Monte-Carlo Method for Direct Computation of the Small Signal Kinetic Coefficients

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Abstract

An approach for analysis of the small signal response of the carriers in semiconductors is presented. The response to an impulse signal is explained in terms of a relaxation process, governed by a Boltzmann equation. The approach assists the understanding of the phenomenon and allows development of novel stochastic algorithms.

1. Introduction

The knowledge of the small signal response characteristics of the carriers system as depending on the frequency and the DC electric field $\mathbf{E}_s$ is of relevant importance to forecast modern device performance. Linked by the Fourier transform, analyses in the time and the frequency domains provide equivalent information. Furthermore, the response to a signal of a general time dependence $\mathbf{E}_1(t)$ can be calculated from the knowledge of the response to an impulse, $\mathbf{E}_i(t) = \delta(t)\mathbf{E}_1$. The advantages of Monte-Carlo simulations of response phenomena in the time domain have been utilized for more than two decades [1]. Within the Monte-Carlo method single-particle simulations are popular, supported by the well established theory of correlation functions of the physical characteristics over a steady state trajectory [2],[3]. Another alternative is in a transient description, given by the following derivate of the Boltzmann equation:

$$\frac{\partial f_1(\mathbf{k},t)}{\partial t} + \frac{e}{\hbar}\mathbf{E}_s \cdot \nabla f_1(\mathbf{k},t) = Q[f_1(\mathbf{k},t)] - \frac{e}{\hbar}\mathbf{E}_1(t) \cdot \nabla f_s(\mathbf{k}) \qquad (1)$$

$Q[f_1(\mathbf{k},t)] = \int S(\mathbf{k}',\mathbf{k}) f_1(\mathbf{k}',t)\mathrm{d}\mathbf{k} - \lambda(\mathbf{k}) f_1(\mathbf{k},t)$ is the common Boltzmann scattering term and f_1 is the correction to the distribution function f around a steady-state value f_s: $f(\mathbf{k},t) = f_s(\mathbf{k}) + f_1(\mathbf{k},t)$. Accordingly, the mean of a physical characteristic $A(\mathbf{k})$ is given by $\langle A\rangle(t) = \langle A\rangle_s + \langle A\rangle_1(t)$. With an impulse $\mathbf{E}_i(t)$ on the right hand side (1) cannot be treated numerically. The used stochastic or deterministic methods [2] solve (1) for the case of a step-like signal: $\mathbf{E}_{step}(t) = \theta(t)\mathbf{E}_1$. Then an impulse response characteristic $\langle A\rangle_i(t)$ is obtained by taking the time derivative of the step response $\langle A\rangle_{step}(t)$.

In this work we utilize an integral formulation of (1) for an impulse signal. It suggests a physical model of the response phenomena. The model allows to develop a new Monte-Carlo method.

2. The Physical Model

We introduce a phase space trajectory $\mathbf{K}(t') = \mathbf{k} - \frac{e}{\hbar}\mathbf{E}_s(t-t')$ which is initialized by $\mathbf{k}$ at time t, so that $\mathbf{K}(t) = \mathbf{k}$. The left hand side of (1) becomes a total derivative and the equation can be formally written as $\frac{\mathrm{d}}{\mathrm{d}t}f(t) = -\lambda(t)f(t) + g(t)$. The latter has a solution $f(t) = f(t_0)\mathrm{e}^{-\int_{t_0}^{t}\lambda(y)\mathrm{d}y} + \int_{t_0}^{t} g(t')e^{-\int_{t'}^{t}\lambda(y)\mathrm{d}y}\mathrm{d}t'$ with $f(t_0)$ given at some initial time t_0. This result allows to reformulate (1) as an integral equation. For the case of an impulse at the time origin we obtain:

$$f_i(\mathbf{k},t) = \int_0^t \mathrm{d}t' \int \mathrm{d}\mathbf{k}' f_i(\mathbf{k}',t')S(\mathbf{k}',\mathbf{K}(t'))\mathrm{e}^{-\int_{t'}^{t}\lambda(\mathbf{K}(y)dy} - \frac{e}{\hbar}\mathbf{E}_1\cdot(\nabla f_s)(\mathbf{K}(0))\mathrm{e}^{-\int_0^t\lambda(\mathbf{K}(y)dy} \tag{2}$$

Here we have used that f_i is zero for negative time, and accounted for the delta function by the time integration. Equation (2) is equivalent to the integral form of the Boltzmann equation [4],[5], with the only difference that the initial distribution function is now replaced by the function $G_i(\mathbf{k}) = -\frac{e}{\hbar}\mathbf{E}_1\cdot(\nabla f_s)(\mathbf{k})$. Since $\int G_i(\mathbf{k})\mathrm{d}\mathbf{k} = 0$, G_i takes also negative values, obstructing a direct physical interpretation of (2). To continue, we decompose G_i into positive and negative parts $G_i = G_i^+ - G_i^-$, and consider the following set of integral equations:

$$f_i^{\pm}(\mathbf{k},t) = \int_0^t \mathrm{d}t' \int d\mathbf{k}' f_i^{\pm}(\mathbf{k}',t')S(\mathbf{k}',\mathbf{K}(t'))\mathrm{e}^{-\int_{t'}^{t}\lambda(\mathbf{K}(y)dy} + G_i^{\pm}(\mathbf{K}(0))\mathrm{e}^{-\int_0^t\lambda(\mathbf{K}(y)dy} \tag{3}$$

These are two Boltzmann equations with initial conditions given by $G_i^{\pm} \geq 0$. Equation (2) is obtained by a subtraction of the two equations such that $f_i(\mathbf{k},t) = f_i^+(\mathbf{k},t) - f_i^-(\mathbf{k},t)$ holds. Thus we can assign to the impulse response equation (1) the following physical model. The impulse at time zero creates instantaneously an initial condition G_i, corresponding to two carrier ensembles P and M, which are initially distributed according to G_i^+ and G_i^-. The ensembles are of equal number of particles which evolve in time under the action of the DC field. The response $\langle A\rangle_i(t)$ of any physical quantity at evolution time t is given by the difference of the two ensemble mean values of A at that time. Since for long evolution times the two ensembles relax to the same steady state, it holds $\langle A\rangle_i(t) = \langle A\rangle_P(t) - \langle A\rangle_M(t) \to 0$ when $t \to \infty$.

3. The Monte-Carlo method

The Monte-Carlo method consists of algorithms providing in a different way the initial condition G. For a general direction of $\mathbf{E}_1$, one possibility is to approximate the gradient of f_s by a finite difference quotient. The wave vector increment has to be taken colinear to $\mathbf{E}_1$. Then the task is to apply algorithms, simulating f_s. If the Ensemble Monte-Carlo is used, the algorithm of Price [1] is particularly obtained. Alternatively, one can sample f_s by a single-particle trajectory. In the important case of colinear DC and perturbation vectors it holds: $G(\mathbf{k}) = \frac{F_1}{F_0}(\lambda(\mathbf{k})f_s(\mathbf{k}) - \int f_s(\mathbf{k}')S(\mathbf{k}',\mathbf{k})\mathrm{d}\mathbf{k}')$. This leads to a natural splitting into G^+ and G^- terms. We give two algorithms using different factors of the terms as probability densities. In general, G^+ and G^- are sampled over a main steady state trajectory. N evolution trajectories are started from G^+, and the same number of trajectories are started from G^-. The chosen probability densities, generating the initial trajectory points, are enclosed below in curly brackets. We note that it is possible to merge the main and the evolution trajectories and to collect the whole information over one trajectory.

Algorithm 1. $G^+(\mathbf{k}_0) = \frac{F_1}{F_0}\lambda(\mathbf{k}_0)\{f_s(\mathbf{k}_0)\}$, $G^-(\mathbf{k}') = \frac{F_1}{F_0}\int\{f_s(\mathbf{k}_0)\}\left\{\frac{S(\mathbf{k}_0,\mathbf{k}')}{\lambda(\mathbf{k}_0)}\right\}\lambda(\mathbf{k}_0)\mathrm{d}\mathbf{k}_0$ For $l = 1$ to N do: 1) Choose $\mathbf{k}_0$ with density f_s, e.g., by sampling the main trajectory at constant time steps. 2) Realize a scattering event from $\mathbf{k}_0$ to $\mathbf{k}'$. a) Start a trajectory from $\mathbf{k}_0$ and give it the weight $w^+ = \frac{F_1}{NF_0}\lambda(\mathbf{k}_0)$. b) Start a trajectory from $\mathbf{k}'$ and give it the negative weight $w^- = -w^+$. 3) Follow each trajectory in an interval $[0,T]$ and sample with constant time step. Add $w^+A(\mathbf{K}^+(t_i))$ and $w^-A(\mathbf{K}^-(t_i))$ to a histogram which estimates $\langle A\rangle_i(t_i)$.

Algorithm 2. $G^+(\mathbf{k}_0) = \frac{F_1}{F_0}\langle\lambda\rangle_s\left\{\frac{\lambda(\mathbf{k}_0)f_s(\mathbf{k}_0)}{\langle\lambda\rangle_s}\right\}$, $G^-(\mathbf{k}') = \frac{F_1}{F_0}\langle\lambda\rangle_s\int\left\{\frac{\lambda(\mathbf{k}_0)f_s(\mathbf{k}_0)}{\langle\lambda\rangle_s}\right\}\left\{\frac{S(\mathbf{k}_0,\mathbf{k}')}{\lambda(\mathbf{k}_0)}\right\}$ $\mathrm{d}\mathbf{k}_0$ where $\langle\lambda\rangle_s = \int f_s(\mathbf{k})\lambda(\mathbf{k})\mathrm{d}\mathbf{k}$ is the inverse of the mean free flight time. The algorithm modifies the first step of Algorithm 1 to: 1) Choose $\mathbf{k}_0$ with density λf_s, e.g., by taking a before-scattering state. The weight is now $w^+ = \frac{F_1}{F_0}\langle\lambda\rangle_s$. Step 2 and 3 remain unchanged.

The second algorithm has been applied to obtain simulation results. For Si electrons at $300K$, Fig. 1 and Fig. 2 show the time response of the differential energy $\partial\langle\epsilon\rangle_i/\partial E_1$ and differential velocity along the electric field $\partial\langle v\rangle_i/\partial E_1$, at different DC field values. After 3 ps the two ensembles reach the steady state and the response characteristics become zero. Fig. 3 and Fig. 4 show the spectral dependence of the differential velocity obtained by a Fourier transform of the data shown in Fig. 2. The low frequency limits of the real parts tend to the corresponding differential mobility values $\partial\langle v\rangle_s/\partial E_s$.

For $GaAs$ electrons at $10K$ and $E_s = 120V/cm$, Fig. 5 and Fig. 6 show time oscillations in the evolution of the P and M energy distribution functions. The oscillation is observed in all response characteristics $\langle A\rangle_i(t)$ and is explained by the model as follows. The initial distributions G^- and G^+ show two peaks placed near zero energy and slightly above the polar optical phonon threshold (0.036 eV) respectively. The M ensemble gains energy by the field and looses it when reaching the phonon energy, giving rise to oscillations between the zero energy and the phonon threshold. The initial peak broadens towards the steady state, reached after 80 ps. The P ensemble is initially transferred by the phonon scattering to low energy for few ps and follows the M ensemble with such a delay. The delay is finally responsible for the oscillations in $\langle A\rangle_i(t)$.

4. Acknowledgments

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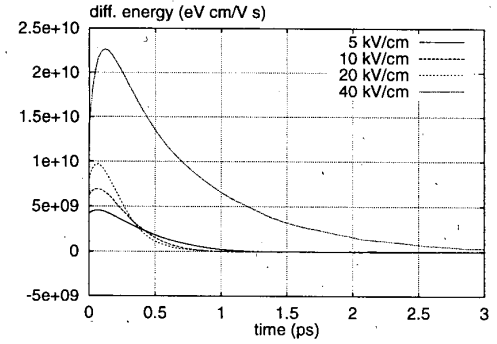

Figure 1: Impulse response of the differential energy

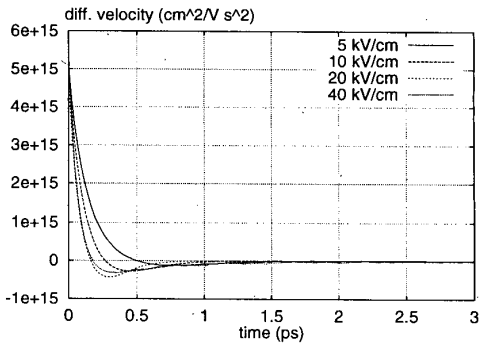

Figure 2: Impulse response of the differential velocity

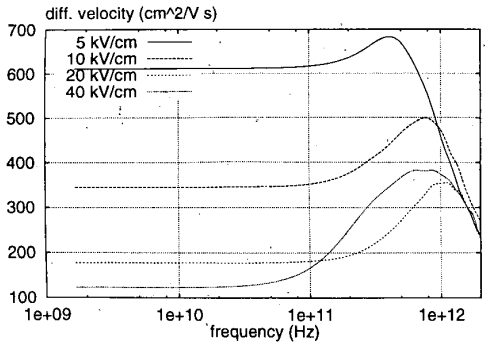

Figure 3: Real part of the differential velocity spectra

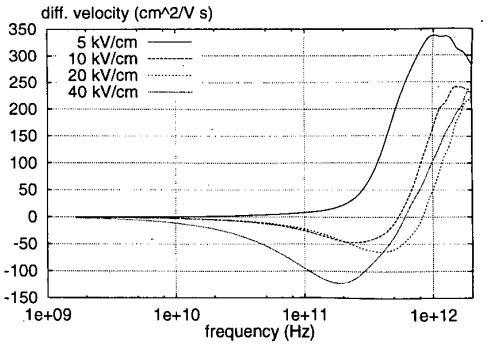

Figure 4: Imaginary part of the differential velocity spectra

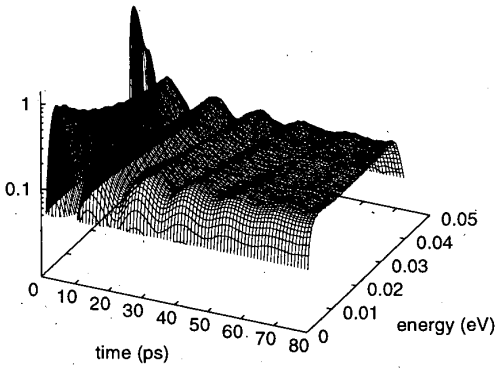

Figure 5: Evolution of the distribution function of the P ensemble.

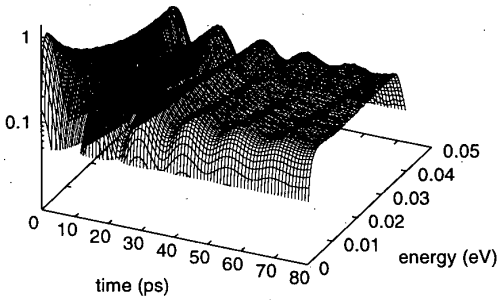

Figure 6: Evolution of the distribution function of the M ensemble.

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