A Legendre Polynomial Solver for the Langevin Boltzmann Equation

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Introduction

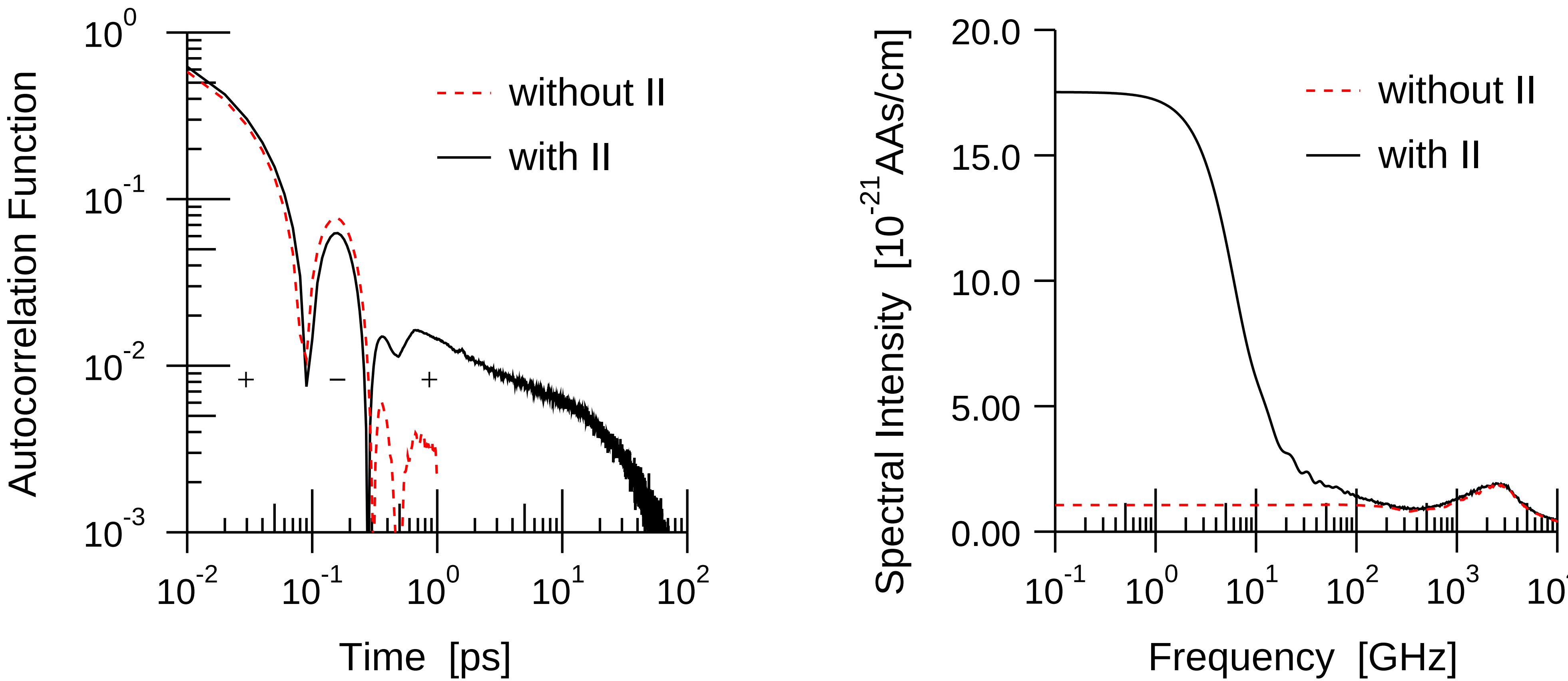
Noise calculation in the semiclassical framework

Boltzmann transport equation

- Physical Monte Carlo method
  - + Inherently contains noise
  - + Well understood and widely used
  - - Solves the BTE in the time domain

- Known numerical approaches (Spherical harmonics expansion of the BTE for the joint distribution function, only 2 papers)
  - - Also solve the BTE in the time domain

MC simulation of a 1D N^+NN^+ structure



Small tail of the ACF determines low-frequency noise

CPU time: 3 weeks (Low pass filter behavior, easy to simulate with MC)

$\Rightarrow$ MC method too CPU intensive for noise calculations below 100GHz

The Langevin Boltzmann equation

LBE:

$$\left\{\frac{\partial}{\partial t} - \frac{q}{\hbar}\vec{E}\cdot\nabla\right\} f_\nu(\vec{k},t) - \widehat{W}\{f\} = \xi_\nu(\vec{k},t)$$

Properties of the Langevin force:

$$\langle \xi_\nu(\vec{k},t)\rangle = 0 \qquad (\Rightarrow \qquad \langle LBE\rangle = BTE)$$

$$\langle \xi_\nu(\vec{k},t)\xi_{\nu'}(\vec{k}',t')\rangle = S^{\xi,\xi}_{\nu,\nu'}(\vec{k},\vec{k}')\delta(t-t')$$

$$S^{\xi,\xi}_{\nu,\nu'}(\vec{k},\vec{k}') = 4\Omega\Bigg[\left(\sum_{\nu''=1}^{6}\int W_{\nu'',\nu}(\vec{k}''|\vec{k})f^0_\nu(\vec{k}) + W_{\nu,\nu''}(\vec{k}|\vec{k}'')f^0_{\nu''}(\vec{k}'')d^3k''\right)$$
$$\delta_{\nu,\nu'}\delta(\vec{k}-\vec{k}') - W_{\nu',\nu}(\vec{k}'|\vec{k})f^0_\nu(\vec{k}) - W_{\nu,\nu'}(\vec{k}|\vec{k}')f^0_{\nu'}(\vec{k}')\Bigg]$$

LBE contains no new information compared to BTE!

For what do we need the LBE?

Can be solved CPU efficiently for noise in the frequency domain!

Green's functions of the LBE for the frequency domain:

$$\left\{ \mathrm{i}\omega - \frac{q}{\hbar}\vec{E}\cdot\nabla \right\} G_{\nu,\nu'}(\vec{k},\vec{k}',\omega) - \widehat{W}\{G\} = \delta_{\nu,\nu'}\delta(\vec{k}-\vec{k}')$$

Spectral intensity of the distribution function (Wiener Lee theorem):

$$S^{f,f}_{\nu,\nu'}(\vec{k},\vec{k}',\omega) = \sum_{\nu_1=1}^{6}\sum_{\nu_2=1}^{6}\int\int G_{\nu,\nu_1}(\vec{k},\vec{k}_1,\omega) S^{\xi,\xi}_{\nu_1,\nu_2}(\vec{k}_1,\vec{k}_2) G^{*}_{\nu',\nu_2}(\vec{k}',\vec{k}_2,\omega) d^3k_1 d^3k_2$$

Spectral intensity of microscopic quantities:

$$S^{x,y}(\omega) = \frac{1}{(2\pi)^6}\sum_{\nu=1}^{6}\sum_{\nu'=1}^{6}\int\int x_\nu(\vec{k}) S^{f,f}_{\nu,\nu'}(\vec{k},\vec{k}',\omega) y_{\nu'}(\vec{k}') d^3k d^3k'$$

The adjoint technique

Green's functions for microscopic quantities:

$$\underbrace{G^x_{\nu_1}(\vec{k}_1,\omega)}_{\text{discretized: vector}} = \frac{1}{(2\pi)^3}\sum_{\nu=1}^{6}\int x_\nu(\vec{k})\ \underbrace{G_{\nu,\nu_1}(\vec{k},\vec{k}_1,\omega)}_{\text{discretized: matrix}}\ d^3k$$

Spectral intensity of microscopic quantities:

$$S^{x,y}(\omega) = \frac{1}{(2\pi)^6}\sum_{\nu=1}^{6}\sum_{\nu'=1}^{6}\int\int x_\nu(\vec{k})S^{f,f}_{\nu,\nu'}(\vec{k},\vec{k}',\omega)y_{\nu'}(\vec{k}')d^3k d^3k'$$
$$= \sum_{\nu_1=1}^{6}\sum_{\nu_2=1}^{6}\int\int G^x_{\nu_1}(\vec{k}_1,\omega)S^{\xi,\xi}_{\nu_1,\nu_2}(\vec{k}_1,\vec{k}_2)G^{y*}_{\nu_2}(\vec{k}_2,\omega)d^3k_1 d^3k_2$$

$G^x_{\nu_1}(\vec{k}_1,\omega)$ can be directly calculated by solving the adjoint LBE

CPU time for noise calculation similar to solving the BTE for the EDF!

Electron transport model

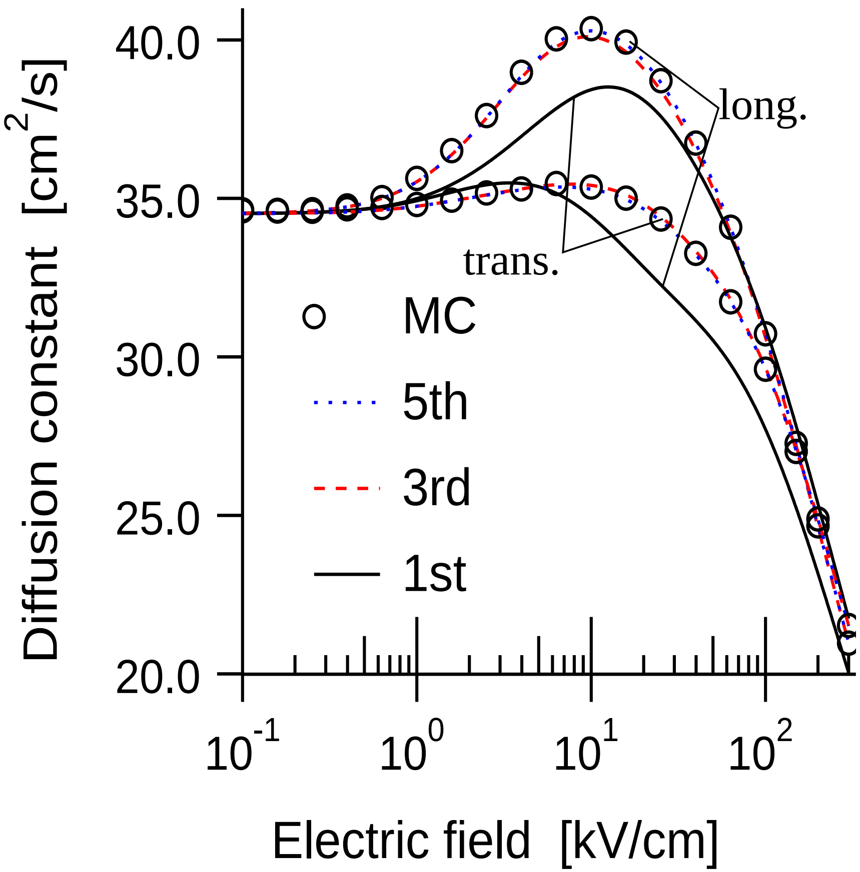
- Jacoboni's six valley model
- Anisotropic nonparabolic band structure
- Optical and acoustic phonons
- Brooks-Herring like impurity scattering with an empirical correction for high doping concentrations

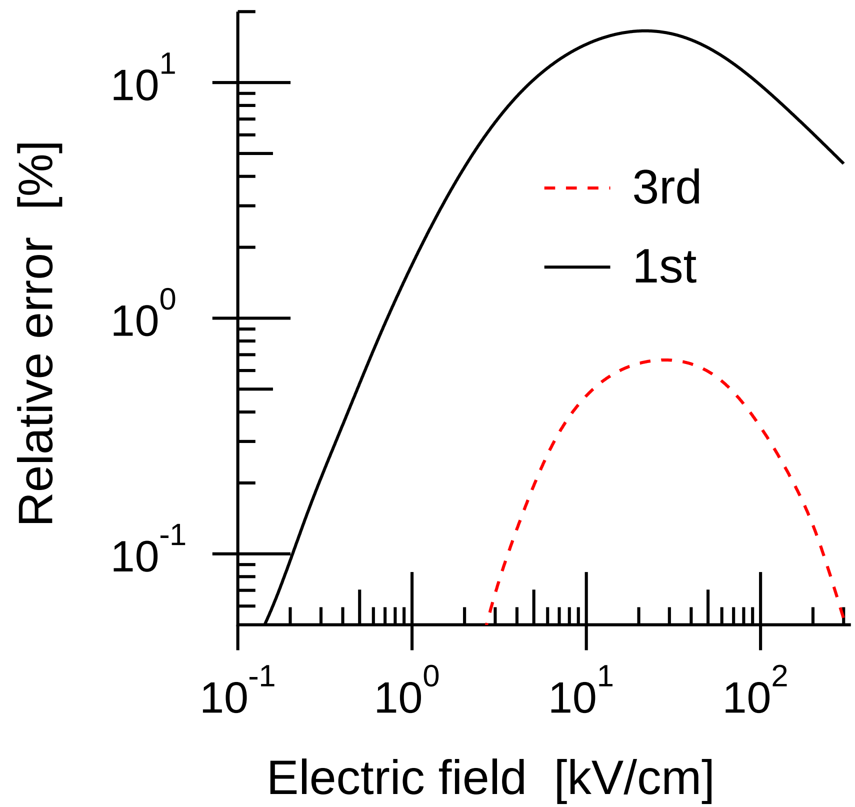
Numerics

- Finite differences in energy
- Legendre polynomial expansion in the angle between electric field and wave vector up to the nth order
- Still direct solvers for the system of linear equations

Results

Longitudinal and transverse diffusion constant $\langle \tau \vec{v}\vec{v}^{\mathsf{T}} \rangle$ (electric field in $\langle 100 \rangle$ direction, undoped Si, 300K)

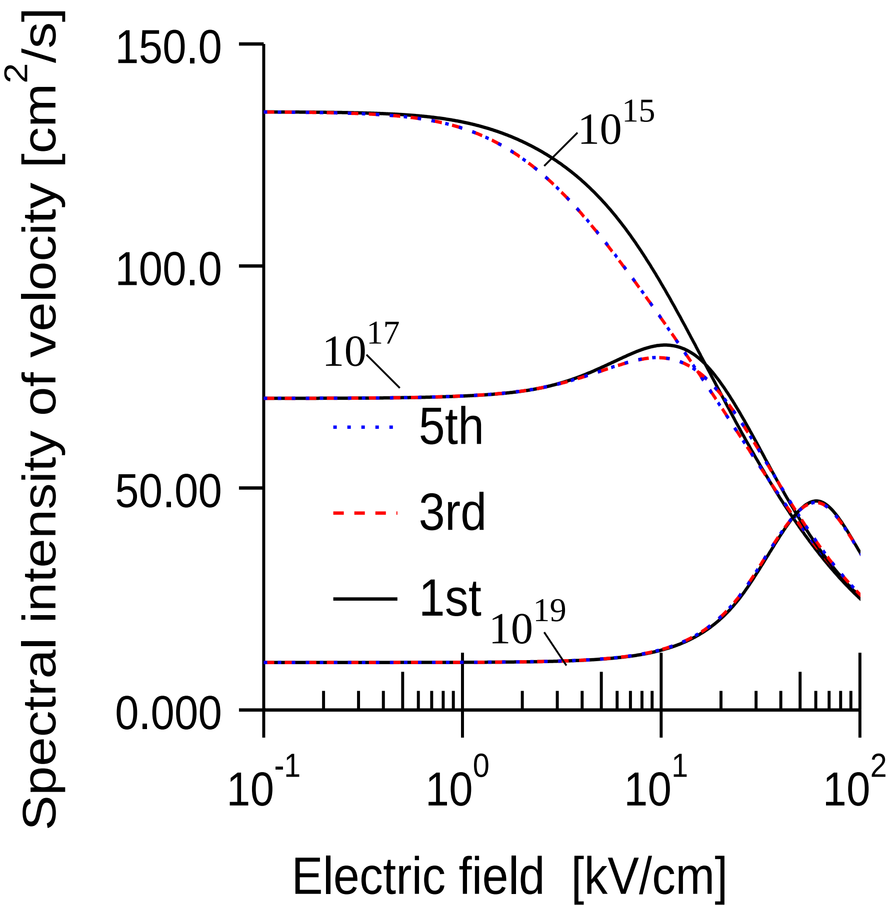




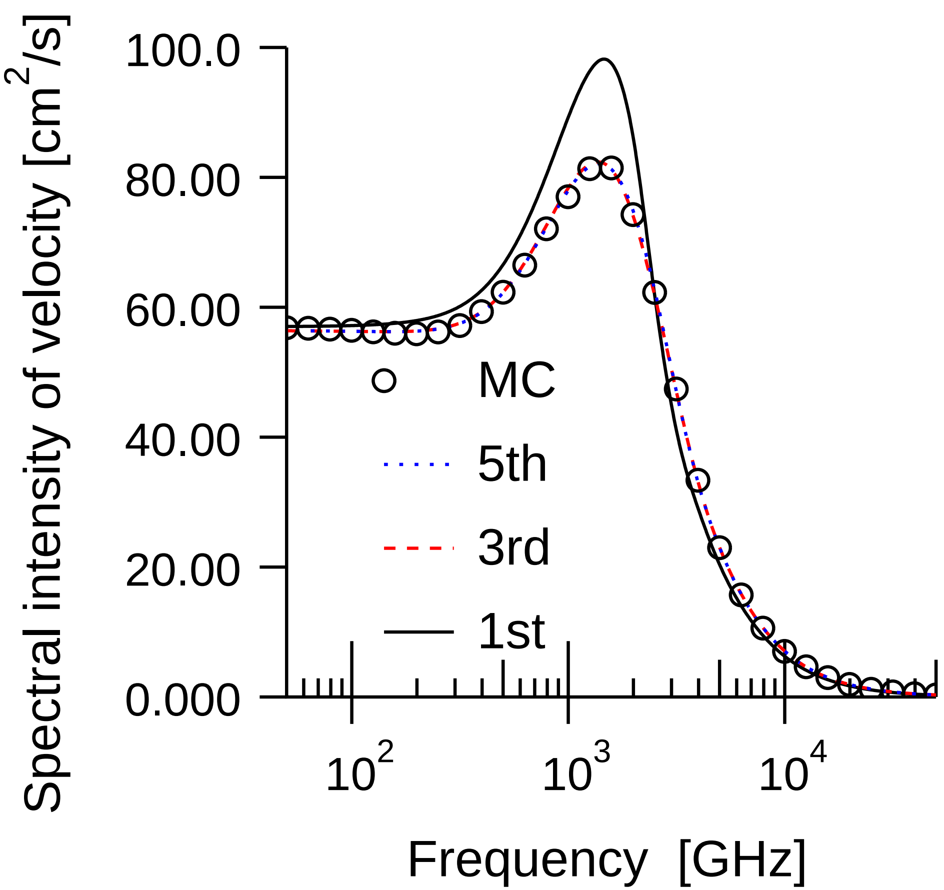
Longitudinal component

MC and LPE yield the same result! 3rd order expansion sufficiently accurate!

Spectral intensity of the longitudinal velocity fluctuations



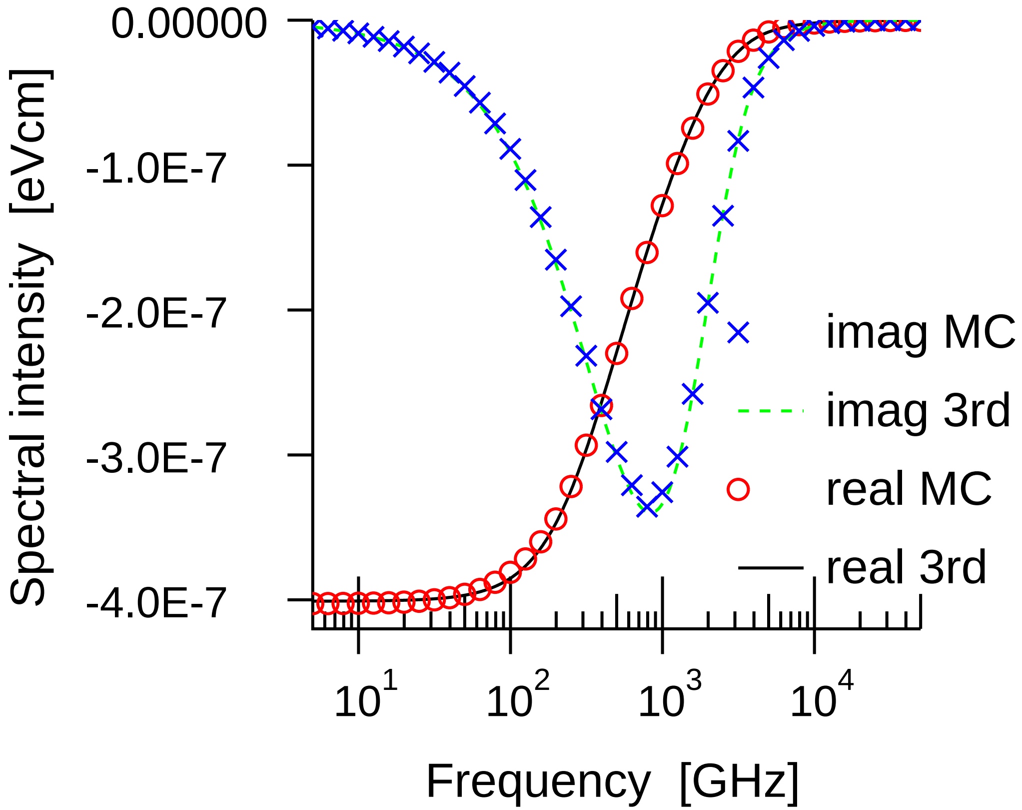
At zero frequency



for 30kV/cm undoped

3rd order expansion sufficiently accurate for noise!

Cross power of the fluctuations of energy and longitudinal velocity



for 30kV/cm undoped

- Imaginary part vanishes for small frequencies
- MC CPU time is for such quantities inversely proportional to the cube of the minimum frequency

LPE at least 1000 times faster than MC!

Conclusions

- First Legendre polynomial solver for the LBE to calculate noise in the frequency domain.

- For the first time the CPU efficient adjoint technique is applied to the LBE.

- Full anisotropy of the band structure is considered.

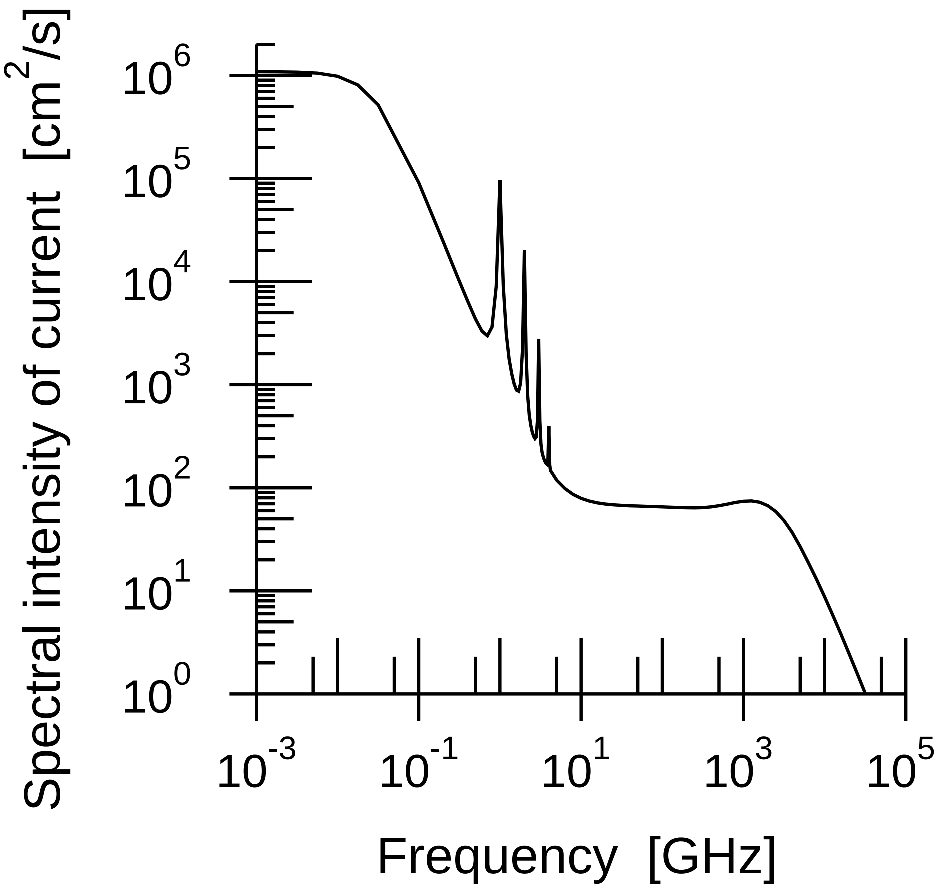
- Noise calculation requires 3rd order expansion, which is also sufficiently accurate.

- Both methods, MC and LPE yield exact solutions of the full LBE, and their results are in excellent agreement.

- CPU time of the LPE is independent of the frequency and allows to investigate low frequencies without prohibitive CPU times.

Outlook:

- Low-frequency generation / recombination noise
- Harmonic balance analysis of cyclostationary noise
- Device noise



$$E(t) = 30kV/cm \cdot (1 + \cos(2\pi f_0 t))$$