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A Wigner equation with quantum electron–phonon interaction

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Abstract

We present a kinetic equation which is obtained after a hierarchy of approximations from the generalized electron–phonon Wigner function. The equation accounts for quantum effects in the electron–phonon interaction which are investigated by numerical experiments. An analysis shows that in contrast to the potential term, which is non local in momentum but local in space, the interaction term is non local also in the real space.

Keywords: Wigner function; Nanostructure; Quantum electron–phonon interaction

1. The equation for the reduced Wigner function

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. It has been shown that the electron phonon interaction greatly affects the device parameters of the resonant tunneling diodes [1,2]. A rigorous inclusion of the phonon interaction is provided by the generalized Wigner function (WF) [3] $f_w(\mathbf{r}, \mathbf{p}, \{n\}, \{m\}, t)$ 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 diagonal elements are indirectly linked to all off-diagonal elements. The equation is obtained after a hierarchy of approximations. As a first approximation we consider the weak scattering limit which neglects all links to the elements placed outside the nearest off-diagonals. In the next step a trace operation at the consecutive time steps of the evolution replaces the occupation numbers $n_{\mathbf{q}}$ involved in the transitions with the equilibrium phonon numbers $n(\mathbf{q})$. Obtained is a set of a main equation for the reduced WF coupled to two auxiliary equations. The solution to the two auxiliary equations can be explicitly

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expressed in terms of the reduced WF using a mean field **E** approximation in the potential term. This approximation concerns only the phonon interaction, while the potential term in the main equation is treated exactly. A single equation is derived:

$$f_w(\mathbf{r}, \mathbf{p}, t) = f_0(\mathbf{r}_{(\mathbf{p},0)}, \mathbf{p}_{(0)}, 0) + \int_0^t \mathrm{d}t' \int \mathrm{d}\mathbf{p}' \left\{ V'_w(\mathbf{r}_{(\mathbf{p},t')}, \mathbf{p}', \mathbf{p}_{(t')}) f_w(\mathbf{r}_{(\mathbf{p},t')}, \mathbf{p}', t') + \int_0^{t'} \mathrm{d}t'' \left(S(\mathbf{p}', \mathbf{p}, t', t'') f_w(\mathbf{r}_{(\mathbf{p},\mathbf{q}')}, \mathbf{p}'_{(t'')}, t'') - S(\mathbf{p}, \mathbf{p}', t', t'') f_w(\mathbf{r}_{(\mathbf{p},\mathbf{q}')}, \mathbf{p}_{(t'')}, t'') \right) \right\};$$

$$\frac{4\pi^3}{VF^2_{\mathbf{q}'}} S(\mathbf{p}', \mathbf{p}, t', t'') = n(\mathbf{q}') \cos(\Omega(\mathbf{p}', \mathbf{p}, t', t'')) + (n(\mathbf{q}') + 1) \cos(\Omega(\mathbf{p}, \mathbf{p}', t', t''))$$

with

$$\Omega(\mathbf{p}', \mathbf{p}, t', t'') = \int_{t''}^{t'} \mathrm{d}\tau (\epsilon(\mathbf{p}_{(\tau)}) - \epsilon(\mathbf{p}'_{(\tau)}) - \hbar\omega_{\mathbf{q}'})/\hbar$$

and

$$\mathbf{q}' = (\mathbf{p}' - \mathbf{p})/\hbar.$$

V'_w is the Wigner transform of the device potential corrected by the potential of the homogeneous field **E**. The rest of the notations are explained below.

2. Quantum effects

The obtained equation is first analyzed by theoretical considerations. f_w 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 non local 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 $f_w(\mathbf{r}_{(\mathbf{p},t')}, \mathbf{p}_{(t')}, t')$ at the past of the evolution defined on the real space part of the trajectory. The scattering term introduces a space non locality due to the correlation between the phonon momentum $\hbar\mathbf{q}'$ and the space component of the trajectory: $\mathbf{r}_{(\mathbf{p},\mathbf{q}')} = \mathbf{r}_{(\mathbf{p},t')} + \hbar\mathbf{q}'(t' - t'')/2m$. At the beginning of the scattering, the real trajectory is shifted by $\hbar\mathbf{q}/2/m(t' - t'')$. The interaction proceeds in two steps, e.g. at t'' the first half of a phonon momentum is absorbed (emitted). 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. In contrast to the Wigner

equation without phonon interaction, the obtained equation becomes non local in the real space. The classical limit $\hbar \to 0$ in the phonon interaction leads to a Wigner equation with a Boltzmann term.

For a bulk semiconductor with an applied electric field **E** the equation resembles the Levinson equation [4], or equivalently the Barker–Ferry equation [5] with infinite electron lifetime. In this case the quantum effects introduced by the electron–phonon interaction are numerically investigated. The bulk equation is solved by a randomized backward Monte Carlo algorithm [6]. Simulation results for GaAs with a PO phonon with constant energy $\hbar\omega$ are presented on cut lines parallel and opposite to the field direction. A reference frame moving with the field is assumed. The initial condition is a sharp Gaussian function of the energy. At very low temperature, the physical system is assumed to have a transparent semiclassical behavior. Semiclassical electrons can only emit phonons and lose energy equal to a multiple of the phonon energy $\hbar\omega$. They evolve according to a distribution, patterned by replicas of the initial peak. The electrons cannot appear in the region above the initial peak.

The quantum solutions demonstrate effects of deviation from the semiclassical behavior. Collisional broadening and retardation exist already at zero electric field. Fig. 1 compares the zero field quantum solution with the corresponding semiclassical solution. The quantity $|k|^2$ is proportional to the electron energy in units 10^{14} m^{-2}. There is a retardation in the build up of the remote 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. 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 the scattering term lead to a delay of the build up of the replicas as compared to the single time integral in the Boltzmann case.

The electric field is responsible for the appearance of the intra-collisional field effect (ICFE). The first replica peak of the 12 kV/cm solution on Fig. 1 is shifted in the field direction. The numerical solution in the semiclassically forbidden region, above the initial condition, demonstrates an increase of the electron population. For states below the initial condition the energy of the field is added to the

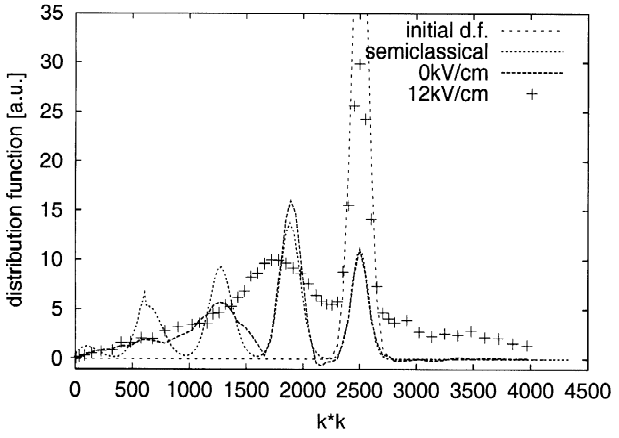

Fig. 1. 300 fs semiclassical (0 kV/cm) and quantum solutions (0 kV/cm and 12 kV/cm). The field points to the left.

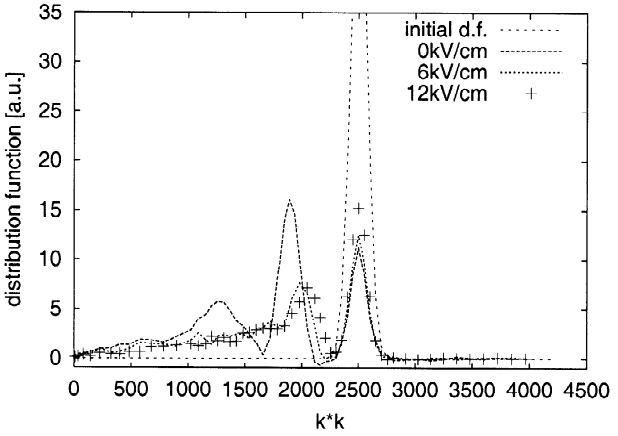

Fig. 2. 300 fs quantum solutions (0 kV/cm, 6 kV/cm and 12 kV/cm). The field points to the right.

phonon energy. Accordingly the solution behaves as in the 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 are demonstrated by the solution if the field changes its direction. In Fig. 2 the first replica peaks of the 6 kV/cm and 12 kV/cm are shifted to the right and the shift is proportional to the field strength. There is no increase of the electron population above the initial condition. A comparison of the first replicas and the main peaks under the initial condition in the two figures shows that the field enhances the broadening and the retardation.

We conclude that the quantum effects are well demonstrated in the solution of the homogeneous equation. A more rigorous study of these effects will consider the general space dependent equation with a quantum correlation term replacing the simple initial condition [7].

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