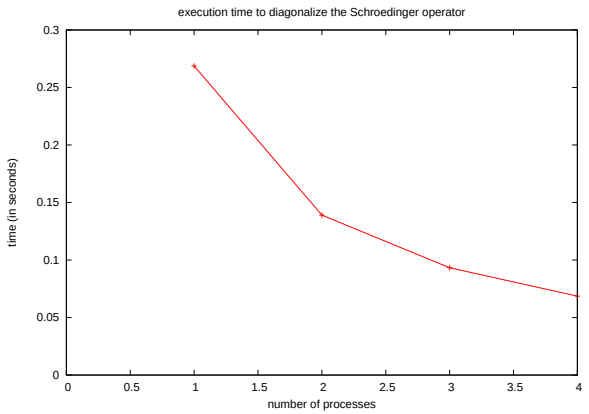
The Schrödinger equation

In the eigenvalue problem, x only acts as a parameter:

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_{z,\nu}}\frac{d\chi_{\nu,p}[V]}{dz}\right]-q\left(V+V_c\right)\chi_{\nu,p}[V]=\epsilon_{\nu,p}[V]\chi_{\nu,p}[V].$$

1D block decomposition in the x-space

We perform a simple 1D block decomposition in the x-domain: each process diagonalizes its set of equations, then the information is gathered (we use MPI). This way, we observe a $\frac{1}{N_p}$-decrease in the computational times:



Parallelization of ?GBSV

The goal

The goal is not the reduction of the computational times in the solution of the linear system, rather in assembling the matrix, which is the bottleneck of this block.

ScaLAPACK's P?GBSV

The banded matrix for ?DGBSV has dimension $(2 \cdot KL + 2 \cdot KU + 1) \times (N_x \cdot N_z)$. The parallel version, requires cutting in the $(N_x \cdot N_z)$-dimension, i.e. a decomposition by column blocks.

1D block decomposition in the (x, z)-space

We consider the (x, z)-space as a 1D space and perform a block decompisition (same strategy as for the (ν, p)-decomposition):

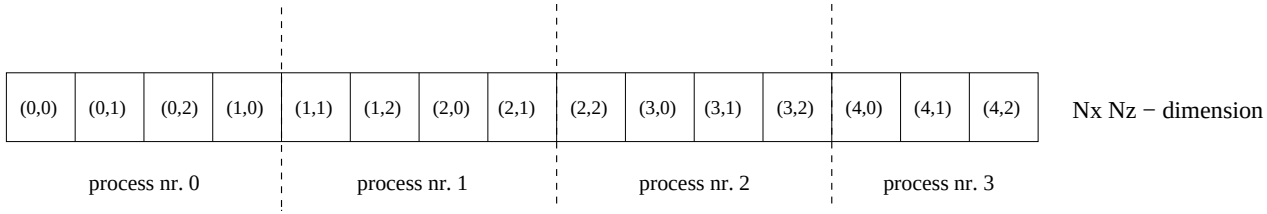
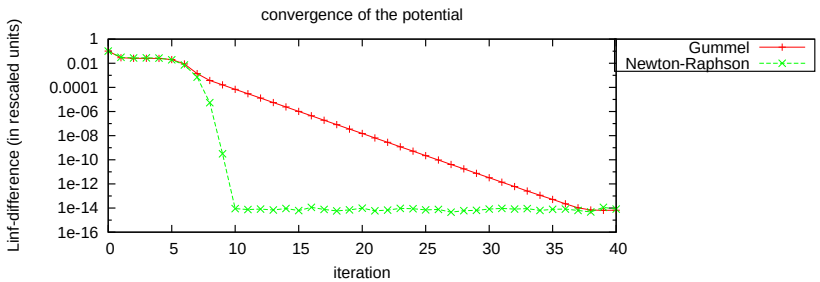


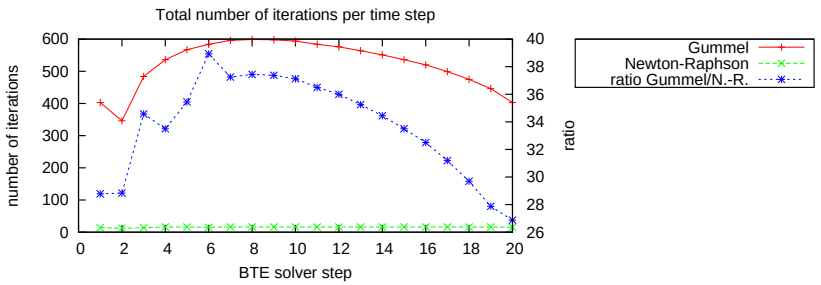
Figure: In this example $(N_x, N_z) = (5, 3)$ and $N_p = 4$.

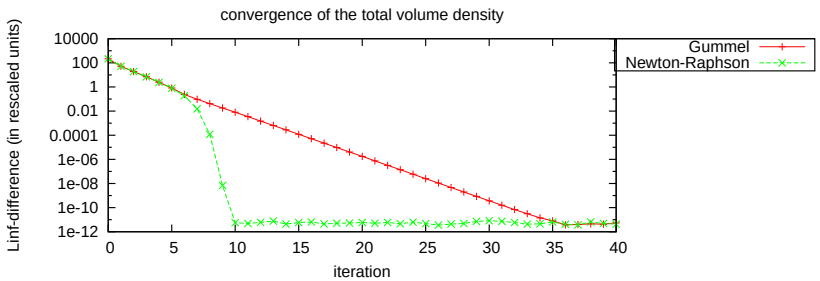
Outline

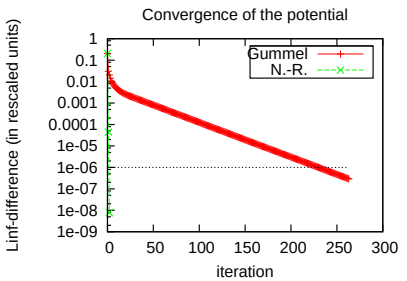
Number of iterations

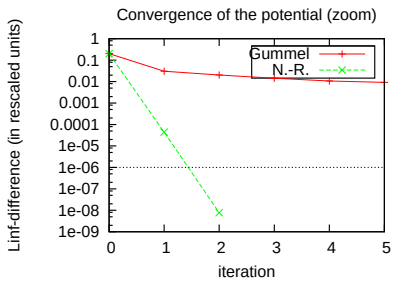
Newton schemes require much less iterations than Gummel in order to compute the thermodynamical equilibrium and any update of the potential; the results are the same up to machine error.











Outline

Thermodynamical equilibrium: three-valley case

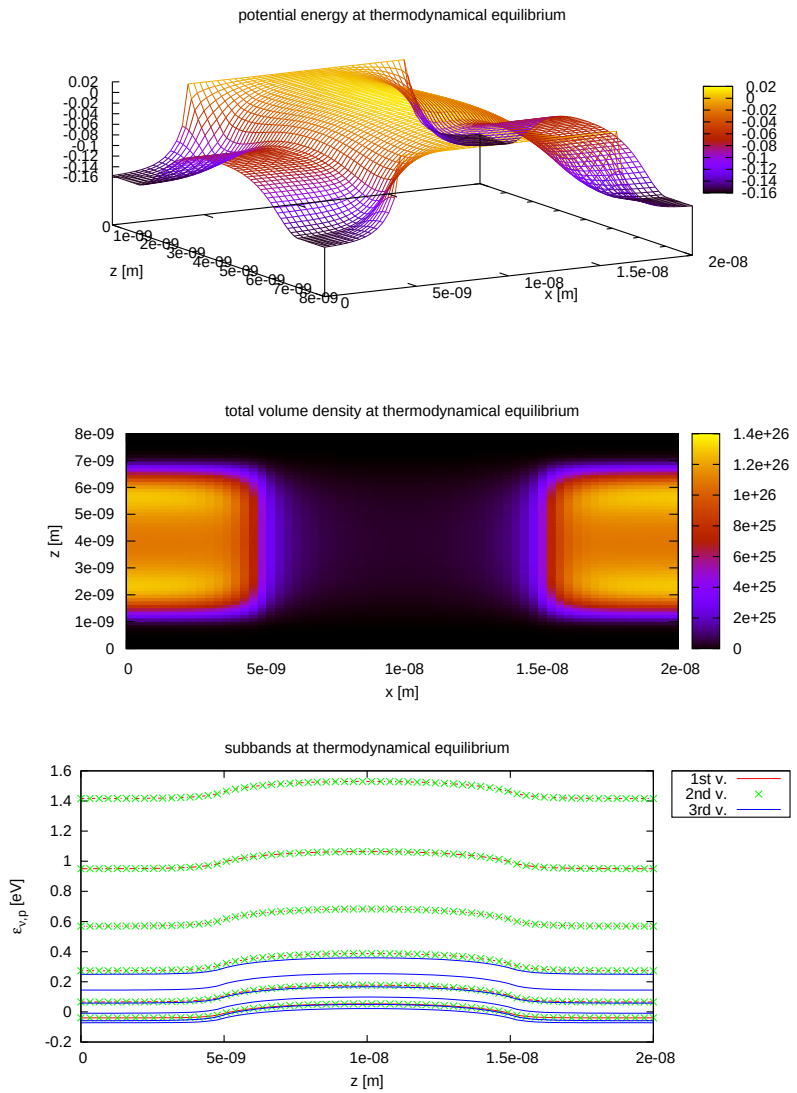


Figure: In this example $(N_{sbn}, N_x, N_z) = (6, 64, 64)$.

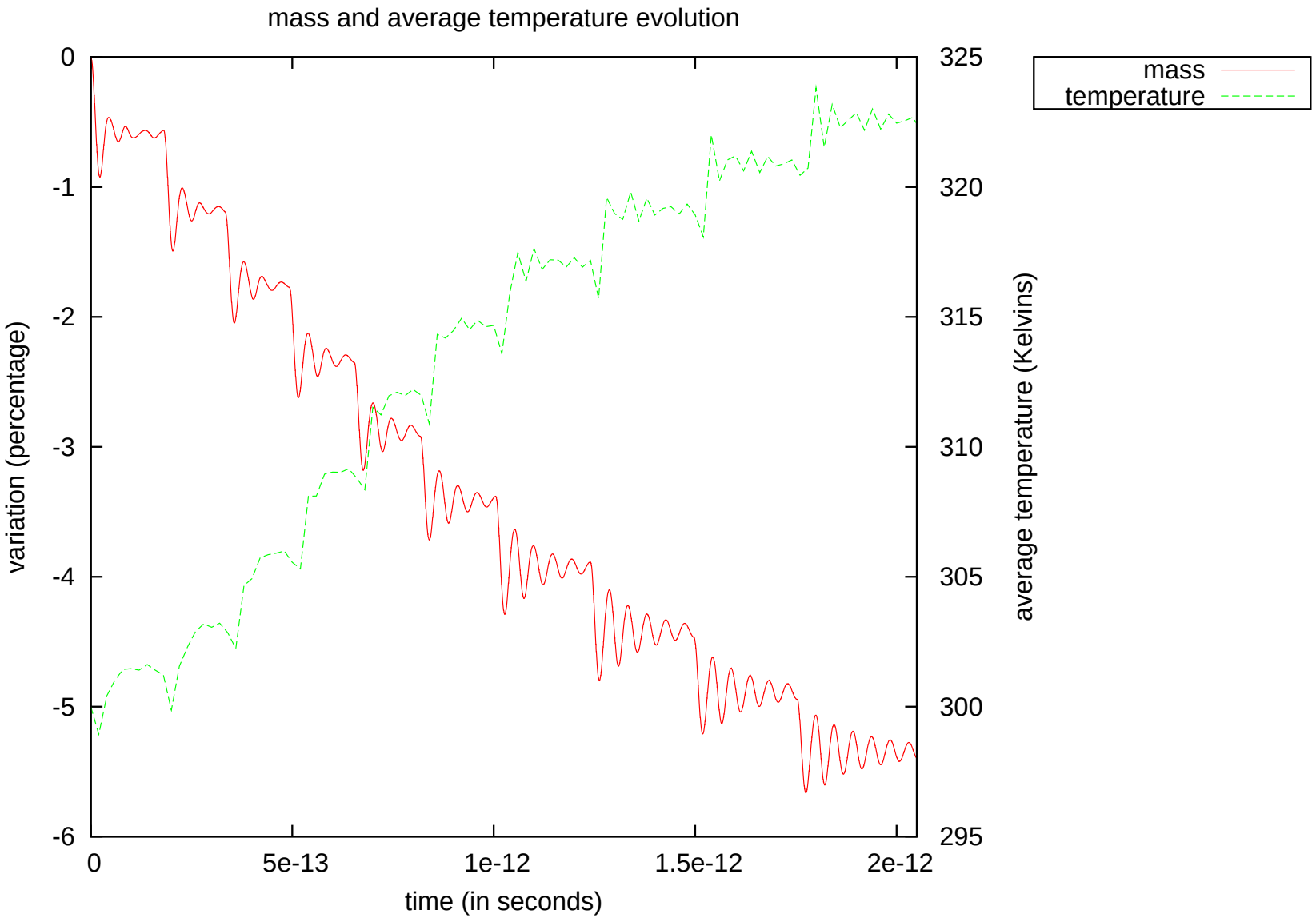
Outline

Long-time behavior

We propose now some results relative to the long-time behavior of the system.

Outline

Mass and temperature oscillations



Numerically-computed oscillations

The plasma frequency is given by

$$\omega_p = \sqrt{\frac{q^2 N_e}{\varepsilon_R \varepsilon_0 m_*}}.$$

N_D^{high} ($\times 10^{26} m^{-3}$)	ε_R	$m_\star$	N_e ($\times 10^{26} m^{-3}$)	ω_{num} ($\times 10^{14} s^{-1}$)	ω_p ($\times 10^{14} s^{-1}$)	Ratio $\frac{\omega_{num}}{\omega_{ref}}$	Expected Ratio
1	11.7	0.5	.400	$\omega_{ref} = 1.344$	1.475	1	/
2	11.7	0.5	.783	2.051	2.064	1.52	$\sqrt{2}$
4	11.7	0.5	1.544	2.813	2.899	2.09	2
1	5.85	0.5	.400	1.848	2.086	1.37	$\sqrt{2}$