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

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Non-equilibrium Green's function formalism (NEGF)

$$G^R = (E - H - \Sigma^R)^{-1}$$

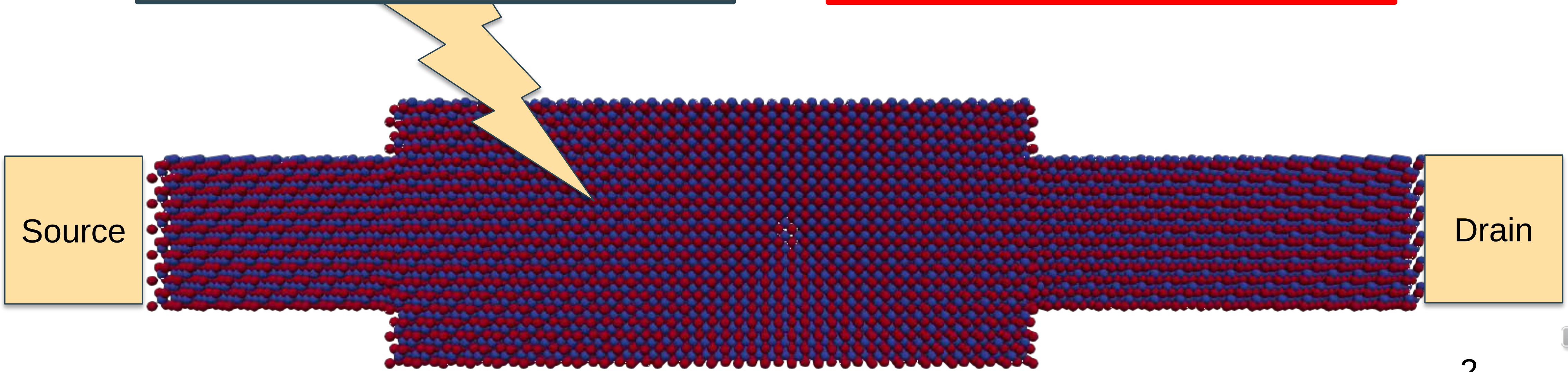
$$G^< = G^R \Sigma^< G^{R\dagger}$$

Self-energies represent external perturbations in atomic devices

- Electrons entering/exiting device (lead/contact self-energy)
- **Incoherent scattering** phenomena, e.g., phonons

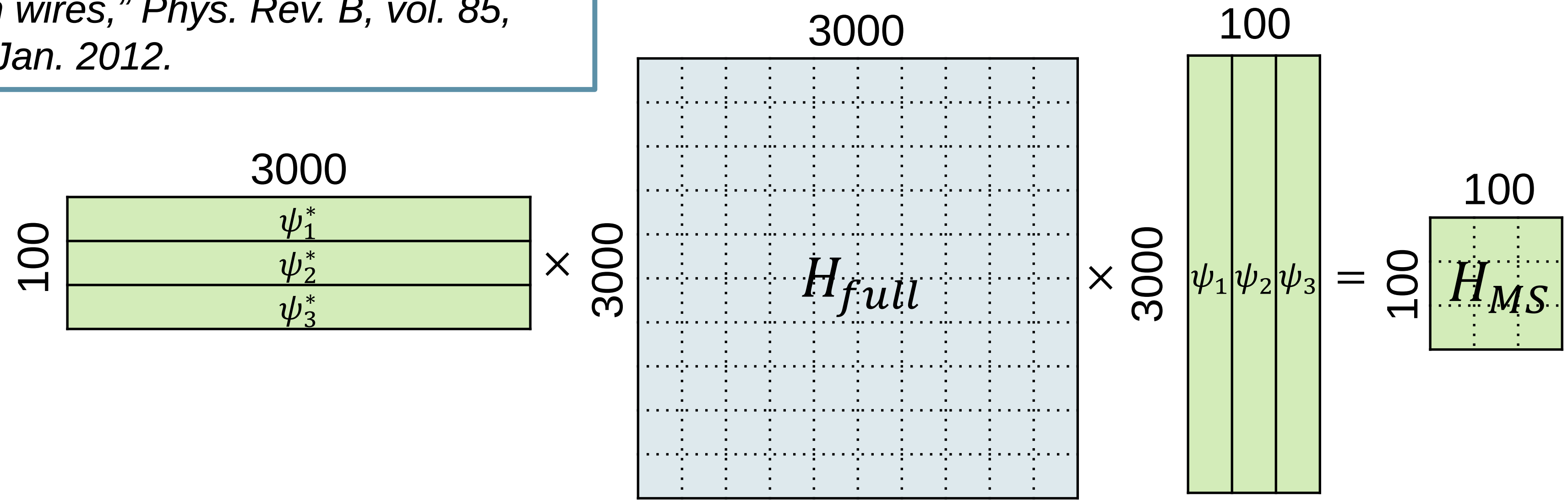
$$\boxed{\Sigma^R = G^R D^R + G^R D^< + G^< D^R}$$

Computationally expensive



Mode space rank reduction

Clever mode filtering method detailed in:
G. Mil'nikov, et al., "Equivalent transport models in atomistic quantum wires," Phys. Rev. B, vol. 85, no. 3, p. 035317, Jan. 2012.



3 nm × 3 nm cross section device using 10-orbital tight binding:
~3000 × 3000 matrices (single unit cell)
$O(N^3) = \boxed{2.7 \times 10^{10}}$ operations

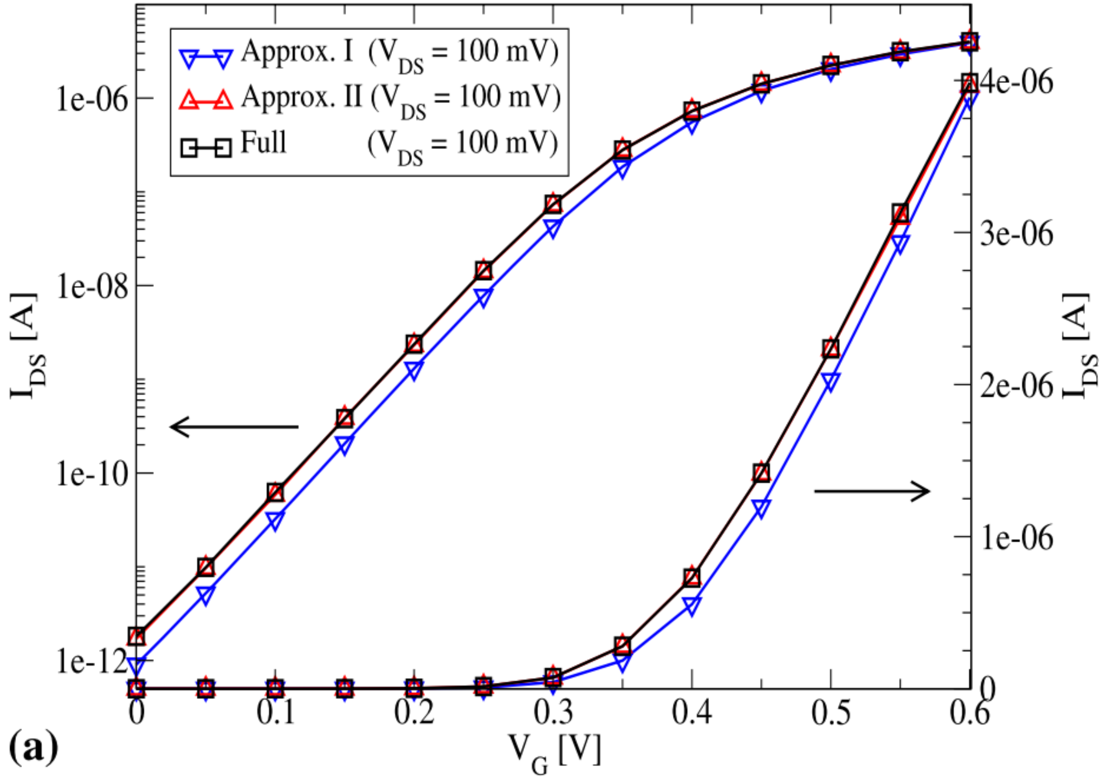
Rank reduced by ~97%
3% reduction ratio

3 nm × 3 nm device using 100 modes:
100 × 100 matrices
$O(N^3) = \boxed{10^6}$operations

Huge reduction in computational complexity

Effects of approximations to retarded self-energies

- Approx. I: No real part
- Approx. II: Approximation avoids principal value integral
- Full: Includes principal value integral



- Common in mode space to **avoid the real part of Σ^R**

Take advantage of mode space and solve Σ^R **exactly**

A. Esposito, M. Frey, and A. Schenk, “Quantum transport including nonparabolicity and phonon scattering: Application to silicon nanowires,” J. Comput. Electron., vol. 8, no. 3–4, pp. 336–348, 2009.

In this work: calculation of retarded self-energies

$$Im[\Sigma^R(E)] = \frac{1}{2}(\Sigma^>(E) - \Sigma^<(E))$$

- Responsible for dephasing of electrons

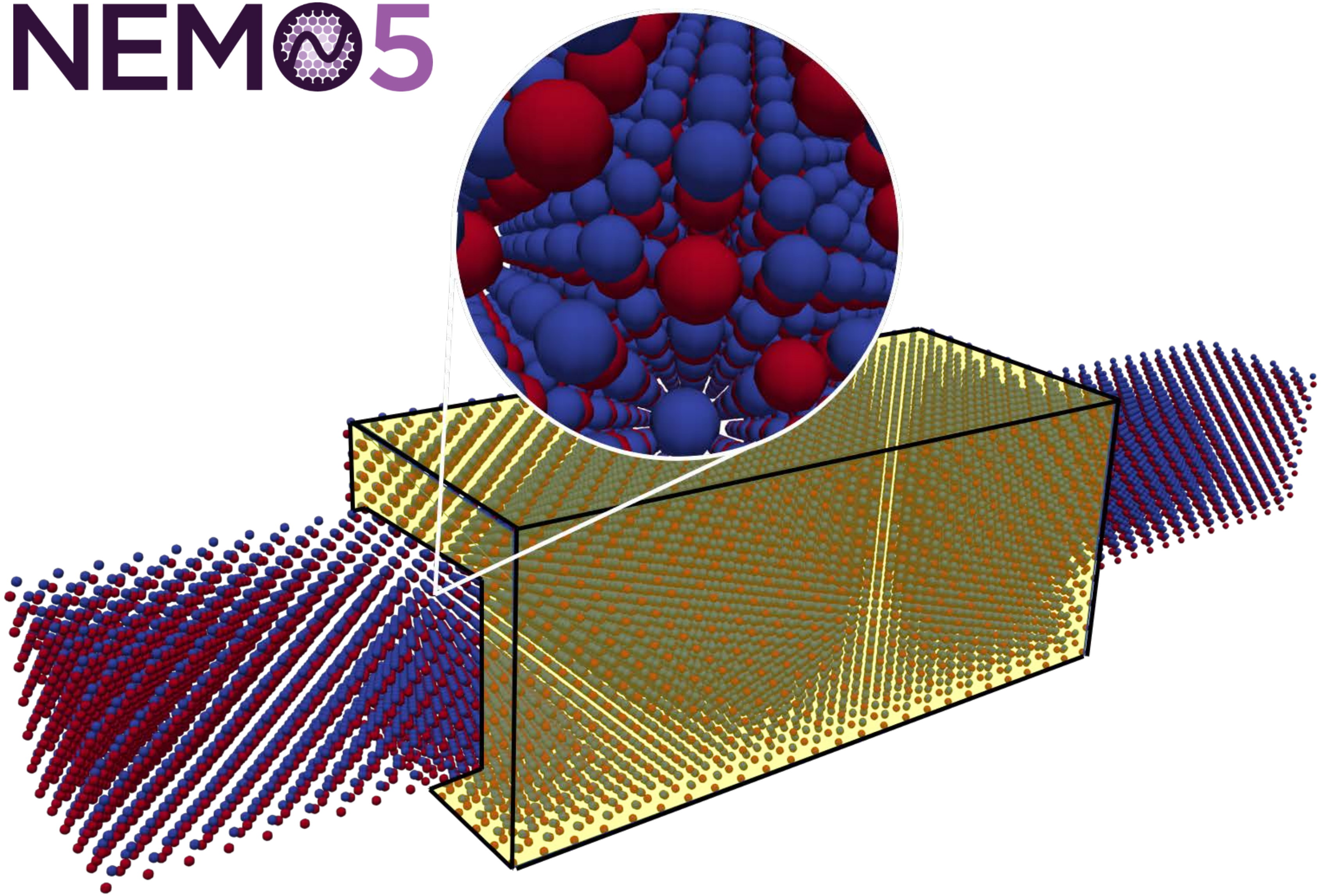
$$Re[\Sigma^R(E)] = \frac{i}{\pi}\mathcal{P}\int dE' \frac{Im[\Sigma^R(E')]}{E - E'}$$

- Responsible for shifting resonance energies
- In the form of Kramers-Kronig relations/Hilbert transform

$$H(u)(t) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{u(\tau)}{t - \tau}\, d\tau$$

Hilbert transform in mode space is faster: < 1% of operations

D. A. Lemus, J. Charles, and T. Kubis, “Mode-space-compatible inelastic scattering in atomistic nonequilibrium Green’s function implementations,” J. Comput. Electron., no. 19, 1389–1398, 2020.

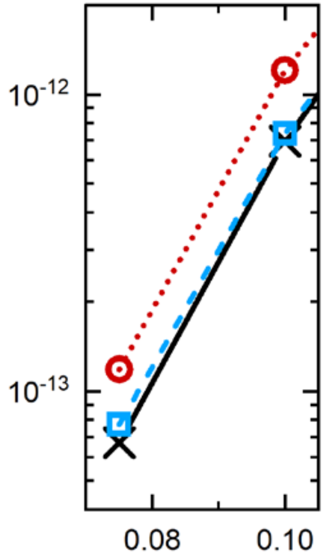


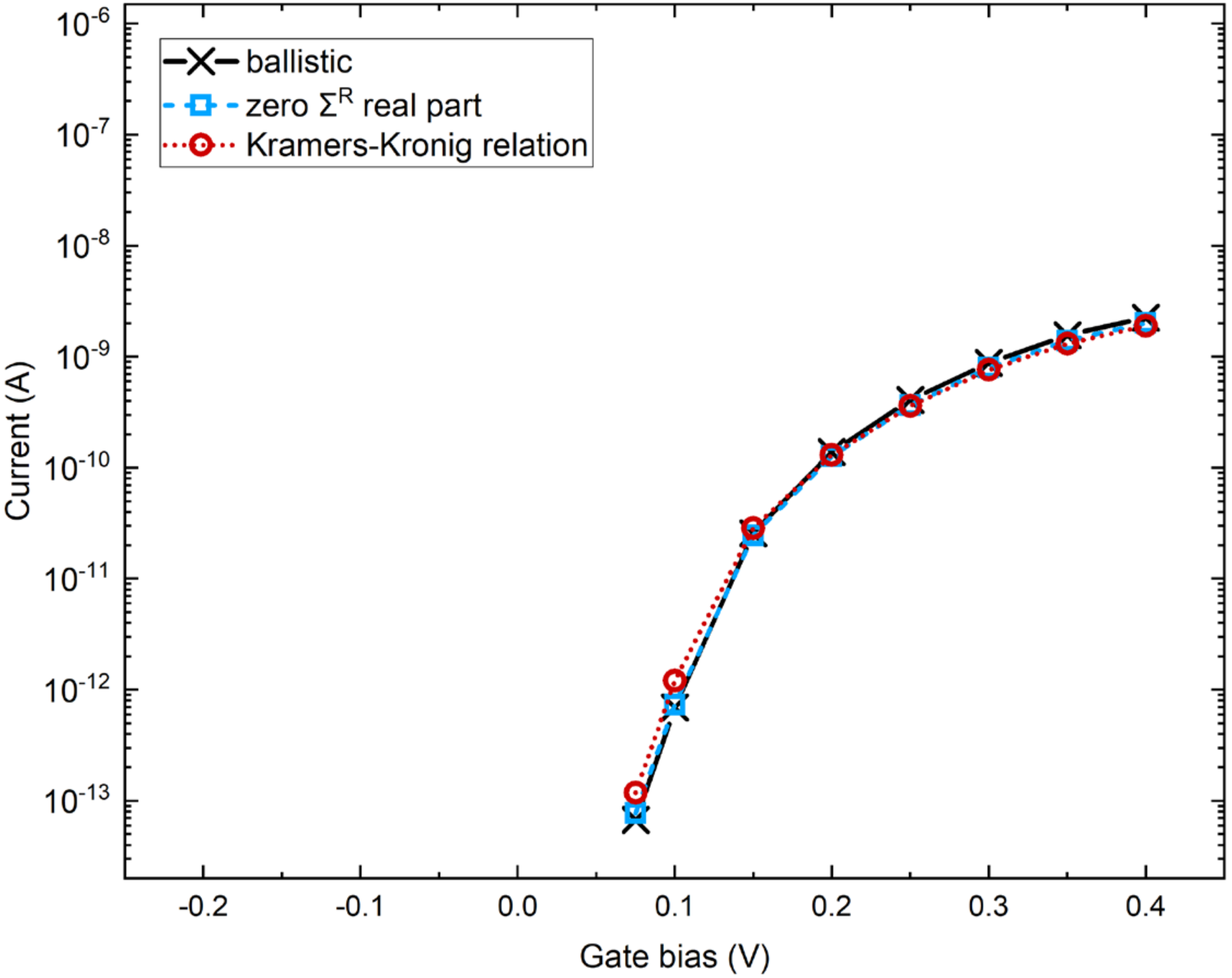
- InAs tunnel FET
- Atomistic tight binding
- Acoustic phonon scattering, optical phonon scattering, polar-optical phonon scattering
- Three cases:
  - Ballistic only
  - Scattering, zero real Σ^R
  - Scattering Σ^R from Kramers-Kronig relation
- All in mode space

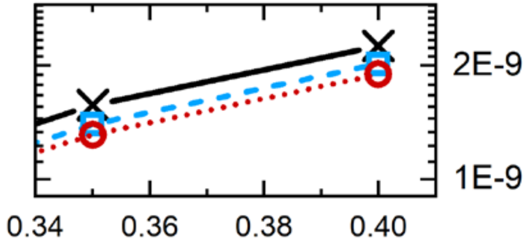
D. A. Lemus, J. Charles, and T. Kubis, "Mode-space-compatible inelastic scattering in atomistic nonequilibrium Green's function implementations," J. Comput. Electron., no. 19, 1389–1398, 2020.

InAs TFET: 2.4nm x 2.4nm

Scattering increases OFF current







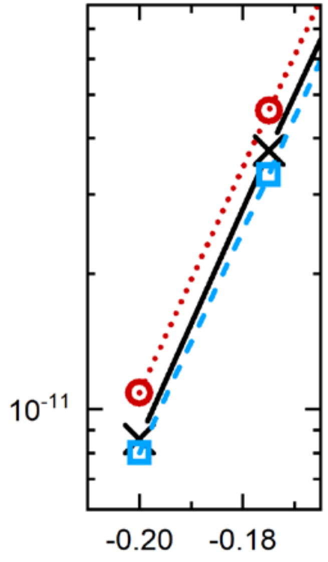
Scattering decreases ON current

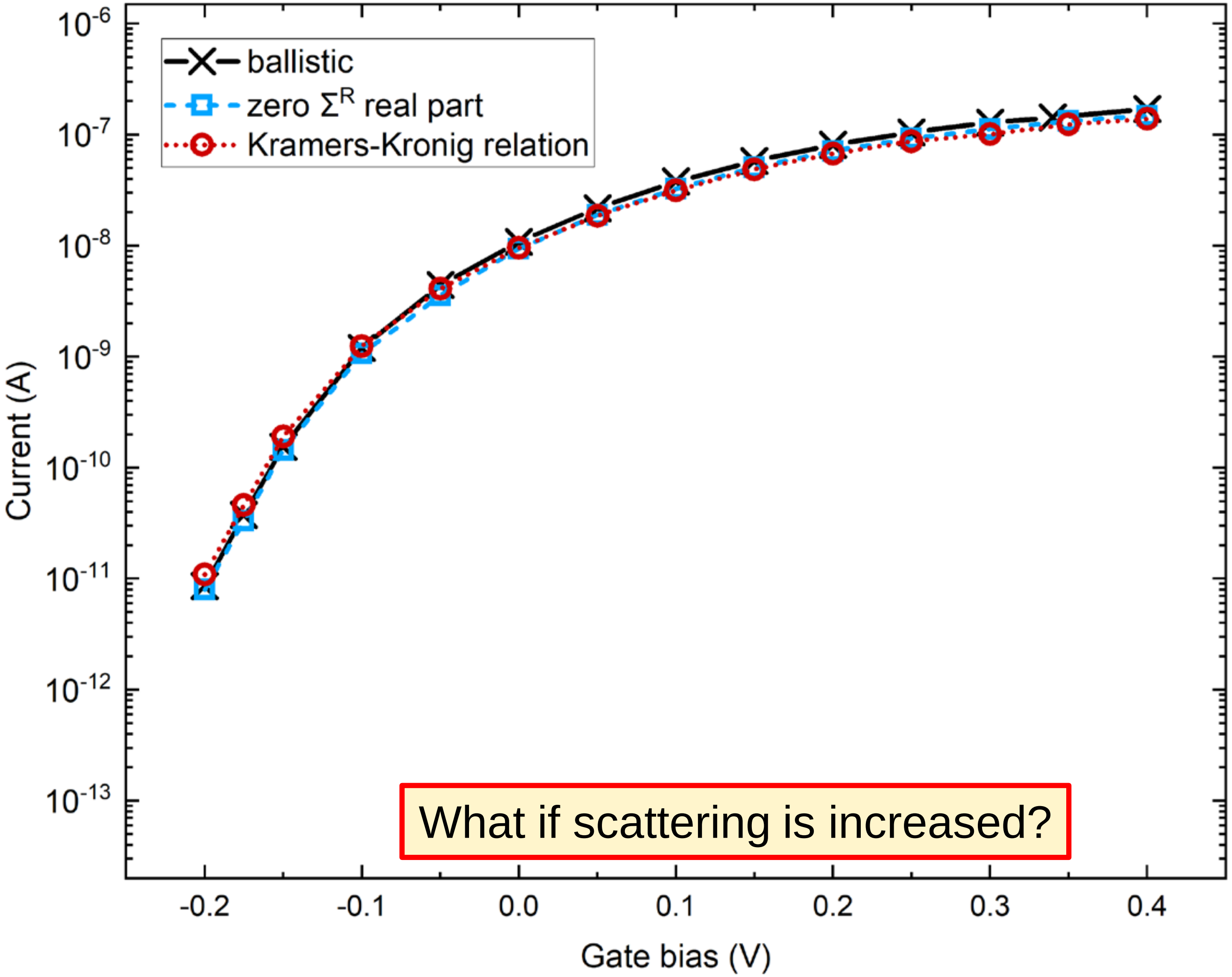
D. A. Lemus, J. Charles, and T. Kubis, "Mode-space-compatible inelastic scattering in atomistic nonequilibrium Green's function implementations," J. Comput. Electron., no. 19, 1389–1398, 2020.

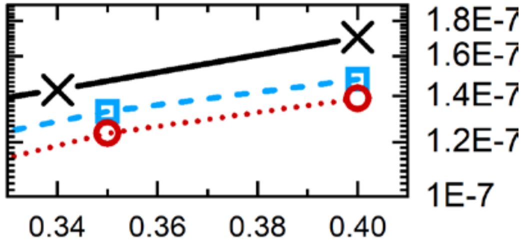
InAs TFET: 3.6nm x 3.6nm

$Re\{\Sigma^R\} = 0$ decreases OFF current

$Re\{\Sigma^R\} \neq 0$ increases OFF current

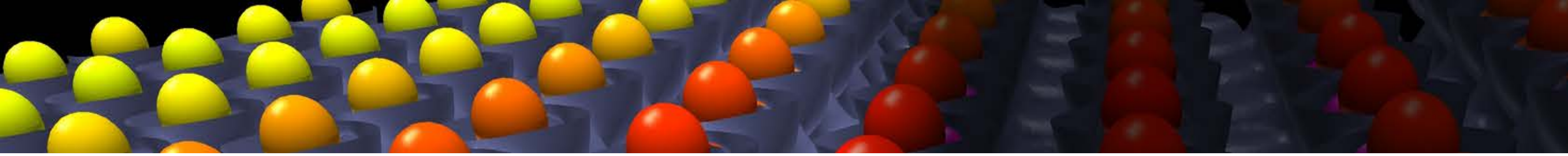






Scattering decreases ON current

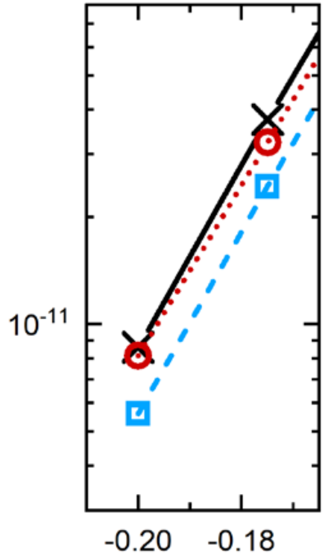
D. A. Lemus, J. Charles, and T. Kubis, "Mode-space-compatible inelastic scattering in atomistic nonequilibrium Green's function implementations," J. Comput. Electron., no. 19, 1389–1398, 2020.

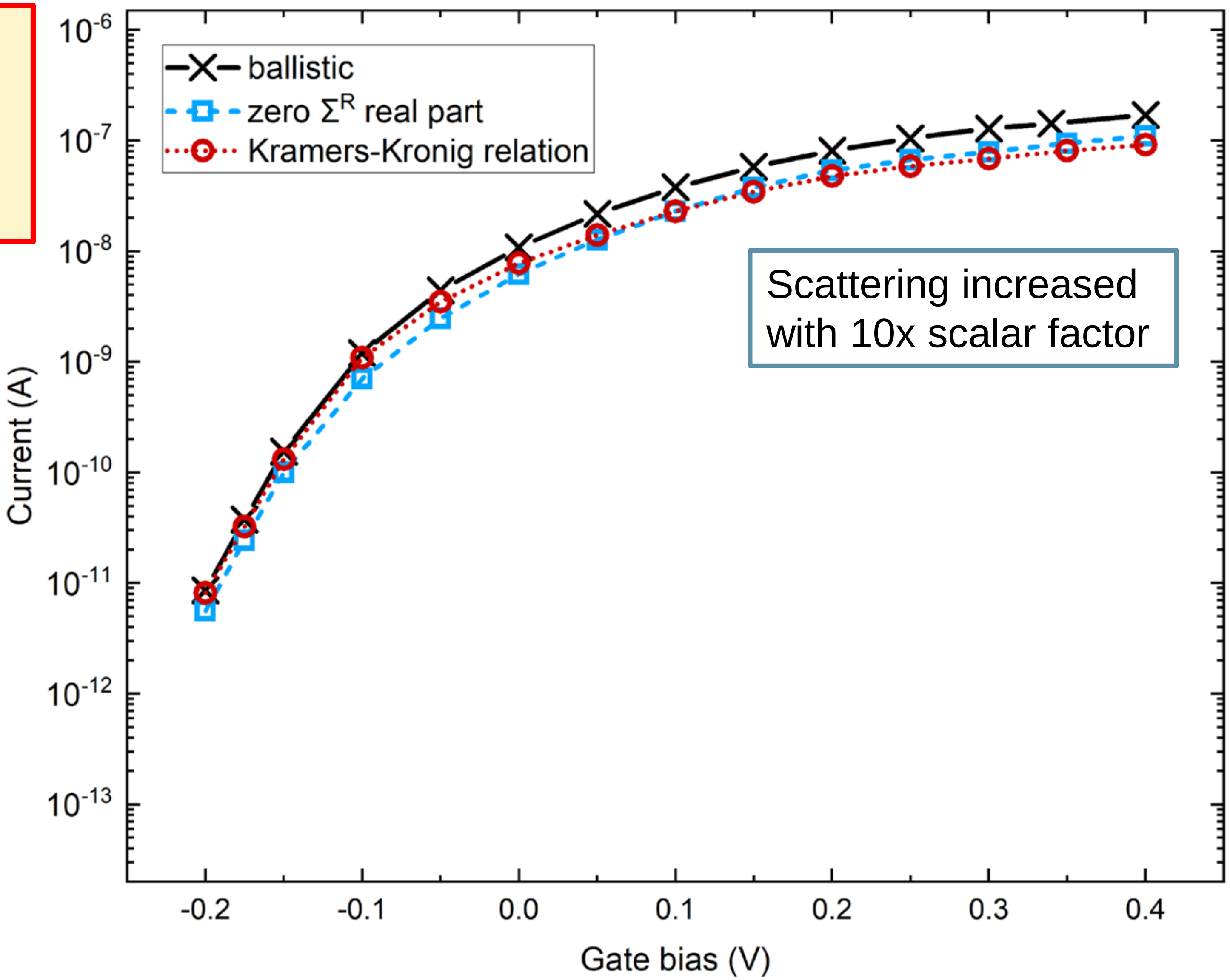


InAs TFET: 3.6nm x 3.6nm with 10x scattering

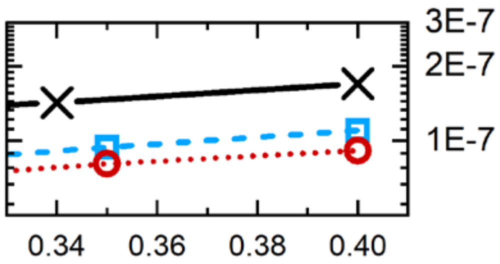
Situation-dependent; real part of Σ^R must be included

Scattering decreases OFF current





Scattering increased with 10x scalar factor



Scattering decreases ON current

Greater effect from real part

D. A. Lemus, J. Charles, and T. Kubis, "Mode-space-compatible inelastic scattering in atomistic nonequilibrium Green's function implementations," J. Comput. Electron., no. 19, 1389–1398, 2020.

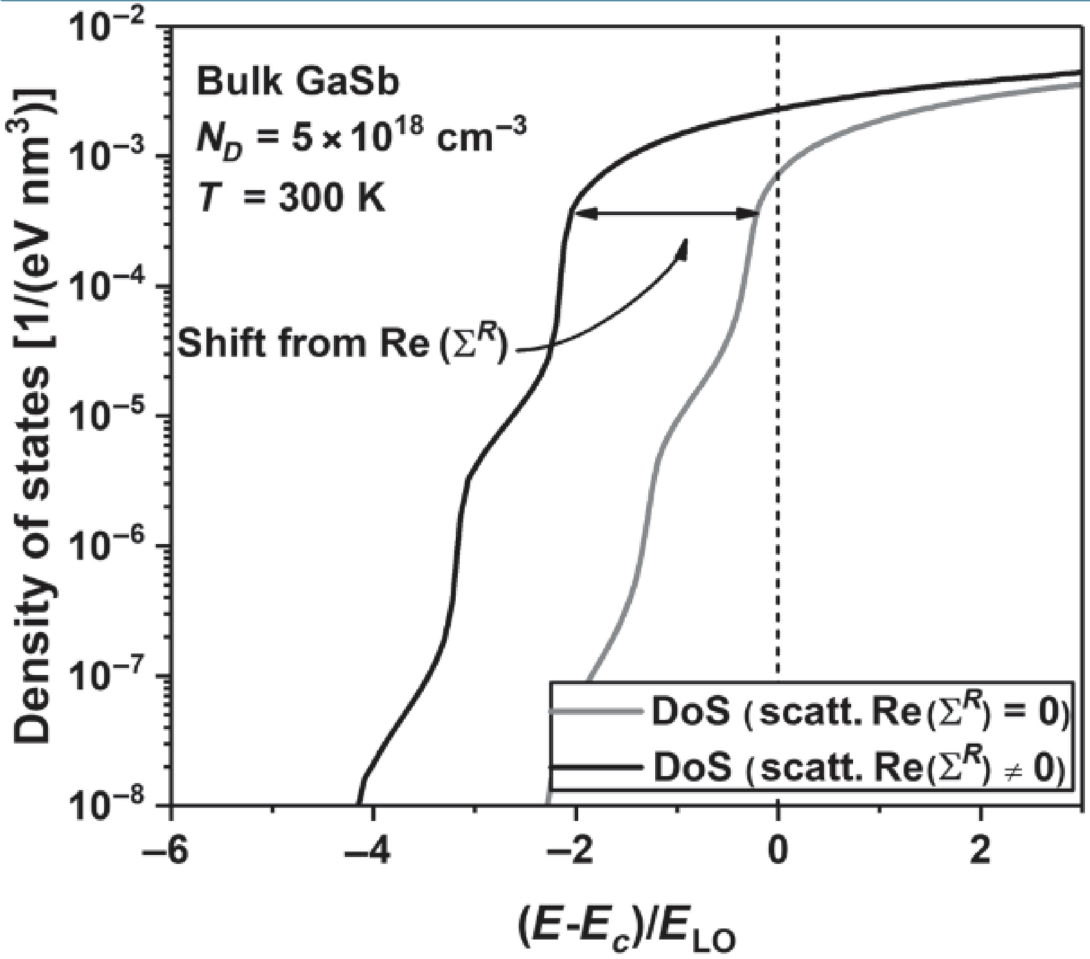
Reason for shift in current

Previous NEMO5 results, shown in IWCN 2019

Previous results did not include mode space, but current results do

Exact solution of Σ^R, in mode space, available in NEMO5

Energy-resolved conduction band density of states

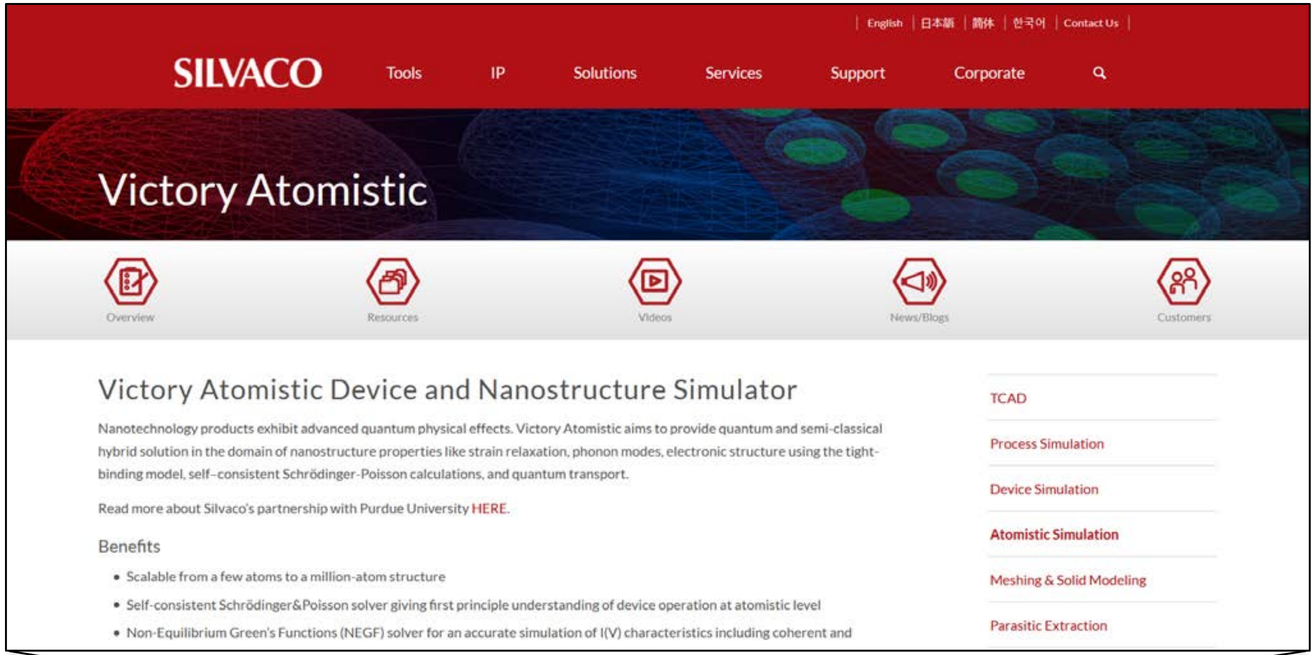


P. Sarangapani, et al., "Band-tail Formation and Band-gap Narrowing Driven by Polar Optical Phonons and Charged Impurities in Atomically Resolved III-V Semiconductors and Nanodevices," Phys. Rev. Appl., vol. 12, no. 4, p. 1, 2019.

Where to find our software

NEMO5

SILVACO



https://silvaco.com/tcad/atomistic-simulation/

Thank you!