A Wigner Equation for the Nanometer and Femtosecond Transport Regime

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Abstract

We present a quantum-kinetic equation which describes the transport phenomena in nanoelectronic devices. The equation can be regarded as a generalization of the Boltzmann equation, which describes the operation of the conventional microelectronic devices. The presented equation treats the coherent part of the transport imposed by the nanostructure potential on a rigorous quantum level, utilizing the Wigner picture. It is shown that the equation is general enough to account for quantum effects in the dissipative part of the transport imposed by the electron-phonon interaction. Numerical experiments demonstrate the effects of collision broadening, retardation and the intra-collisional field effect. Theoretical analysis of the equation reveals a novel quantum effect which is due to the correlation between the interaction process and the space component of the Wigner path.

1. Introduction

Nanoelectronic devices are designed to achieve an ultra-high circuit density and can operate at ultra-high speed. Their feature size is comparable to the wavelength of an electron. The transient response time which determines the ultimate switching speed is reported to be within a few hundred femtoseconds for resonant tunneling diodes [1]. The introduced length and time scales are beyond the limit where the classical transport picture can be used to explain the operational characteristics of nanoelectronic devices: The Boltzmann equation requires the space and time scales to be much larger than nanometer and femtosecond respectively. At such scales a quantum-mechanical treatment becomes necessary. Moreover, in far from equilibrium operating conditions, when there is a current flow through the device, the Schrödinger equation is not suitable and a kinetic approach is relevant. For such conditions we utilize the Wigner picture as a convenient description of the transport phenomena. Many of the concepts of the transport in classical devices, such as phase space, distribution function and current injecting boundary conditions at the contacts remain valid. The boundary conditions determine the operational characteristics of the nanodevice and are of crucial importance for existence of a stable solution of the coherent Wigner equation [2].

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 [2]. 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 [3].

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. The interaction is commonly treated in the classical Boltzmann limit and thus femtoseconds transport regimes can not be treated correctly. Moreover additional approximations, such as relaxation time [3] or assumptions for equilibrium conditions in the direction normal to the current flow [2] are introduced. A rigorous inclusion of the phonon interaction is provided by the generalized Wigner function (WF) $f_w(\mathbf{r}, \mathbf{p}, \{n\}, \{n'\}, t)$ 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 only for the reduced WF can not be obtained from the generalized Wigner equation, since the trace

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operation does not commute with the electron-phonon interaction Hamiltonian. The numerical treatment of the generalized WF introduces a heavy computational burden. CPU times in the order of $30h$ per point in the $I(V)$ characteristics are required on a 100 CPU-Cray machine [4].

The alternative approach is to obtain from the generalized Wigner equation an approximate, but closed equation for the reduced WF. In the next section we present an equation for the reduced WF which is obtained after a hierarchy of approximations. The equation treats the coherent part of the transport imposed by the nanostructure potential at a rigorous quantum level. The analysis reveals a novel quantum effect which is due to the correlation between the phonon interaction and the space component of the Wigner path. It is general enough to account for the quantum effects in the interaction with phonons at the femtosecond time scale. These effects are investigated numerically in Section 3q.

2. The Quantum Equation

The generalized Wigner equation [4] 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. The evolution process begins with an initially decoupled electron-phonon system and involves transitions between the diagonal and the first off-diagonal elements. It is assumed that the phonons are in equilibrium during the evolution. 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 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 integral 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 complex conjugate.

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, the solution to the two auxiliary equations can be explicitly expressed in terms of the reduced WF. The 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. 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 equation has the following integral form:

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

The contributions to the value of $f_w(\mathbf{r},\mathbf{p},t)$ occur on the trajectory initialized by $\mathbf{r},\mathbf{p}$ at time t. They are solved by using Newton's trajectories defined by:

$$\mathbf{p}_{(\tau)} = \mathbf{p} - e\mathbf{E}(t-\tau)$$

$$\mathbf{r}_{(\mathbf{p},\mathbf{q}',\tau)} = \mathbf{r} - \int_{\tau}^{t} \mathrm{d}y \frac{\mathbf{p}_{(y)}}{m}$$

The initial condition evolves on this trajectory and adds to f_w the initial value at point $(\mathbf{r}_{(\mathbf{p},0)},\mathbf{p}_{(0)})$. V'_w is obtained by the Wigner transform of the device potential V corrected by the potential of the homogeneous field $\mathbf{E}$:

$$V'_w(\mathbf{r},\mathbf{p}) = \frac{1}{\hbar^3}\int \mathrm{d}\mathbf{s} \mathrm{e}^{-i/\hbar\mathbf{p}\cdot\mathbf{s}} \frac{1}{i\hbar} \times$$

$$\left(V(\mathbf{r}-\frac{\mathbf{s}}{2}) - V(\mathbf{r}+\frac{\mathbf{s}}{2}) + e\mathbf{E}\cdot\mathbf{s}\right)$$

The term 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 because of the integration on $\mathbf{p}'$, but it is local in the real space. At a fixed time t' the information is collected at the point $\mathbf{r}_{(\mathbf{p},t')}$ defined by the real space part of the trajectory.
Up to now the same properties are also demonstrated by the integral form of the Boltzmann equation. The novel effect stems from the terms related to the electron-phonon interaction. They are nonlocal also with respect to the real space. The following physical processes are associated with these terms. Consider the contribution of $f_w(\mathbf{r}_{(\mathbf{p},t'')}+\frac{\hbar\mathbf{q}'}{2m}(t'-t''),\mathbf{p}_{(t'')}-\hbar\mathbf{q}',t'')$. Formally a test particle that carries the value of f_w can be assigned to that phase space point and time. The interaction begins at t'' when the particle absorbs one half of the phonon momentum $\hbar\mathbf{q}'/2$. The particle momentum becomes $\mathbf{p}_{(t'')} - \hbar\mathbf{q}'/2$. With this momentum and real space coordinate which are denoted by $\mathbf{r}'',\mathbf{p}''$ the particle evolves until time t' to a phase space point defined by:

$$\mathbf{p}'' + e\mathbf{E}(t'-t'') = \mathbf{p}_{(t')} - \frac{\hbar\mathbf{q}'}{2}$$

$$\mathbf{r}'' + \int_{t''}^{t'} d\tau \frac{\mathbf{p}'' + e\mathbf{E}(t'-t'')}{m} = \mathbf{r}_{(\mathbf{p},t')}$$

At time t' the second half of the phonon momentum is absorbed by the particle. It appears with the right coordinates $\mathbf{r}_{(\mathbf{p},t')},\mathbf{p}_{(t')}$ to continue to $\mathbf{r},\mathbf{p}$ at time t. The process corresponds to a real absorption of a phonon with mode $\mathbf{q}'$. The next term,

$$f_w(\mathbf{r}_{(\mathbf{p},t'')} + \frac{\hbar\mathbf{q}'}{2m}(t'-t''),\mathbf{p}_{(t'')},t'')$$

is treated in the same way with the only difference that at t'' the half of the phonon momentum is emitted, while at t' it is absorbed back. The process is called virtual emission since the emission process begins but does not finish with a final release of a phonon in mode $\mathbf{q}'$. The last two terms are related to processes of virtual absorption and real emission. It is seen that the finite duration of the phonon interaction gives rise to a space non-locality of the quantum transport process. The momentum conservation law holds after the interaction completes as in the Boltzmann case. There is no energy conservation in the electron-phonon interaction. The energy conserving delta function is obtained after a limit which neglects the duration of the collision process.
Numerical studies of the electron-phonon interaction beyond the Boltzmann limit have been recently reported in the literature [5]. Here the proposed equation is investigated for quantum effects which are purely due to the electron-phonon interaction. For this the space homogeneous case is considered. Eq.(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. More specifically the solution is explored for the effects of collisional broadening, retardation and the intracollisional field effect. These effects are theoretically expected in quantum regimes of the electron-phonon interaction [6].

3. Results

Simulation results for $GaAs$ material with a PO phonon with constant energy $\hbar\omega$ are presented. The initial condition is a Gaussian function of the energy. A choice of a very low temperature, when the physical system has a transparent semiclassical behavior allows conveniently to study the quantum effects. 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, $(k=0,r>0)$. The effects of collisional broadening and retardation exist already at zero electric field. Figures 1, 2, and 3 present snapshots of the evolution of the semiclassical (inverse hyperbolic cosine [7]) and quantum solutions $|k|f(0,|k|,t)$ for times $100fs$, $200fs$ and $400fs$ 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. The electrons cannot appear in the region above the initial distribution.

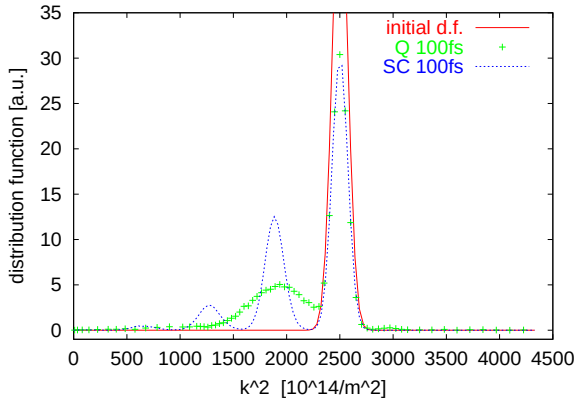

Figure 1: Initial distribution function (initial d.f.), semiclassical (SC) and quantum (Q) solutions $kf(0,k,t)$ for $100fs$ evolution time at zero electric field.

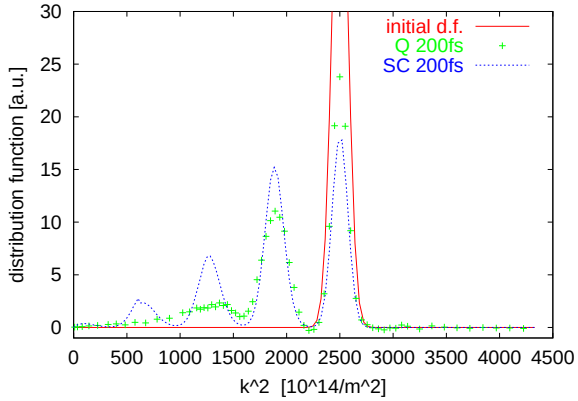

Figure 2: Initial distribution function (initial d.f.), semiclassical (SC) and quantum (Q) solutions $kf(0,k,t)$ for $200fs$ evolution time at zero electric field.

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 Eq.(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 $100fs$ is broadened. It resembles the corresponding replica of the semiclassical solution after $400fs$ evolution time. The retardation of the quantum solutions is associated

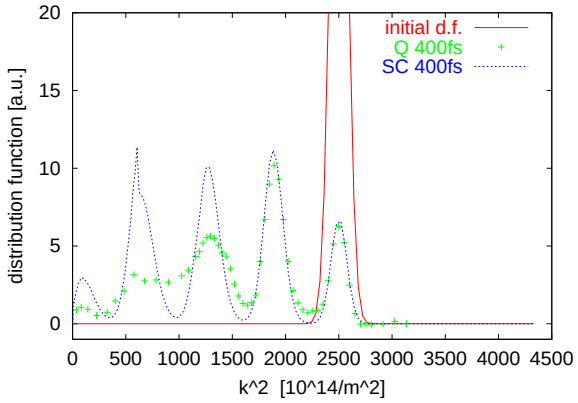

Figure 3: Initial distribution function (initial d.f.), semiclassical (SC) and quantum (Q) solutions $kf(0,k,t)$ for $400fs$ evolution time at zero electric field.

with the memory character of the equation. The two time integrals in Eq.(1) lead to a delay of the build up of the replicas.

Figure 4 compares the $200fs$ solutions as a function of $k < 0$ for different positive values of the electric force $\mathbf{E}$. 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.

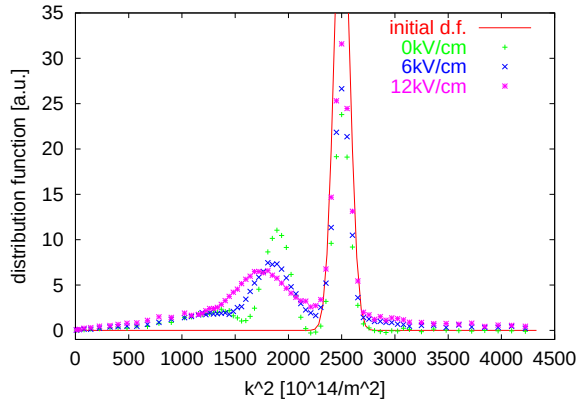

Figure 4: Solutions $|k|f(0,k,t)$, at negative k values, and evolution time $200fs$. The electric field is 0, $6kV/cm$, and $12kV/cm$.

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 ini-

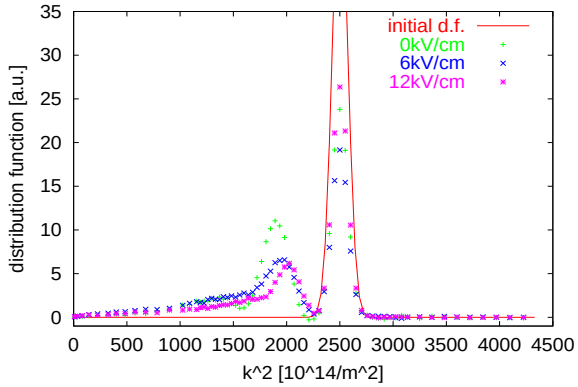

Figure 5: Solutions $kf(0,k,t)$ for positive k values and evolution time $200fs$. The electric field is 0, $6kV/cm$, and $12kV/cm$.

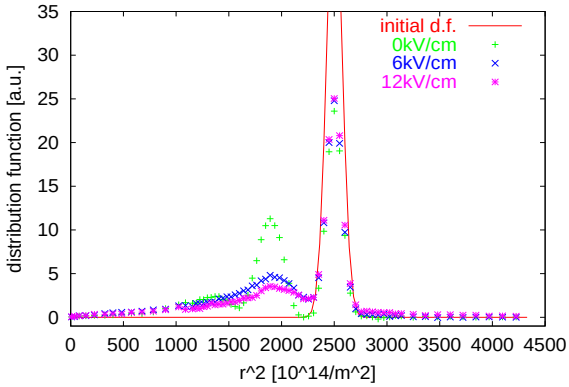

Figure 6: Solutions $rf(r,0,t)$ for an evolution time of $200fs$. The electric field $\mathbf{E}$ is 0, $6kV/cm$, and $12kV/cm$.

tial 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 on Figure 5. The first replicas peaks are shifted to the right and there is no enhancement of the electron population above the initial condition.

No shift in the replicas of the solutions in the direction normal to the field is expected due to the symmetry of the task. Indeed, as seen from Figure 6, the distance between the first replica peaks and the main peak does not depend on the field. Nevertheless 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 Figures 4, 5, and 6 show that the field influences the effects of collisional broadening and the retardation.

4. Conclusions

We conclude that the intra collisional field effect is well demonstrated in the early time evolution of the electron-phonon relaxation. The electric field causes a shift in the replicas, which depends on the field strength and orientation. It affects the electron population of the semiclassically forbidden regions in the direction of the field. It also has an influence on the broadening and retardation of the solution.

5. Acknowledgment

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6. References

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