Journal of Computational Electronics 1: 27–31, 2002

A Space Dependent Wigner Equation Including Phonon Interaction

M. NEDJALKOV, H. KOSINA, R. KOSIK AND S. SELBERHERR
Institute for Microelectronics, TU Vienna, Gusshausstrasse 27–29, A-1040 Vienna, Austria
Nedjalkov@iue.tuwien.ac.at

Abstract. We present a kinetic equation which is obtained after a hierarchy of approximations from the generalized Wigner function equation which accounts for interaction with phonons. The equation treats the coherent part of the transport imposed by the nanostructure potential at a rigorous quantum level. It is general enough to account for the quantum effects in the dissipative part of the transport due to the electron-phonon interaction. Numerical experiments demonstrate the effects of collisional broadening, retardation and the intra-collisional field effect. The obtained equation can be regarded as a generalization of the Levinson equation for space dependence. An analysis shows that the equation is nonlocal in the real space. This quantum effect is due to the correlation between the interaction process and the space component of the Wigner path.

Keywords: Wigner function, nanostructure, quantum electron-phonon interaction, Monte Carlo method

Introduction

The quantum transport in far from equilibrium conditions is determined not only by the nanoscale of the device potential, but also by dissipative processes due to interaction with phonons. Usually the boundary conditions are given by electrons in traveling states entering into a nanodevice from the leads. If only the coherent part of the transport is considered, these states remain isolated from the notch states, which exist at the lower energy regions of the device potential. In this case unphysical simulation results can be obtained (Frensley 1990). Thus dissipative processes which are due to interaction with phonons must be taken into account. The electron-phonon interaction links the traveling and the notch states and correctly redistributes the electrons into the device. It has been shown that the electron phonon interaction greatly affects the device parameters of the resonant tunneling diodes (Zhao *et al*. 2001). While the theoretical and numerical aspects of the application of the coherent Wigner equation are well established, the inclusion of the electron-phonon interaction is still under investigation.

Approximations

A rigorous inclusion of the phonon interaction is provided by the generalized Wigner function (WF) (Bordone *et al*. 1999) $f_w(\mathbf{r}, \mathbf{p}, \{n\}, \{m\}, t)$ which along with the electron coordinates $\mathbf{r}$, $\mathbf{p}$ depends also on the phonon coordinates $\{n\} = \{n_1, \ldots, n_{\mathbf{q}}, \ldots\}$ with $n_{\mathbf{q}}$ being the number of phonons in mode $\mathbf{q}$. Of interest is the reduced WF $f_w(\mathbf{r}, \mathbf{p}, t)$, which is obtained by taking the trace of the generalized WF over the phonon system and thus depends only on the electron coordinates. An exact equation for the reduced WF can not be obtained from the generalized Wigner equation, since the trace operation does not commute with the electron-phonon interaction Hamiltonian.

The task is to obtain from the generalized Wigner equation a closed equation for the reduced WF. The approximations include a weak scattering limit in the phonon interaction, assumption of an equilibrium phonon system, mean phonon number approximation, and an effective field in the scattering-Wigner potential correlation.

The generalized Wigner equation couples an element $f_w(\ldots, \{n\}, \{m\}, t)$ to four neighborhood elements

given by $f_w(\ldots,\{n\}\pm 1_{\mathbf{q}},\{m\},t)$, $f_w(\ldots,\{n\},\{m\}\pm 1_{\mathbf{q}},t)$ for any phonon mode $\mathbf{q}$. The equations for the four neighboring elements involve elements which are secondary neighbors with respect to the $(\{n\},\{m\})$ element. In this way the diagonal elements, involved in the trace operation are linked to all off-diagonal elements. As a first approximation we consider the weak scattering limit, which neglects all links to the elements placed outside the nearest off-diagonals. This assumption ignores higher order electron phonon interactions.

The evolution process begins with an initially decoupled electron-phonon system and involves transitions between the diagonal and the first off-diagonal elements. The next approximation is to replace the occupation numbers $n_{\mathbf{q}}$ involved in the transitions with the equilibrium phonon number $n(\mathbf{q})$: This is done by performing the trace operation at the consecutive time steps of the evolution. With this it is assumed that the phonons stay in equilibrium during the evolution (phonon bath). This allows to perform the trace operation and to obtain a closed equation set for the reduced WF. The set consists of a main equation for the reduced WF coupled to two auxiliary equations. The latter arise from the first off-diagonal terms of the generalized WF and describe the electron-phonon interaction. While the equation for the reduced WF is real, the two auxiliary equations are complex and mutually conjugated. The formal solution of the auxiliary equations is given by the Neumann series, which can be substituted into the main equation.

The implicit inclusion of the Neumann expansions in the main equation is rather inconvenient and we look for an approximation where the two auxiliary equations can be solved explicitly. If the potential term in the two auxiliary equations is approximated by the mean homogeneous electric field $\mathbf{E}$ throughout the device (mean field approximation), the solution to the two auxiliary equations can be explicitly expressed in terms of the reduced WF. This approximation concerns only the phonon interaction, while the potential term in the equation for the reduced WF is treated exactly. A single equation for the reduced WF is obtained.

$$
\begin{aligned}
&f_w(\mathbf{r},\mathbf{p},t)\\
&\quad= f_0\big(\mathbf{r}_{(\mathbf{p},0)},\mathbf{p}_{(0)},0\big)+\int_0^t \mathrm{d}t'\int \mathrm{d}\mathbf{p}' V'_w\\
&\qquad\times\big(\mathbf{r}_{(\mathbf{p},t')},\mathbf{p}'-\mathbf{p}_{(t')}\big) f_w\big(\mathbf{r}_{(\mathbf{p},t')},\mathbf{p}',t'\big)\\
&\qquad+2\int_0^t \mathrm{d}t'\int_0^{t'}\mathrm{d}t''\sum_{\mathbf{q}'}F^2(\mathbf{q}')\\
&\qquad\times\cos\!\left(\int_{t''}^{t'}\mathrm{d}\tau\frac{1}{\hbar}\big(\epsilon\big(\mathbf{p}_{(\tau)}\big)-\epsilon\big(\mathbf{p}_{(\tau)}-\hbar\mathbf{q}'\big)-\hbar\omega_{\mathbf{q}'}\big)\right)\\
&\qquad\times\left\{n(\mathbf{q}')f_w\left(\mathbf{r}_{(\mathbf{p},t'')}+\frac{\hbar\mathbf{q}'}{2m}(t'-t''),\mathbf{p}_{(t'')}-\hbar\mathbf{q}',t''\right)\right.\\
&\qquad\left.-(n(\mathbf{q}')+1)f_w\left(\mathbf{r}_{(\mathbf{p},t'')}+\frac{\hbar\mathbf{q}'}{2m}(t'-t''),\mathbf{p}_{(t'')},t''\right)\right\}\\
&\qquad-2\int_0^t \mathrm{d}t'\int_0^{t'}\mathrm{d}t''\sum_{\mathbf{q}'}F^2(\mathbf{q}')\\
&\qquad\times\cos\!\left(\int_{t''}^{t'}\mathrm{d}\tau\frac{1}{\hbar}\big(\epsilon\big(\mathbf{p}_{(\tau)}\big)-\epsilon\big(\mathbf{p}_{(\tau)}+\hbar\mathbf{q}'\big)+\hbar\omega_{\mathbf{q}'}\big)\right)\\
&\qquad\times\left\{n(\mathbf{q}')f_w\left(\mathbf{r}_{(\mathbf{p},t'')}-\frac{\hbar\mathbf{q}'}{2m}(t'-t''),\mathbf{p}_{(t'')},t''\right)\right.\\
&\qquad\left.-(n(\mathbf{q}')+1)f_w\left(\mathbf{r}_{(\mathbf{p},t'')}-\frac{\hbar\mathbf{q}'}{2m}(t'-t''),\right.\right.\\
&\qquad\left.\left.\mathbf{p}_{(t'')}+\hbar\mathbf{q}',t''\right)\right\}
\end{aligned}
\tag{1}
$$

Here V'_w is obtained by the Wigner transform of the device potential V corrected by the potential of the homogeneous field $\mathbf{E}$. The rest of the notations will be explained below.

Analysis of the Equation

The reduced WF is expressed as a sum of contributions coming from the initial distribution, the interaction of the electron with the device potential and the electron-phonon interaction.

The contributions from the first two terms to the value of $f_w(\mathbf{r},\mathbf{p},t)$ occur on the Newton trajectory $(\mathbf{r}_{(\mathbf{p},t')},\mathbf{p}_{(t')})$ initialized by $\mathbf{r}$, $\mathbf{p}$ at time t. The initial condition f_0 evolves on this trajectory and adds to f_w its value at point $(\mathbf{r}_{(\mathbf{p},0)},\mathbf{p}_{(0)})$.

The term from the potential provides information to $f_w(t)$ from $f_w(t')$ at previous times $t'\in(0,t)$. This information is nonlocal in the momentum part of the phase space, but it is local in the real space part of the trajectory $\mathbf{r}_{(\mathbf{p},t')}$, $t'\in(t,0)$. The contribution of this term can be evaluated from the knowledge of $f_w(\mathbf{r}_{(\mathbf{p},t')},\mathbf{p}',t')$ at the past of the evolution defined on the real space part of the trajectory.

A novel effect arrises due to the correlation between the phonon momentum $\hbar\mathbf{q}'$ and the space component of the trajectory in the scattering terms. At the beginning of the scattering, the real trajectory is shifted by $\frac{\hbar\mathbf{q}/2}{m}(t'-t'')$. The interaction proceeds in two steps, e.g. for the terms in the first curly brackets: The first half

of a phonon momentum is absorbed (emitted) at t''. At t' the second half is absorbed—real absorption, or the first half is absorbed back (virtual emission). In both cases the position at t' is just the right one, $\mathbf{r}_{(\mathbf{p},t')}$, $\mathbf{p}_{(t')}$), which evolves to $\mathbf{r}$, $\mathbf{p}$ at t. The term related to the last curly brackets is analyzed in similar way. In contrast to the Wigner equation without phonon interaction, the obtained equation becomes nonlocal in the real space.

The classical limit $\hbar \to 0$ in the phonon interaction leads to a Wigner equation with a Boltzmann scattering term. For a bulk semiconductor with an applied electric field $\mathbf{E}$ the equation resembles the Levinson equation (Rammer 1991), or equivalently the Barker-Ferry equation without damping of the electron lifetime.

Simulation Results

We investigate equation for quantum effects which are purely due to the electron-phonon interaction. Equation (1) is written for a bulk semiconductor in presence of an applied electric field. Cylindrical coordinates (r, k, ϕ) with r chosen normal to the field direction are used in the wave vector space. A transformation is used which shifts the coordinate system in time with the electric field. To solve (1) a randomized backward Monte Carlo algorithm is applied (Gurov and Whitlock 2001).

Simulation results for *GaAs* with a PO phonon with constant energy $\hbar\omega$ are presented. The initial condition is a sharp Gaussian function of the energy. A very low temperature, where the physical system has a transparent semiclassical behavior is assumed. The solutions are obtained on cut lines parallel to the field, $(k > 0, r = 0)$, opposite to the field, $(k < 0, r = 0)$ and normal to the field, $(k = 0, r > 0)$.

Collisional Broadening and Retardation

The effects of collisional broadening and retardation exist already at zero electric field. Figures 1–3 present snapshots of the evolution of the semiclassical and quantum solutions $|k| f(0, |k|, t)$ for times 100 fs, 200 fs and 300 fs as a function of $|k|^2$. The quantity $|k|^2$ is proportional to the electron energy in units 10^{14} m^{-2}. Semiclassical electrons can only emit phonons and loose energy equal to a multiple of the phonon energy $\hbar\omega$. They evolve according to a distribution, patterned by replicas of the initial condition shifted towards low energies.

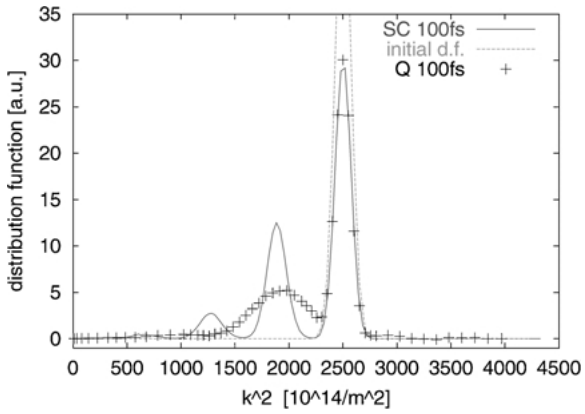

Figure 1. Initial distribution function (initial d.f.), semiclassical (SC) and quantum (Q) solutions $kf(0, k, t)$ for 100 fs evolution time at zero electric field.

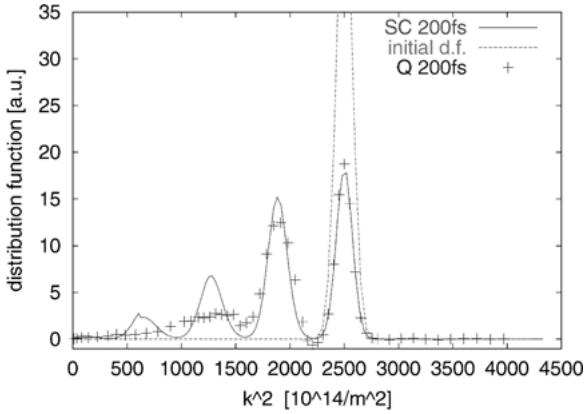

Figure 2. Initial distribution function (initial d.f.), semiclassical (SC) and quantum (Q) solutions $kf(0, k, t)$ for 200 fs evolution time at zero electric field.

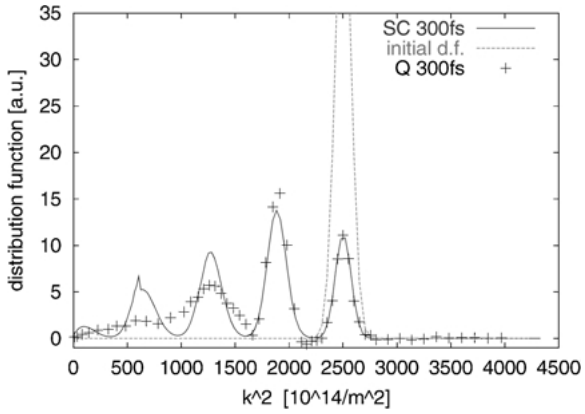

Figure 3. Initial distribution function (initial d.f.), semiclassical (SC) and quantum (Q) solutions $kf(0, k, t)$ for 300 fs evolution time at zero electric field.

The electrons cannot appear in the region above the initial distribution. The quantum solutions demonstrate two effects of deviation from the semiclassical behavior. There is a retardation in the build up of the remote peaks with respect to the initial condition peaks. The replicas are broadened and the broadening increases with the distance to the initial peak. The broadening is due to the lack of energy conservation in the interaction. At low evolution times the cosine function in (1) weakly depends on the phase space variables. With the increase of the time, the cosine term becomes a sharper function of these variables and in the long time limit tends to the semiclassical delta function. Accordingly the first replica of the 100 fs is broadened. The quantum solution resembles the main pack and the first replica of the semiclassical solution after 300 fs evolution time while the remote replicas remain broadened. The retardation of the quantum solutions is associated with the memory character of the equation. The two time integrals in (1) lead to a delay of the build up of the replicas as compared to the single time integral in the Boltzmann case.

Intra-Collisional Field Effect

Figure 4 compares the 200 fs solutions as a function of $k < 0$ for different positive values of the field. The first replica peaks are shifted to the left by the increasing electric field. The numerical solution in the semiclassically forbidden region, above the initial condition, demonstrates enhancement of the electron population with the growth of the field.

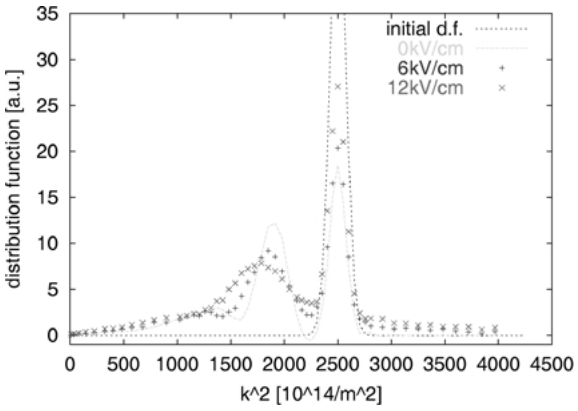

Figure 4. Solutions $|k|f(0,k,t)$, at negative k values, and evolution time 200 fs. The electric field is 0, 6 kV/cm, and 12 kV/cm.

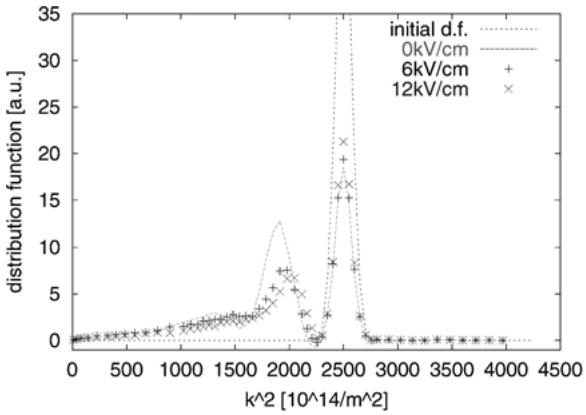

Figure 5. Solutions $kf(0,k,t)$ for positive k values and evolution time 200 fs. The electric field is 0, 6 kV/cm, and 12 kV/cm.

For states below the initial condition the energy of the field is added to the phonon energy. Accordingly the solution behaves as in presence of a phonon with energy higher than $\hbar\omega$; the distance between the first replica and the initial condition increases. For states above the initial condition the energy of the field reduces the phonon energy and thus the electron population in the vicinity of the initial condition increases. Just the opposite effects appear in the region of positive k values. This is demonstrated in Fig. 5. The peaks of the first replica are shifted to the right and there is no enhancement of the electron population above the initial condition. The field has a pronounced effect on the broadening and retardation of the solutions: A comparison of the first replicas and the main peaks under the initial condition on Figs. 4 and 5 show that the field influences the effects of collisional broadening and the retardation.

Conclusion

Starting from a full quantum mechanical model we have identified the physical assumptions necessary to derive an approximate but closed model for the reduced Wigner function. The obtained equation can be regarded as a generalization of the Levinson equation that includes the real space dependence. It is shown that the finite duration of the phonon interaction gives rise to a space non-locality of the quantum transport process. Quantum effects in electron phonon interaction have been demonstrated numerically. Observed are collisional broadening, retardation and the intra-collisional field effect.

Acknowledgment

This work has been supported by the IST program, project NANOTCAD, IST-1999-10828, and the "Christian Doppler Forschungsgesellschaft", Vienna, Austria.

References

Bordone P., Pascoli M., Brunetti R., Bertoni A., and Jacoboni C. 1999. Quantum transport of electrons in open nanostructures with the Wigner function formalism. Physical Review B 59(4): 3060–3069.

Frensley W.R. 1990. Boundary conditions for open quantum systems driven far from equilibrium. Reviews of Modern Physics 62(3): 745–791.

Gurov T. and Whitlock P. 2001. Statistical algorithms for simulation of electron quantum kinetics in semiconductors—Part I. In: Proceedings of the 3rd International Conference on Large-Scale Scientific Computations, 2001, LNCS, Springer.

Rammer J. 1991. Quantum transport theory of electrons in solids: A single-particle approach. Reviews of Modern Physics 63(4): 781–817.

Zhao P., Cui H.L., Woolard D.L., Jensen K.L., and Buot F.A. 2001. Equivalent circuit parameters of resonant tunneling diodes extracted from self-consistent Wigner-Poisson simulation. IEEE Transactions on Electron Devices 48(4): 614–627.