

Femtosecond Evolution of Spatially Inhomogeneous Carrier Excitations Part II: Stochastic Approach and Grid Implementation

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Abstract. We present a stochastic approach for solving the quantum-kinetic equation introduced in Part I. A Monte Carlo method based on backward time evolution of the numerical trajectories is developed. The computational complexity and the stochastic error are investigated numerically. Variance reduction techniques are applied, which demonstrate a clear advantage with respect to the approaches based on symmetry transformation. Parallel implementation is realized on a GRID infrastructure.

1 Introduction

A Wigner equation for nanometer and femtosecond transport regime has been previously derived from a three equations set model based on the generalized Wigner function [7]. The complete equation poses serious numerical challenges so that we consider limiting versions of the equation corresponding to simplified physical. Two limiting cases, namely the Wigner-Boltzmann equation [8] and the homogeneous Levinson (or Barker-Ferry) equation [5, 4] have been analyzed with various Monte Carlo (MC) approaches. In particular, spherical and cylindrical transformations have been used to reduce the dimensions in the momentum space. The equation derived in Part I presents a third limiting case, where the electron-phonon interaction is described on the quantum-kinetic level by the Levinson equation, but the evolution problem becomes inhomogeneous due to the spatial dependence of the initial condition. The problem is relevant e.g. for description of the ultrafast dynamics of optically generated carriers. Particularly we consider a quantum wire, where the carriers are confined in the plane normal to the wire by infinite potentials. At low temperatures the carriers remain in the ground state in the normal plane. Thus, the evolution is described in the two dimensional phase space of the carrier wave vector and the position, while the phonons are three dimensional. The initial carrier distribution is assumed Gaussian both in energy and space coordinates, and an electric field can be

applied along the wire. We recall the integral form of the derived in Part I quantum-kinetic equation:

$$\begin{aligned}
f_w(z, k_z, t) &= f_w\left(z - \frac{\hbar k_z}{m}t + \frac{\hbar \mathbf{F}}{2m}t^2, k_z, 0\right) + \int_0^t dt'' \int_{t''}^t dt' \int d\mathbf{q}'_{\perp} \int dk'_z \times \quad (1) \\
&\left[S(k'_z, k_z, t', t'', \mathbf{q}'_{\perp}) f_w\left(z - \frac{\hbar k_z}{m}(t - t'') + \frac{\hbar \mathbf{F}}{2m}(t^2 - t''^2) + \frac{\hbar q'_z}{2m}(t' - t''), k'_z, t''\right) \right. \\
&\left. - S(k_z, k'_z, t', t'', \mathbf{q}'_{\perp}) f_w\left(z - \frac{\hbar k_z}{m}(t - t'') + \frac{\hbar \mathbf{F}}{2m}(t^2 - t''^2) - \frac{\hbar q'_z}{2m}(t' - t''), k_z, t''\right) \right] \\
S(k'_z, k_z, t', t'', \mathbf{q}'_{\perp}) &= \frac{2V}{(2\pi)^3} |G(\mathbf{q}'_{\perp}) \mathcal{F}(\mathbf{q}'_{\perp}, k_z - k'_z)|^2 \times \\
&\left[(n(\mathbf{q}') + 1) \cos\left(\frac{\epsilon(k_z) - \epsilon(k'_z) + \hbar \omega_{\mathbf{q}'}}{\hbar}(t' - t'') + \frac{\hbar}{2m} \mathbf{F} \cdot \mathbf{q}'_z (t'^2 - t''^2)\right) \right. \\
&\left. + n(\mathbf{q}') \cos\left(\frac{\epsilon(k_z) - \epsilon(k'_z) - \hbar \omega_{\mathbf{q}'}}{\hbar}(t' - t'') + \frac{\hbar}{2m} \mathbf{F} \cdot \mathbf{q}'_z (t'^2 - t''^2)\right) \right]
\end{aligned}$$

Here, $f(z, k_z, t)$ is the Wigner function described in the 2D phase space of the carrier wave vector k_z and the position z , and t is the evolution time.

$F = e\mathbf{E}/\hbar$, where \mathbf{E} is a homogeneous electric field along the direction of the wire z , e being the electron charge and \hbar - the Plank's constant.

$n_{\mathbf{q}'} = 1/(\exp(\hbar \omega_{\mathbf{q}'}/\mathcal{K}T) - 1)$ is the Bose function, where \mathcal{K} is the Boltzmann constant and T is the temperature of the crystal, corresponds to an equilibrium distributed phonon bath.

$\hbar \omega_{\mathbf{q}'}$ is the phonon energy which generally depends on $\mathbf{q}' = \mathbf{q}'_{\perp} + q'_z = \mathbf{q}'_{\perp} + (k_z - k'_z)$, and $\epsilon(k_z) = (\hbar^2 k_z^2)/2m$ is the electron energy.

\mathcal{F} is obtained from the Fröhlich electron-phonon coupling by recalling the factor $i\hbar$ in the interaction Hamiltonian, Part I:

$$\mathcal{F}(\mathbf{q}'_{\perp}, k_z - k'_z) = - \left[\frac{2\pi e^2 \omega_{\mathbf{q}'}}{\hbar V} \left(\frac{1}{\epsilon_{\infty}} - \frac{1}{\epsilon_s} \right) \frac{1}{(\mathbf{q}')^2} \right]^{\frac{1}{2}},$$

where (ϵ_{∞}) and (ϵ_s) are the optical and static dielectric constants. The shape of the wire affects the electron-phonon coupling through the factor

$$G(\mathbf{q}'_{\perp}) = \int d\mathbf{r}_{\perp} e^{i\mathbf{q}'_{\perp} \cdot \mathbf{r}_{\perp}} |\Psi(\mathbf{r}_{\perp})|^2,$$

where Ψ is the ground state of the electron system in the plane normal to the wire.

In the inhomogeneous case the wave vector (and respectively the energy) and the density distributions are given by the integrals

$$f(k_z, t) = \int \frac{dz}{2\pi} f_w(z, k_z, t); \quad n(z, t) = \int \frac{dk_z}{2\pi} f_w(z, k_z, t). \quad (2)$$

Our aim is to estimate these quantities, as well as the Wigner function (1) by MC approach.

2 Monte Carlo Approach

Consider the problem of evaluating the following functional of the solution of the integral equation (1)

$$J_g(f) \equiv (g, f) = \int_0^T \iint_D g(z, k_z, t) f_w(z, k_z, t) dz dk_z dt, \quad (3)$$

by a MC method. Here we specify that the phase space point (z, k_z) belongs to a rectangular domain $D = (-Q_1, Q_1) \times (-Q_2, Q_2)$, and $t \in (0, T)$. The arbitrary function $g(z, k_z, t)$ belongs to the space L_∞ .

Now (1) can be written in the following form:

$$\begin{aligned} f_w(z, k_z, t) &= f_w(z - z(k_z, t), k_z, 0) + \\ &+ \int_0^t dt'' \int_{t''}^t dt' \int_G d^3 \mathbf{k}' \{ K_1(k_z, \mathbf{k}', t', t'') f_w(z + h(k_z, q'_z, t, t', t'', \mathbf{F}), k'_z, t'') \} \\ &+ \int_0^t dt'' \int_{t''}^t dt' \int_G d^3 \mathbf{k}' \{ K_2(k_z, \mathbf{k}', t', t'') f_w(z + h(k_z, -q'_z, t, t', t'', \mathbf{F}), k'_z, t'') \}, \end{aligned} \quad (4)$$

where

$$\begin{aligned} z(k_z, t) &= \frac{\hbar k_z}{m} t - \frac{\hbar \mathbf{F}}{2m} t^2, \\ h(k_z, q'_z, t, t', t'', \mathbf{F}) &= -\frac{\hbar k_z}{m} (t - t'') + \frac{\hbar \mathbf{F}}{2m} (t^2 - t''^2) + \frac{\hbar q'_z}{2m} (t' - t''), \\ K_1(k_z, \mathbf{k}', t', t'') &= S(k'_z, k_z, t', t'', \mathbf{q}'_\perp) = -K_2(\mathbf{k}', k_z, t', t''), \end{aligned}$$

and $\int_G d^3 \mathbf{k}' = \int d\mathbf{q}'_\perp \int_{-Q_2}^{Q_2} dk_z$. We note that the Neumann series of such integral equations as (4) converges [5]. Thus, the functional (3) can be evaluated by a MC estimator [6].

Let us construct a biased MC estimator for evaluating the functional (3) using backward time evolution of the numerical trajectories in the following way:

$$\xi_s[J_g(f)] = \frac{g(z, k_z, t)}{p_{in}(z, k_z, t)} W_0 f_w(\cdot, k_z, 0) + \frac{g(z, k_z, t)}{p_{in}(z, k_z, t)} \sum_{j=1}^s W_j^\alpha f_w(\cdot, k_{z,j}^\alpha, t_j), \quad (5)$$

where

$$\begin{aligned} f_w(\cdot, k_{z,j}^\alpha, t_j) &= \\ &\begin{cases} f_w(z + h(k_{z,j-1}, k_{z,j-1} - k_{z,j}, t_{j-1}, t'_j, t_j, \mathbf{F}), k_{z,j}, t_j), & \text{if } \alpha = 1, \\ f_w(z + h(k_{z,j-1}, k_{z,j} - k_{z,j-1}, t_{j-1}, t'_j, t_j, \mathbf{F}), k_{z,j-1}, t_j), & \text{if } \alpha = 2, \end{cases} \\ W_j^\alpha &= W_{j-1}^\alpha \frac{K_\alpha(k_{z,j-1}, \mathbf{k}_j, t'_j, t_j)}{p_\alpha p_{tr}(\mathbf{k}_{j-1}, \mathbf{k}_j, t'_j, t_j)}, \quad W_0^\alpha = W_0 = 1, \quad \alpha = 1, 2, \quad j = 1, \dots, s. \end{aligned}$$

The probabilities p_α , ($\alpha = 1, 2$) are chosen to be proportional to the absolute value of the kernels in (4). The initial density $p_{in}(z, k_z, t)$ and the transition density $p_{tr}(\mathbf{k}, \mathbf{k}', t', t'')$ are chosen to be tolerant¹ to the function $g(z, k_z, t)$ and

¹ $r(x)$ is tolerant to $g(x)$ if $r(x) > 0$ when $g(x) \neq 0$ and $r(x) \geq 0$ when $g(x) = 0$.

the kernels, respectively. The first point $(z, k_{z,0}, t_0)$ in the Markov chain is chosen using the initial density, where $k_{z,0}$ is the third coordinate of the wave vector \mathbf{k}_0 . Next points $(k_{z,j}, t'_j, t_j) \in (-Q_2, Q_2) \times (t_j, t_{j-1}) \times (0, t_{j-1})$ of the Markov chain:

$$(k_{z,0}, t_0) \rightarrow (k_{z,1}, t'_1, t_1) \rightarrow \cdots \rightarrow (k_{z,j}, t'_j, t_j) \rightarrow \cdots \rightarrow (k_{z,s}, t'_s, t_s)$$

do not depend on the position z of the electrons. They are sampled using the transition density $p_{tr}(\mathbf{k}, \mathbf{k}', t', t'')$ as we take only the z -coordinate of the wave vector \mathbf{k} . Note the time t'_j conditionally depends on the selected time t_j . The Markov chain terminates in time $t_s < \varepsilon_1$, where ε_1 is a fixed small positive number called a truncation parameter.

In order to evaluate the functional (3) by N independent samples of the estimator (5), we define a Monte Carlo method

$$\frac{1}{N} \sum_{i=1}^N (\xi_s[J_g(f)])_i \xrightarrow{P} J_g(f_s) \approx J_g(f), \quad (6)$$

where \xrightarrow{P} means stochastic convergence as $N \rightarrow \infty$; f_s is the iterative solution obtained by the Neumann series of (4), and s is the number of iterations. The relation (6) still does not determine the computational algorithm. To define a MC algorithm we have to specify the initial and transition densities, as well the modeling function (or sampling rule). The modeling function describes the rule needed to calculate the states of the Markov chain by using uniformly distributed random numbers in the interval $(0, 1)$.

Here, the transition density is chosen:

$$\begin{aligned} p_{tr}(\mathbf{k}, \mathbf{k}', t', t'') &= p(\mathbf{k}'/\mathbf{k})p(t, t', t'') \\ p(t, t', t'') &= p(t, t'')p(t'/t'') = \frac{1}{t} \frac{1}{(t-t'')} \\ p(\mathbf{k}'/\mathbf{k}) &= c_1/(\mathbf{k}' - \mathbf{k})^2 \end{aligned}$$

(c_1 is the normalized constant). Thus, if we know t , the next times t'' and t' are computed by using the inverse-transformation rule. The wave vector \mathbf{k}' are sampled in the same way as described in [3]. The difference here is that we have to compute all three coordinates of the wave vector although we need only the third coordinate.

The choice of $p_{in}(z, k_z, t)$ depends on the function $g(z, k_z, t)$. The cases when

$$\begin{aligned} (i) \quad g(z, k_z, t) &= \delta(z - z_0)\delta(k_z - k_{z,0})\delta(t - t_0), \\ (ii) \quad g(z, k_z, t) &= \frac{1}{2\pi}\delta(k_z - k_{z,0})\delta(t - t_0), \\ (iii) \quad g(z, k_z, t) &= \frac{1}{2\pi}\delta(z - z_0)\delta(t - t_0), \end{aligned}$$

are of special interest, because they estimate the values of the Wigner function (1), the wave vector and the density distribution (2) in fixed points.

3 Grid Implementation and Numerical Results

The computational complexity of an MC algorithm can be measured by the quantity $CC = N \times \tau \times M(s_{\varepsilon_1})$. The number of the random walks, N , and the average number of transitions in the Markov chain, $M(s_{\varepsilon_1})$, are related to the stochastic and systematic errors [5]. The mean time for modeling one transition, τ , depends on the complexity of the transition density functions and on the sampling rule, as well as on the choice of the random number generator (rng).

It is proved [5, 4] that the stochastic error has order $O(N^{-1/2} \exp(c_2 t))$, where t is the evolution time and c_2 is a constant depending on the kernels of the quantum kinetic equation under consideration. This estimate shows that when t is fixed and $N \rightarrow \infty$ the error decreases, but for large t the factor $\exp(c_2 t)$ looks ominous. Therefore, the algorithm solves an *NP*-hard problem concerning the evolution time. To solve this problem for long evolution times with small stochastic error we have to combine both MC variance reduction techniques and distributed or parallel computations.

It is well known that the MC algorithms are very convenient for implementations on parallel computer systems [1], because every realization of the MC estimator can be done independently and simultaneously. Although MC algorithms are well suited to parallel computation, there are a number of potential problems. The available computers can run at different speeds; they can have different user loads on them; one or more of them can be down; the rng's that they use can run at different speeds; etc. On the other hand, these rng's must produce independent and non-overlapping random sequences. Thus, the parallel realization of the MC algorithms is not a trivial process on different parallel computer systems.

By using the grid environment provided by the EGEE project middleware² [2] we were able to reduce the computing time of the MC algorithm under consideration. The simulations are parallelized on the existing Grid infrastructure by splitting the underlying random number sequences. The numerical results discussed in Fig. 1 are obtained for zero temperature and GaAs material parameters: the electron effective mass is 0.063, the optimal phonon energy is $36meV$, the static and optical dielectric constants are $\varepsilon_s = 10.92$ and $\varepsilon_\infty = 12.9$. The initial condition is a product of two Gaussian distributions of the energy and space. The k_z^2 distribution corresponds to a generating laser pulse with an excess energy of about $150meV$. The z distribution is centered around zero. A quantum wire with orthogonal cross section is assumed.

² The Enabling Grids for E-science (EGEE) project is funded by the European Commission and aims to build on recent advances in grid technology and develop a service grid infrastructure which is available to scientists 24 hours-a-day. The project aims to provide researchers in both academia and industry with access to major computing resources, independent of their geographic location. The EGEE project identifies a wide-range of scientific disciplines and their applications and supports a number of them for deployment. To date there are five different scientific applications running on the EGEE Grid infrastructure. For more information see <http://public.eu-egee.org/>.

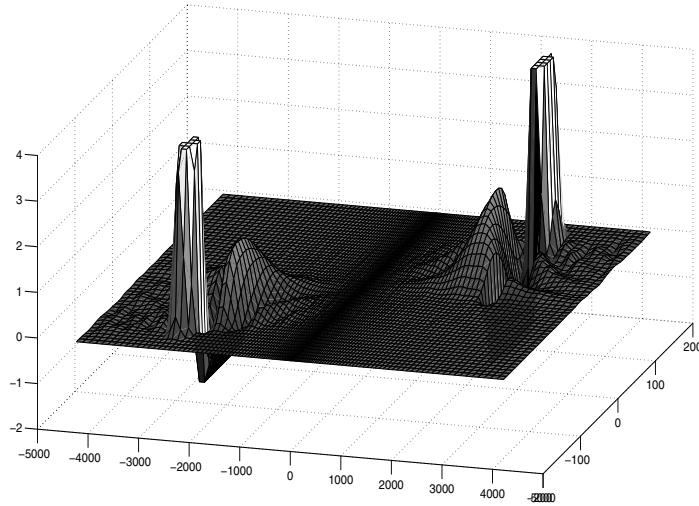


Fig. 1. Evolution of optically generated distribution of electrons in a quantum wire. The electric field E is 0, the number of the random walks per point is $N = 10$ millions, t is 150 femtoseconds.

Table 1. The CPU time (seconds) for all 800×260 points, the speed-up, and the parallel efficiency. The number of random walks is $N = 100000$. The evolution time is 100 $f.s.$

Number of CPUs	CPU Time (s)	Speed-up	Parallel Efficiency
2	9790	-	-
4	4896	1.9996	0.9998
6	3265	2.9985	0.9995

The solution $f(z, k_z, t)$ is estimated in 800×260 points (see Figure 1) that are symmetrically located in the rectangular domain $(-Q_1, Q_1) \times (-Q_2, Q_2)$, where $Q_1 = 400 \times 10^9 m^{-1}$ and $Q_2 = 66 \times 10^7 m^{-1}$.

In our research, the MC algorithm has been implemented in C . The SPRNG library has been used to produce independent and non-overlapping random sequences [9]. Successful tests of the algorithm were performed at the Bulgarian SEE-GRID³ sites using the Resource Broker at ULAKBIM — Turkey. The MPI

³ South Eastern European GRid-enabled eInfrastructure Development (SEE-GRID) project is funded by the European Commission and aims to provide specific support actions to pave the way towards the participation of the SE European countries to the Pan-European and worldwide Grid initiatives. The SEE-GRID consortium consists of eleven contractors: ten representatives or incubators of National Grid initiatives (NGIs) from SE European countries and CERN. The consortium contractors that represent NGIs are: GRNET (Greece), SZTAKI (Hungary), ICI (Romania), IPP (former CLPP, Bulgaria), TUBITAK (Turkey), INIMA (Albania), BIHARNET (Bosnia-Herzegovina), Ss Cyril and Methodius University (FYRoM), University of Belgrade (Serbia-Montenegro), RBI (Croatia). For more information see <http://www.see-grid.org/>.

implementation was MPICH 1.2.6, and the execution is controlled from the Computing Element via the Torque batch system.

The timing results for evolution time $t=100$ femtoseconds are shown in Table 1. The parallel efficiency is close to 100%.

4 Conclusion

A Wigner equation for the evolution of spatially inhomogeneous electron distribution excited by a laser pulse in a quantum wire has been solved by a Monte Carlo approach. Numerical results are obtained for the Wigner function without applied electric field, but the proposed approach is suitable for exploration of the influence of the field. The numerical problem is CPU intensive and thus suitable for implementation on Grid infrastructures, especially since high parallel efficiency is achieved.

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