11th International Workshop on Computational Electronics
TU Wien, 25-27 May 2006

Ultrafast Wigner Transport in Quantum Wires

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Transport Models

The early time dynamics of highly non-equilibrium confined carriers incorporates a number of quantum phenomena, which are subject of active investigations [1]. We explore two models of evolution of an initial distribution of carriers interacting with optical phonons in a quantum wire. The carriers can be injected or optically excited, an electric field E can be applied along the direction z of the wire. The models are introduced by the Boltzmann-like equation

$$\mathcal{L}f_w(z,k_z,t) = \int dk_z' \int_0^t dt' \left\{S'f_w' - Sf_w\right\} \quad (1)$$

Here $\mathcal{L}$ is the Liouville operator, the Wigner function on the right $f' = f_w(\mathcal{Z}(t'), k_z'(t'), t')$ depends on the Newton trajectory $z(t'), k_z(t')$ as follows:

$$\mathcal{Z}(t') = z(t') + \frac{\hbar(k_z - k_z')}{2m}\Delta_c; \quad \Delta_c = t - t'. \quad (2)$$

$S(k_z, k_z', t, t')$ is obtained from the Boltzmann scattering rate in the wire by replacing the energy conserving δ-function by the real part of

$$\mathcal{D} = \frac{1}{2}e^{-\int_{t'}^{t}\Gamma(\frac{k_z(\tau)+k_z'(\tau)}{2})+i\frac{\epsilon(k_z(\tau))-\epsilon(k_z'(\tau))-\hbar\omega}{\hbar}d\tau}, \quad (3)$$

Γ is the total Boltzmann out-scattering rate, and Sf_w is obtained from $S'f_w'$ by the usual exchange of the primed and unprimed momentum variables. As suggested by the energy term in (3), a ground state is assumed in the plane of confinement. The two evolution models are counterparts of the Levinson (L), $\Gamma = 0$, and the Barker-Ferry (B-F), $\Gamma \neq 0$ equations, now generalized to account for a space-dependent evolution. Derived [2] from the electron-phonon Wigner equation, (1) accounts for the finite time of the electron collisions.

Physical Features and Simulations

The interval Δ_c is identified as the collision duration time. The two models differ in the way of treatment of collisions with different Δ_c. While in the L case all collisions are welcome, in the B-F case long correlation times are damped by Γ in (3).

A GaAs quantum wire with 10 nm square cross section has been considered in the numerical experiments. The choice $T = 0$K provides a clear reference picture, where classical electrons can only emit phonons and since the constant POP energy form replicas of the initial distribution. The later is chosen to be Gaussian in both energy and space. A backward Monte Carlo method is used to evaluate directly the Wigner function f_w and its first moments - the density $n(z)$ and the wave vector distribution $f(k_z)$. To analyze certain numerical aspects the later are computed also from the values of f_w. We summarize the quantum effects revealed in the simulation results. The non-Markovian evolution gives rise to a retardation in the build-up of the replicas. The retardation is larger in the B-F model (Figs. 1 and 2). The lack of energy conservation causes broadening of the replicas and appearance of electrons in the classically forbidden energy region. Certain carriers reach larger distances than the classically fastest ballistic electrons (Fig. 3). The modification of the classical trajectory caused by Δ_c in (2) has an important physical effect. The lack of this term leads to negative densities around the front of the fastest quantum electrons (Fig. 4).

References

[1] M. Herbst, M. Glanemann, V. Axt, and T. Kuhn, *Electron-Phonon Quantum Kinetics for Spatially Inhomogeneous Excitations*, Physical Review B, **67**, 195305:1–18 (2003).
[2] The derivation is due to a collaboration with groups from ASU and Modena Univ. and will be published elsewhere.

ISBN 3-901578-16-1

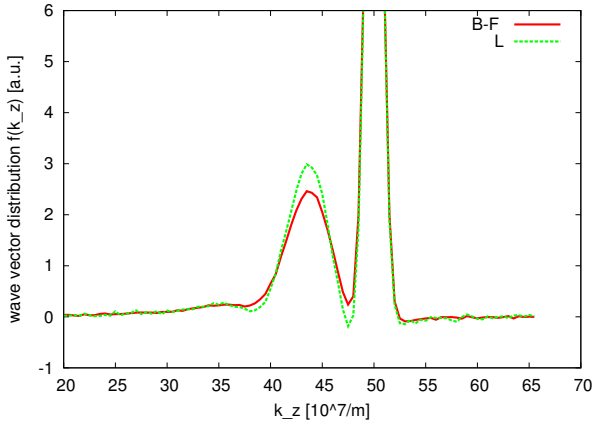

Fig. 1. Wave vector distribution $f(k_z)$, plotted in a window of positive k_z, after 150 femtoseconds evolution time. $f(k_z)$ is computed from the values of the Wigner function which has been evaluated with a high precision in 800×260 z and k_z points and then numerically integrated on z. The initial peak is centered at 5×10^8 m^{-1}. The classical evolution will form exact replicas of the initial peak shifted by the phonon energy to the left. The first quantum replicas are much broadened due to the lack of energy conservation. The peak-to-valley ratio of the L curve is more pronounced, in particular it touches the zero in the valley, which demonstrates the retardation of the B-F evolution. However the appearance of electrons above the initial distribution, which can be observed at smaller evolution times, is already missing. The reason is explained below.

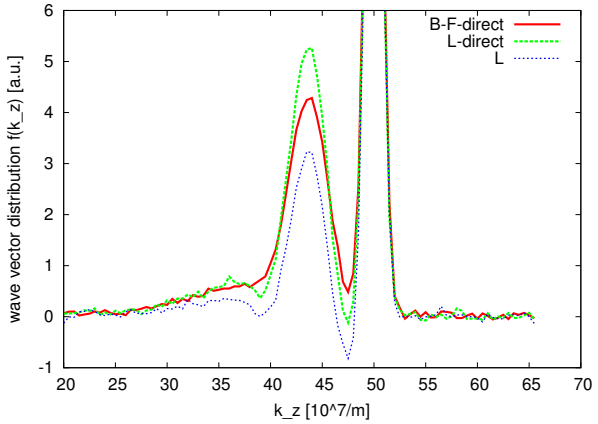

Fig. 2. Broadening and retardation effects after 175 femtoseconds evolution time. The L curve, computed from f_w, differs significantly from the directly computed with the Monte Carlo method counterpart and becomes unphysical. The reason is that with the increase of the evolution time f_w becomes less and less smooth function and thus more and more points are needed for a precise evaluation of the corresponding functionals. This suggests that a direct evaluation of any physical observable is necessary for larger evolution times.

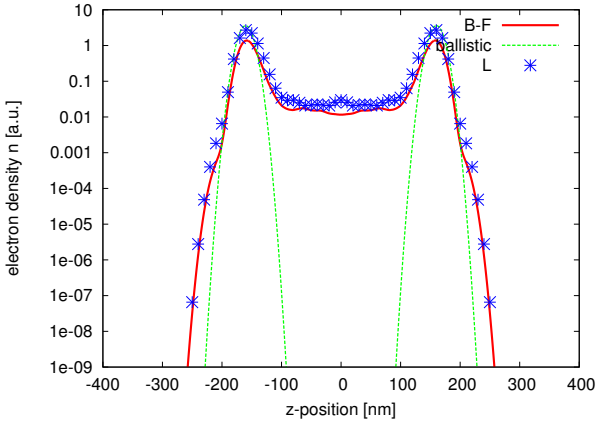

Fig. 3. Electron density after 175 femtoseconds of evolution presented in a logarithmic scale. The initial distribution centered at 0 splits in two peaks, which move in the positive and the negative directions of the wire. There are no ballistic electrons left around the center. On contrary, due to the electrons which lost energy from the collisions, the two quantum solutions demonstrate finite density in the central part. Above and below the ballistic front, at around 230 and -230 nanometers, respectively, there are faster quantum electrons which gained energy during the finite collisions. The difference in the spatial behavior of the two models is due to the effects of retardation.

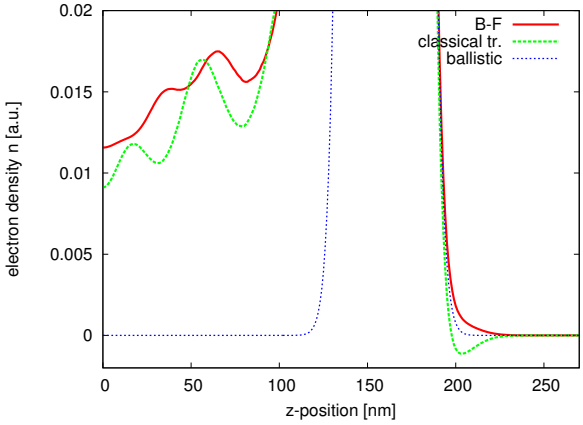

Fig. 4. Electron density obtained after 175 femtoseconds evolution from the B-F model plotted around the ballistic curve in the positive direction of the wire. The excess electron density above 200 nanometers is well demonstrated by the quantum solution. If the term accounting for the effect of the finite collision duration Δ_c is neglected in (2), $\mathcal{Z}(t')$ becomes equivalent to the classical trajectory $z(t')$. The third curve on the plot is obtained by using classical trajectories in the B-F model. This leads to a modification of the electron distribution and appearance of negative densities in the region around 200 nanometers. Thus, this term has an important role in maintaining the physical relevance of the quantum evolution process.