Time-resolved computational method for atomistic open system simulations

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INTRODUCTION

Time-resolved quantum transport simulations are useful for accurate predictions of turn on energy-delay characteristics of logic devices [1]. Furthermore, time-resolved quantum simulations provide means to study novel device phenomena, e.g. electron pumps [5]. They can also be utilized for dissipation calculations due to phonon scattering with a multiscale time-stepping algorithm where phonons are real space lattice vibrations that enter the Hamiltonian as inhomogeneous strain.

We present a method based on the mixed energy-time space scattering matrix approach. It has clear connection to Green's functions [2] and the following advantages. First, as an integral part of our comprehensive simulation tool [4], it can be used to simulate realistic materials and geometries in atomistic tight-binding basis. Second, for not too high excitation rates it directly relies on the efficient transfer matrix method (TMM) for lead self-energies [3].

THEORY AND COMPUTATIONAL ASPECTS

Partitioning the wave function (wf) into injected and scattered lead Bloch modes and exposing the scattering matrix, we arrive at $i\hbar\partial\boldsymbol{\psi}_{\mathrm{E}}(t)/\partial t = [\mathrm{h}_{\mathrm{E}}(t) - E(t)]\,\boldsymbol{\psi}_{\mathrm{E}}(t) + \mathrm{I}_{\mathrm{E}}(t)$, where $\boldsymbol{\psi}_{\mathrm{E}}$, h_{E}, and I_{E} are the wf, Hamiltonian, and lead injection term in the mixed scattered-mode/orbital space, and $\mathrm{E(t)}$ is the injection energy. Equivalently, the scattered-mode space degrees of freedom (DOF) can be eliminated by explicitly calculating the self-energy $\Sigma(\mathrm{t})$ in orbital space.

When the above equation is used directly with the lead TMM the phase coherence between the device and leads may be lost, due to the arbitrary phase of the eigensolver. This can be resolved by consistent phase normalization in the leads. Furthermore, the scattered-mode space DOFs in $\mathrm{h_E(t)}$ contain multiple energies due to the time-dependent Hamiltonian. Closely spaced energies may lead to an unstable matrix preventing straightforward inclusion of ever more energies in the scattered mode space. The wide-band approximation (WBA) can be applied if the excitation rate is not too high. It amounts to keeping only the injected energy in the scattered-mode space, equivalent to $\int du\mathbf{\Sigma(t-u)\Psi_E(u)} \rightarrow \mathbf{\Sigma(E)\Psi_E}$.

RESULTS

Time resolved simulations are performed for a Si nanowire with $2.1\mathrm{x}2.1\mathrm{nm}$ cross section and $\sim 20\mathrm{nm}$ length in atomistic $\mathrm{sp_3d_5s^*}$ basis. The system has $\sim 49 \cdot 10^3$ orbital DOFs and ~ 270 modes per energy. The time-dependent bias is a 4nm wide rectangular barrier in the center of device, whose $10\mathrm{mV}$ amplitude has a variable $\mathrm{mV/ps}$ rising edge. The time resolved data is calculated in the WBA. Fig. 1 shows the 3D atomic wf magnitude and plots its evolution along a chain of atoms. Initial homogeneous left injected state evolves into the wf that shows reflection due to the potential barrier with $10\mathrm{mV}$ amplitude and $1\mathrm{mV/ps}$ rising edge. There are no reflection artifacts at the open boundaries. Crank-Nicholson time-stepping scheme is used with $\mathrm{dt} = 1\mathrm{fs}$. Fig. 2, shows the corresponding time-resolved reflection R and transmission T probabilities, while Fig. 3 shows the probability current conservation $(\mathrm{R+T})$ for $1\mathrm{mV/ps}$, $2\mathrm{mV/ps}$, and $10\mathrm{mV/ps}$ rising edges. Probability conservation is less rigorous for higher excitation rates in the WBA, due to a larger energy variation of the injected state. The upper limit for the validity of the WBA is $\sim 1\mathrm{mV/ps}$, which corresponds to a few GHz in realistic transistors. Interestingly, all three excitation rates show identical long time wf, Fig. 4.

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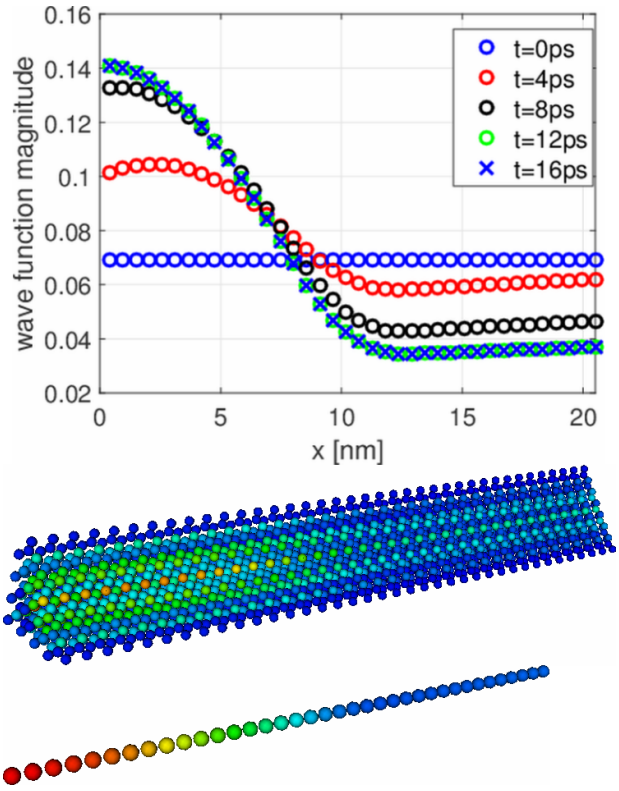

Fig. 1. Top: s orbital wave function magnitude along a chain of atoms at 1.8x0.4nm for left injection at energy 1.515eV (2 propagating modes). The barrier rising edge is $1\mathrm{mV/ps}$ and the total rise time is 10ps. There are no visible artificial reflections at device/lead interfaces. Middle and bottom: diagonal cross section of the nanowire and the selected chain of atoms corresponding to the top figure at 15ps.

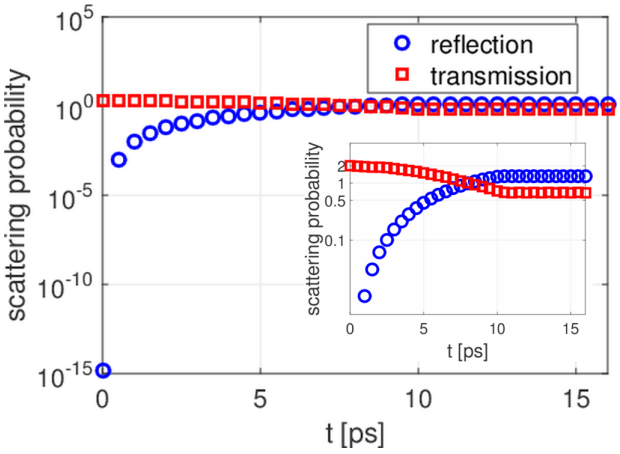

Fig. 2. T and R corresponding to data in Fig. 1.

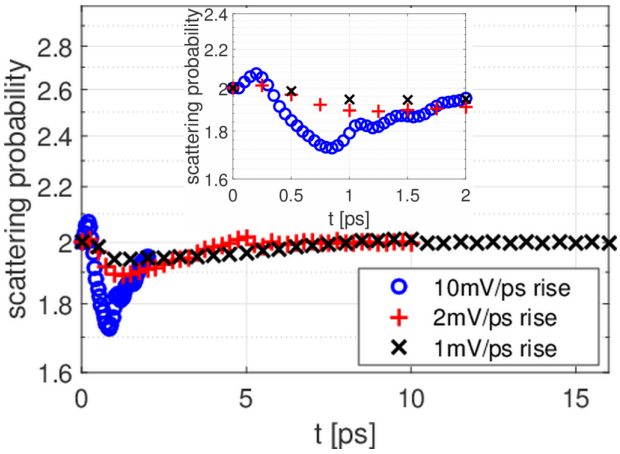

Fig. 3. Probability current conservation (T + R) for $1\mathrm{mV/ps}$, $2\mathrm{mV/ps}$, and $10\mathrm{mV/ps}$ rising edges. Upper validity limit for the wide-band approximation around $1\mathrm{mV/ps}$, corresponding to a few GHz in realistic transistors.

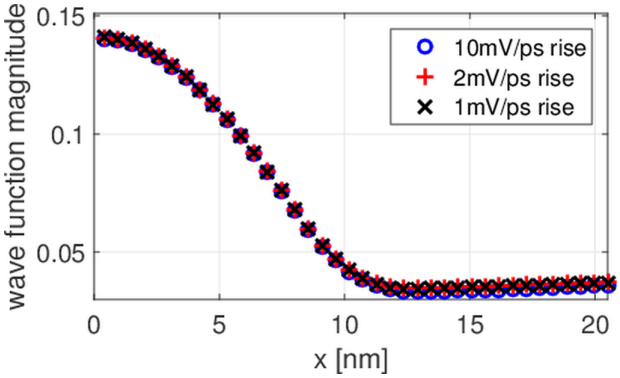

Fig. 4. Unlike Fig. 3, long time open boundary wave function magnitudes match well for three different excitation rates.

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REFERENCES

[1] D. E. Nikonov and I. A. Young, IEEE Journal on Exploratory Sold-State Computational Devices and Circuits, DOI: 10.1109/JXCDC.2015.2418033 (2015).

[2] B. Gaury, J. Weston, M. Santin, M. Houzet, C. Groth, and X. Waintal, Phys. Rep. **534**, 1-37 (2014).

[3] M. Luisier, A. Schenk, and W. Fichtner, Phys. Rev. B **74**, 205323 (2006).

[4] J. E. Fonseca, T. Kubis, M. Povolotskyi, B. Novakovic, A. Ajoy, G. Hegde, H. Ilatikhameneh, Z. Jiang, P. Sengupta, Y. Tan, and G. Klimeck, J. Comput. Electron. **12**, 592 (2013).

[5] G. Stefanucci, S. Kurth, A. Rubio, and E. K. U. Gross, Phys. Rev. B **77**, 075339 (2008).