How to preserve the Kramers-Kronig relation in inelastic atomistic quantum transport calculations

Daniel Lemus[1], James Charles[1], Tillmann Kubis[1,2,3,4]
[1]*School of Electrical and Computer Engineering, Purdue University, W. Lafayette, IN, USA*
[2]*Network for Computational Nanotechnology, Purdue University, W. Lafayette, IN, USA*
[3]*Purdue Center for Predictive Materials and Devices, W. Lafayette, IN, USA*
[4]*Purdue Institute of Inflammation, Immunology and Infectious Disease, W. Lafayette, IN, USA*
dlemus@purdue.edu

The nonequilibrium Green's function method (NEGF) is often used to predict quantum transport in atomically resolved nanodevices. This yields a high numerical load when inelastic scattering is included. Atomistic NEGF had been regularly applied on nanodevices, such as nanotransistors. However, incoherent scattering is still subject to significant approximation. A very common approximation to scattering is to neglect the real part of the retarded scattering self-energies, which fundamentally violates the causality relation. Neglecting that real part is known to alter electronic energies, which in turn impacts transistor I-V characteristics [1,2]. In this work, [3] the atomistic mode space approach of Mil'nikov et al. [4] is extended by including the exact calculation of the real part of retarded scattering self-energies in the reduced basis representation using the Kramers–Kronig relation. The real part of the retarded scattering self-energy, $\Sigma(\mathbf{r},\mathbf{r}',E)^R_{i,j,real} = \mathcal{H}(\Sigma(\mathbf{r},\mathbf{r}',E)^R_{i,j,imag})$, is solved with a Hilbert transform of each matrix element i,j of the imaginary part of Σ for all energies E. Performing this calculation in a typical atomistic basis such as tight binding is prohibitively numerically expensive [2]. However, the mode space basis reduction reduces the numerical load to under 1% of the operations in the original basis which effectively enables scattered atomistic NEGF on nanodevices without losing the predictive power of NEGF. All atomistic quantum transport simulations in this work utilize NEMO5 and Victory Atomistic and include deformation potential scattering on acoustic and optical phonons, as well as Fröhlich scattering on polar optical phonons. The non-local nature of polar optical phonon scattering is included using a cross-section-dependent compensation factor [5]. The impact of the real part of the retarded scattering self-energies is exemplified on atomically resolved InAs nanowire tunneling field effect transistors. Depending on the device physics, the real part of retarded self-energies alters the transistor performance, increasing the OFF and decreasing the ON current.

[1] J. Charles et al., J. Comput. Electron., **15** (2016).
[2] A. Esposito, et al. J. Comput. Electron., **8**, (2009).
[3] D. A. Lemus et al., J. Comput. Electron, **19**, (2020).
[4] G. Mil'nikov, et al., Phys. Rev. B, **85**, 035317, (2012).
[5] P. Sarangapani, et al., Phys. Rev. Appl., **12**, 044045, (2019).

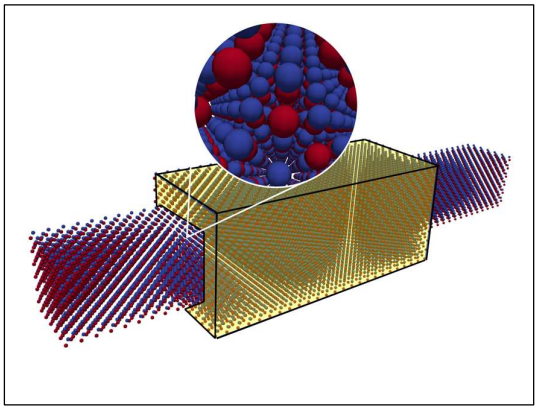

Fig.1: 3.64 nm × 3.64 nm × 30.29 nm InAs TFET device with a 1nm gate oxide layer surrounding the center of the device (in yellow), used in all calculations in this work.

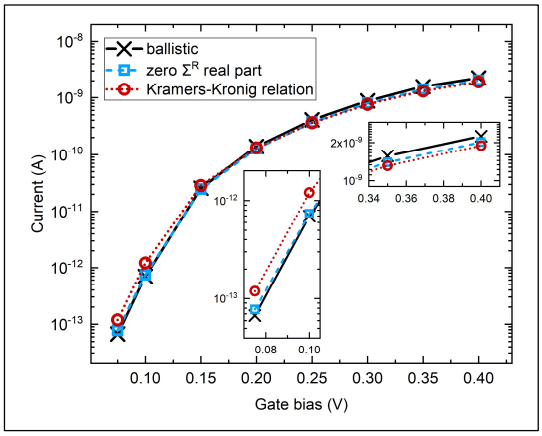

Fig.2: I–V characteristics for a 2.42 nm × 2.42 nm × 30.29 nm InAs TFET device solved in NEGF including incoherent scattering on polar optical phonons, acoustic phonons and optical deformation potential phonons. Scattering, even without a real part of Σ^R , increases the off-current densities and lowers on-current densities. When the real part of the retarded self-energy Σ^R is included, the Kramers–Kronig relations are obeyed and scattering shows an even larger impact. The insets zoom into the first two and the last two points of the curves.

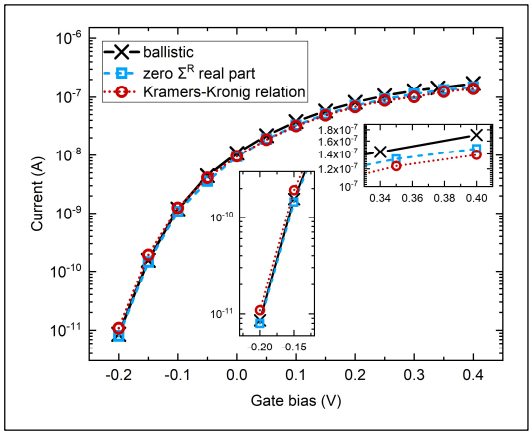

Fig.3: I–V characteristics of a 3.64 nm × 3.64 nm × 30.29 nm InAs TFET device, comparing the same ballistic and scattering configurations of Fig. 2. Scattering has a greater effect on the ON state for this device geometry, in particular when the real part of the retarded self-energy Σ^R is included.

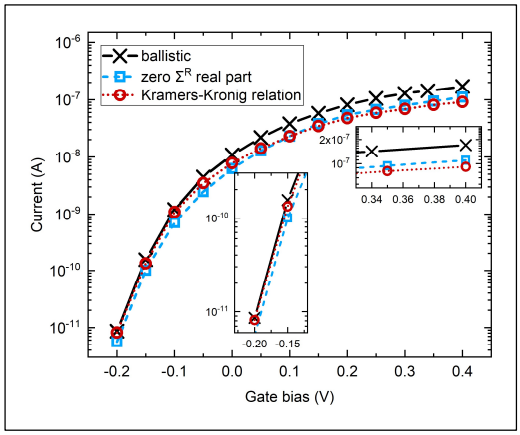

Fig.4: Similar to Fig. 3, the I-V characteristics of 3.64 nm × 3.64 nm × 30.29 nm InAs TFET device, but with the scattering strength multiplied by 10. The inclusion of the real part of the retarded self-energy Σ^R in cases with higher scattering strength is shown to have a significant effect on device performance and must therefore be included.

ISBN 978-89-89453-30-7