An efficient backward Monte Carlo estimator for solving of a quantum kinetic equation with memory kernel

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Abstract

An efficient backward Monte Carlo estimator and a corresponding algorithm for solving a quantum-kinetic equation describing an ultrafast semiconductor carrier transport is proposed and studied. In order to obtain the electron energy distribution for long evolution times, variance reduction techniques are applied. The balancing of errors (both systematic and stochastic) and computational cost are investigated.

The presented algorithm is implemented using the SPRNG random number generator and one by L'Ecuyer based on a combination of two linear congruential sequences.

Numerical results for long and short evolution times are obtained. They show that the SPRNG random number generator is preferable to that by L'Ecuyer.

Key words: Monte Carlo estimator, Monte Carlo algorithm, Quantum-kinetic equation, Electron-phonon quantum transport, Random number generator

1 Introduction

In the last several years the development of device modeling physics involved such small space and time scales that the applicability of semiclassical transport fails and a quantum description is needed. The carrier-phonon kinetics beyond the semiclassical Boltzmann equation (BE) has been investigated in

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many publications for the case of applied electrical fields [1,10,18,19] and for optically generated carriers [8,16,22,25,27]. In general, the solutions of the equations describing quantum processes can be found only numerically.

It is well-known that the Monte Carlo (MC) method is a numerically efficient way for charge-transport modeling in semiconductors [6,7,9,12,15,20]. In this work a quantum-kinetic equation which accounts for the memory character of the electron-phonon interaction is solved by a stochastic approach.

The physics model includes a femtosecond relaxation process of optically excited carriers in an one-band semiconductor [22], which allows us to concentrate on memory effects related to the energy-time uncertainty in the electron-phonon interaction. The process is described by the zero field Barker-Ferry equation [1]. The electron-phonon interaction is switched on after a laser pulse creates an initial electron distribution. The set of kinetic equations for the electron dynamics is given in [22].

Under an assumption for equilibrium phonons, an integral formulation of the quantum-kinetic equation is obtained in [17]. The suggested MC estimator in [17] solves the equatio n it considers only for short evolution times and it fails for long evolution times because the stochastic error increases drastically.

In this work we suggest a efficient backward Monte Carlo estimator and a corresponding algorithm for solving the quantum-kinetic equation from [17]. Here the advantage is that this estimator computes the electron energy distribution for long evolution times. Also the computational cost for short times decreases very fast. These results are achieved using variance reduction techniques such as conditional Monte Carlo and reducing the dimensionality.

It is well known that with MC methods, when using random estimators, the results are obtained with statistical errors [11,21,23]. In the case when the MC method approximates some deterministic iterative method there are two errors - systematic (a truncation error) and stochastic (a probability error) [3,14]. The systematic error depends on the number of iterations of the used iterative method, while the stochastic error depends on the probabilistic nature of the MC method.

Consider the following functional:

$$J(f) \equiv (g, f) = \int_G g(x) f(x) dx, \tag{1}$$

where the domain $G \subset I\!R^d$ and a point $x \in G$ is a point in the Euclidean space $I\!R^d$. The functions $f(x)$ and $g(x)$ belong to any Banach space X and to the adjoint space X^*, respectively, and $f(x)$ is an unique solution of the

following Fredholm integral equation in an operator form:

$$f = I\!K(f) + \phi. \tag{2}$$

Consider the iterative process for the integral equation (2):

$$f_l = I\!K(f_{l-1}) + \phi, \;\; l = 1, 2, \ldots , \tag{3}$$

where l is the number of iterations. In fact (3) defines a Neumann series

$$f_l = \phi + I\!K(\phi) + \ldots + I\!K^{l-1}(\phi) + I\!K^l(f_0), \qquad l > 1 \, ,$$

where $I\!K^l$ means the l-th iteration of $I\!K$. In the case when the corresponding infinite series converges then the sum is an element f from the space X which satisfies the equation (2).

¿From (2) and (3) one can get the value of the truncation error. If $f_0 = \phi$ then

$$f_l - f = I\!K^l(\phi - f).$$

Now, a random variable Θ is said to be a MC estimator for the functional (1) if the mathematical expectation of Θ is equal to $J(f)$: $E\Theta = J(f)$. Therefore we can define a MC method

$$\overline{\Theta} = \frac{1}{N} \sum_{i=1}^{N} \Theta^{(i)} \xrightarrow{P} J(f), \tag{4}$$

where $\Theta^{(1)}, \ldots , \Theta^{(N)}$ are independent values of Θ and $\xrightarrow{P}$ means stochastic convergence as $N \longrightarrow \infty$. The well known "law of three sigmas" gives the rate of convergence (see [11,23]):

$$P(|\overline{\Theta} - J(f)|) < 3\frac{\sqrt{Var\Theta}}{\sqrt{N}} \approx 0.997.$$

Thus, as N increases, this statistical error decreases as $N^{-1/2}$. Here $Var(\Theta) = E\Theta^2 - E^2\Theta$ is the variance.

The relation (4) still does not determine the computation algorithm: we must specify the modeling function (sampling rule)

$$\Theta = F(\beta_1, \beta_2, \ldots ,), \tag{5}$$

where $\beta_1, \beta_2, \ldots ,$ are uniformly distributed random numbers in the interval (0, 1). It is known that random number generators are used to produce such

sequences of numbers. They are based upon specific mathematical algorithms, which are repeatable and sequential.

Now both relations (4) and (5) define a Monte Carlo algorithm for estimating $J(f)$.

The case when $g = \delta(x - x_0)$ is of special interest, because we are interested in calculating the value of f at x_0, where $x_0 \in G$ is a fixed point.

It is clear that every iterative algorithm uses a finite number of iterations l. In practice we define a Monte Carlo estimator Θ_l for computing the functional $J(f_l)$ with a statistical error. On the other hand Θ_l is a biased estimator for the functional $J(f)$ with statistical and truncation errors.

We note that the number of iterations can be a random variable when an ε-criterion is used for truncating the Neumann series or the corresponding Markov chain in the MC algorithm.

The paper is organized as follows. In Section 2 the quantum-kinetic equation is described and a new integral form is introduced by reducing the dimensionality in time integral. Convergence of the corresponding Neumann series is proved in Section 3 and the backward MC estimator is introduced. It is proved that the variance of this estimator is bounded. In Section 4 the MC algorithm is presented as decomposition and inverse-transformation techniques for the transition density function which is used for calculating the sequence of points in the Markov process. Numerical results for the electron energy distribution at different evolution times (until 400 fs) and for the computational cost of the algorithm are given in Section 5 using two types of random number generators. Concluding summary is made in Section 6.

2 Formulation of the problem

The three-dimensional one-band electron quantum kinetic integral equation has the following form (see [17]):

$$f(\mathbf{k},t) = \int_0^t dt' \int_0^{t'} dt'' \int d^3\mathbf{k}' \{S(\mathbf{k}',\mathbf{k},t'-t'')f(\mathbf{k}',t'') - S(\mathbf{k},\mathbf{k}',t'-t'')f(\mathbf{k},t'')\} + \phi(\mathbf{k}), \tag{6}$$

with a kernel

$$S(\mathbf{k}',\mathbf{k},t-t') = \frac{2V}{(2\pi)^3\hbar^2}\|g_{\mathbf{k}'-\mathbf{k}}\|^2 e^{-\Gamma_{\mathbf{k}',\mathbf{k}}(t-t')} \tag{7}$$
$$\times\{(n+1)\cos(\Omega_{\mathbf{k}',\mathbf{k}}(t-t')) + n\cos(\Omega_{\mathbf{k},\mathbf{k}'}(t-t'))\},$$

where $\mathbf{k}$ is the momentum, $f(\mathbf{k},t)$ is the distribution function, $\phi(\mathbf{k})$ is the positive initial condition. In the kernel (7) $\Omega_{\mathbf{k}',\mathbf{k}} = (\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} - \hbar\omega)/\hbar$, where ω is the phonon frequency, $\hbar\omega$ is the phonon energy and $\varepsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m$ is the electron energy. The coupling

$$g_{\mathbf{k}'-\mathbf{k}} = -i\left[\frac{2\pi q^2\hbar\omega}{V}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s}\right)\frac{1}{(\mathbf{k}'-\mathbf{k})^2}\right]^{\frac{1}{2}}$$

applies to the Fröhlich interaction with LO phonons, which means a fixed phonon energy with optical (ϵ_∞) and static (ϵ_s) dielectric constants and the normalization volume of the crystal, V.

The Bose function $n = 1/(exp[\hbar\omega/KT] - 1)$, where K is the Boltzmann constant and T is the temperature of the crystal, corresponds to an equilibrium distributed phonon bath. The damping $\Gamma_{\mathbf{k}',\mathbf{k}} = \Gamma_{\mathbf{k}'} + \Gamma_{\mathbf{k}}$ is related to the finite carrier lifetime for the scattering process:

$$\Gamma_{\mathbf{k}} = \int d^3\mathbf{k}' \frac{V}{2^3\pi^2\hbar}\sum_{\pm}\|g_{\mathbf{k}'-\mathbf{k}}\|^2\delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \pm \hbar\omega)(n + \frac{1}{2} \pm \frac{1}{2}). \tag{8}$$

By using the indentity $\int_0^t dt' \int_0^{t'} dt'' = \int_0^t dt'' \int_{t''}^t dt'$, equation (6) can be written in the following form:

$$f(\mathbf{k},t) = \int_0^t dt'' \int d^3\mathbf{k}' \ [\{\int_{t''}^t dt' S(\mathbf{k}',\mathbf{k},t'-t'')\} f(\mathbf{k}',t'')$$
$$- \{\int_{t''}^t dt' S(\mathbf{k},\mathbf{k}',t'-t'')\} f(\mathbf{k},t'')] + \phi(\mathbf{k}). \tag{9}$$

This form is similar to the BE, (see [17], where it is discussed in detail). Note that the "scattering term" $\{\int_{t''}^t dt' S(\mathbf{k},\mathbf{k}',t'-t'')\}$ (if a probabilistic interpretation is possible) depends on the time which is responsible for the memory character of the quantum equation (9). In contrast to the BE, the scattering term, being provided by a long time limit (called the golden rule), does not depend on the time.

Equation (9) allows an analytical evaluation of the "scattering term" [17], since

$$\int_0^{t-t''} d\tau e^{-\Gamma_{\mathbf{k}',\mathbf{k}}\tau} cos(\Omega_{\mathbf{k}',\mathbf{k}}\tau) = \frac{\Gamma_{\mathbf{k}',\mathbf{k}}}{\Omega^2_{\mathbf{k}',\mathbf{k}} + \Gamma^2_{\mathbf{k}',\mathbf{k}}}$$
$$+ \frac{-\Gamma_{\mathbf{k}',\mathbf{k}} cos(\Omega_{\mathbf{k}',\mathbf{k}}(t-t'')) + \Omega_{\mathbf{k}',\mathbf{k}} sin(\Omega_{\mathbf{k}',\mathbf{k}}(t-t''))}{\Omega^2_{\mathbf{k}',\mathbf{k}} + \Gamma^2_{\mathbf{k}',\mathbf{k}}} \times e^{-\Gamma_{\mathbf{k}',\mathbf{k}}(t-t'')}.$$

Using this transformation equation (6) can be writen in the following form:

$$f(\mathbf{k},t) = \int_0^t dt'' \int d^3\mathbf{k}' \{\mathcal{K}(\mathbf{k}',\mathbf{k},t-t'') f(\mathbf{k}',t'')$$
$$- \mathcal{K}(\mathbf{k},\mathbf{k}',t-t'') f(\mathbf{k},t'')\} + \phi(\mathbf{k}), \tag{10}$$

with a kernel

$$\mathcal{K}(\mathbf{k}',\mathbf{k},t-t'') = \frac{q^2\omega}{2\pi^2\hbar} \left|\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s}\right| \frac{1}{(\mathbf{k}'-\mathbf{k})^2} \tag{11}$$

$$\times \left((n+1) L_{\mathbf{k}',\mathbf{k}} \left[1 + \left(\frac{\Omega_{\mathbf{k}',\mathbf{k}}}{\Gamma_{\mathbf{k}',\mathbf{k}}} sin(\Omega_{\mathbf{k}',\mathbf{k}}(t-t'')) - cos(\Omega_{\mathbf{k}',\mathbf{k}}(t-t'')) \right) e^{-\Gamma_{\mathbf{k}',\mathbf{k}}(t-t'')} \right] \right.$$
$$\left. + n L_{\mathbf{k},\mathbf{k}'} \left[1 + \left(\frac{\Omega_{\mathbf{k},\mathbf{k}'}}{\Gamma_{\mathbf{k},\mathbf{k}'}} sin(\Omega_{\mathbf{k},\mathbf{k}'}(t-t'')) - cos(\Omega_{\mathbf{k},\mathbf{k}'}(t-t'')) \right) e^{-\Gamma_{\mathbf{k},\mathbf{k}'}(t-t'')} \right] \right),$$

where $L_{\mathbf{k},\mathbf{k}'}$ is a Lorentzian function, $L_{\mathbf{k}',\mathbf{k}} = \frac{\Gamma_{\mathbf{k}',\mathbf{k}}}{\Omega^2_{\mathbf{k}',\mathbf{k}} + \Gamma^2_{\mathbf{k}',\mathbf{k}}}$. Thus the kernel (11) can be decomposed into a time-independent part and a part which depends explicitly on the time.

One way of obtaining the long-time-scale solution of this quantum kinetic equation is presented in [16] where the time-dependent terms in the kernel (11) are removed. For a long time limit, $t \to \infty$, the terms involving time which contain the memory character of the equation vanish. Here we treat a simulation method as we save the time-dependent terms in the kernel (11).

3 A backward Monte Carlo estimator

Let us specify that the wave vectors $\mathbf{k}$, $\mathbf{k}'$ belong to a finite domain G with a volume V_G.

Consider an equation (10) that can be written in the following second-order Voltera-Fredholm form:

$$f(\mathbf{k},t) = \int_0^t dt'' \int_G d^3\mathbf{k}' \{\mathcal{K}(\mathbf{k}',\mathbf{k},t-t'')f(\mathbf{k}',t'')\} \tag{12}$$
$$- \int_0^t dt'' \int_G d^3\mathbf{k}' \{\mathcal{K}(\mathbf{k},\mathbf{k}',t-t'')f(\mathbf{k},t'')\} + \phi(\mathbf{k}).$$

We note that the kernel in (12) is polar since it can be rewritten as

$$\mathcal{K}(\mathbf{k}',\mathbf{k},t-t'') = \frac{\lambda(\mathbf{k}',\mathbf{k},t-t'')}{|\mathbf{k}'-\mathbf{k}|^2}, \tag{13}$$

where $\lambda(\mathbf{k}',\mathbf{k},t-t'')$ is a continuous function in the domain $\overline{G}\times\overline{G}\times[0,t]$. Therefore, the following inequalities hold (see [26]):

$$\max_{0\le t''\le t}\max_{\mathbf{k}\in\overline{G}}\int_G d^3\mathbf{k}'|\mathcal{K}(\mathbf{k}',\mathbf{k},t-t'')| \le M_1\,, \quad \max_{0\le t''\le t}\max_{\mathbf{k}\in\overline{G}}\int_G d^3\mathbf{k}'|\mathcal{K}(\mathbf{k},\mathbf{k}',t-t'')| \le M_2\,,$$

where M_1 and M_2 are positive constants. Let $M = \max\{M_1, M_2\}$, then the following proposition holds.

Lemma 1 *Consider the following iterative process for the equation (12):*

$$f_l(\mathbf{k},t) = \int_0^t dt'' \int_G d^3\mathbf{k}' \{\mathcal{K}(\mathbf{k}',\mathbf{k},t-t'')f_{l-1}(\mathbf{k}',t'')\} \tag{14}$$
$$- \int_0^t dt'' \int_G d^3\mathbf{k}' \{\mathcal{K}(\mathbf{k},\mathbf{k}',t-t'')f_{l-1}(\mathbf{k},t'')\} + \phi(\mathbf{k}),$$
$$f_0(\mathbf{k},t) = \phi(\mathbf{k}), \quad l = 1,2,\ldots$$

If $\|\phi\| = \max_{\mathbf{k}\in\overline{G}}\phi(\mathbf{k})$ *then*

$$|f_l(\mathbf{k},t) - \phi(\mathbf{k})| \le \|\phi\| \sum_{j=1}^{l} \frac{(2M)^j t^j}{j!}. \tag{15}$$

Proof: To prove inequality (15) we will use induction. For $l = 1$ we may quickly verify that

$$|f_1(\mathbf{k},t) - f_0(\mathbf{k},t)| \le \|\phi\|(2M)\frac{t}{1!}.$$

Assume that we have the following estimate for l :

$$|f_l(\mathbf{k},t) - f_{l-1}(\mathbf{k},t)| \le \|\phi\|(2M)^l\frac{t^l}{l!}.$$

For $l+1$ we obtain

$$|f_{l+1}(\mathbf{k},t) - f_l(\mathbf{k},t)|$$

$$\leq \left| \int_0^t dt'' \int_G d^3\mathbf{k}' \{\mathcal{K}(\mathbf{k}',\mathbf{k},t-t'')f_l(\mathbf{k}',t'')\} - \int_0^t dt'' \int_G d^3\mathbf{k}' \{\mathcal{K}(\mathbf{k},\mathbf{k}',t-t'')f_l(\mathbf{k},t'')\} \right.$$

$$\left. - \int_0^t dt'' \int_G d^3\mathbf{k}' \{\mathcal{K}(\mathbf{k}',\mathbf{k},t-t'')f_{l-1}(\mathbf{k}',t'')\} + \int_0^t dt'' \int_G d^3\mathbf{k}' \{\mathcal{K}(\mathbf{k},\mathbf{k}',t-t'')f_{l-1}(\mathbf{k},t'')\} \right|$$

$$\leq \int_0^t dt'' \int_G d^3\mathbf{k}' |\mathcal{K}(\mathbf{k}',\mathbf{k},t-t'')| \, |f_l(\mathbf{k}',t'') - f_{l-1}(\mathbf{k}',t'')|$$

$$+ \int_0^t dt'' \int_G d^3\mathbf{k}' |\mathcal{K}(\mathbf{k},\mathbf{k}',t-t'')| \, |f_{l-1}(\mathbf{k},t'') - f_l(\mathbf{k},t'')|$$

$$\leq \int_0^t dt'' M_1 \|\phi\| (2M)^l \frac{t''^l}{l!} + \int_0^t dt'' M_2 \|\phi\| (2M)^l \frac{t''^l}{l!}$$

$$= M_1\|\phi\|(2M)^l \frac{t^{l+1}}{(l+1)!} + M_2\|\phi\|(2M)^l \frac{t^{l+1}}{(l+1)!} \leq \|\phi\|(2M)^{l+1}\frac{t^{l+1}}{(l+1)!}$$

and further

$$|f_l(\mathbf{k},t) - \phi(\mathbf{k})|$$

$$\leq |f_1(\mathbf{k},t) - \phi(\mathbf{k})| + |f_2(\mathbf{k},t) - f_1(\mathbf{k},t)| + \ldots + |f_l(\mathbf{k},t) - f_{l-1}(\mathbf{k},t)|$$

$$\leq \|\phi\| \sum_{j=1}^{l} \frac{(2M)^j t^j}{j!}.$$

This completes the proof. □

Lemma 1 yields that the iterative process (14) converges to the solution of the equation (12) absolutely, because the corresponding Neumann series is bounded by the summation of the series $\|\phi\| exp(2Mt)$.

Now let us construct a backward Monte Carlo estimator for the solution of the equation (12) at a fixed point $\mathbf{k}$ at time t using backward time evolution of the numerical trajectories.

Define a terminated Markov chain

$$(\kappa_0,\tau_0) \to \ldots \to (\kappa_j,\tau_j) \to \ldots \to (\kappa_l,\tau_l), \tag{16}$$

such that every point $(\kappa_j,\tau_j), j = 1,2,\ldots,l$ is chosen in the domain $\overline{G} \times (0,\tau_{j-1})$ in accordance with a transition density functions $r_\alpha(\mathbf{k},t,\mathbf{k}',t'')$, $(\alpha = 1,2)$ which are tolerant [1] to both kernels $K_1(\mathbf{k},t,\mathbf{k}',t'') = \mathcal{K}(\mathbf{k}',\mathbf{k},t-t'')$ and

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

$K_2(\mathbf{k},t,\mathbf{k}',t'') = -\mathcal{K}(\mathbf{k},\mathbf{k}',t-t'')$, respectively. The parameter l is chosen from the condition $\tau_l < \varepsilon$, where ε is a very small positive number.

Consider the following estimators

$$\begin{aligned}\nu_0 &= \phi(\kappa_0),\\ \nu_j^{\alpha_1,\ldots,\alpha_j} &= \frac{K_{\alpha_1}(\kappa_0,\tau_0,\kappa_1,\tau_1)\ldots K_{\alpha_j}(\kappa_{j-1},\tau_{j-1},\kappa_j,\tau_j)}{p_{\alpha_1} r_{\alpha_1}(\kappa_0,\tau_0,\kappa_1,\tau_1)\ldots p_{\alpha_j} r_{\alpha_j}(\kappa_{j-1},\tau_{j-1},\kappa_j,\tau_j)}\phi(\kappa_j^{\alpha_j}),\end{aligned}$$

where

$$\phi(\kappa_j^{\alpha_j}) = \begin{cases}\phi(\kappa_j), & \text{if } \alpha_j = 1\\ \phi(\kappa_{j-1}), & \text{if } \alpha_j = 2\end{cases} \quad \text{and } p_{\alpha_j} \geq 0, \sum_{\alpha_j=1}^{2} p_{\alpha_j} = 1.\ j = 1,2,\ldots,l,$$

Thus the biased backward Monte Carlo estimator for the solution of equation (12) at the fixed point $(\mathbf{k},t) = (\kappa_0,\tau_0)$ has the form

$$\Theta_l[\kappa_0,\tau_0] = \nu_0 + \sum_{j=1}^{l} \nu_j^{\alpha_1,\ldots,\alpha_j}. \tag{17}$$

Using N independent samples of the estimator (17) we obtain

$$\overline{\Theta}_l[\kappa_0,\tau_0] = \frac{1}{N}\sum_{i=0}^{N}(\Theta_l[\kappa_0,\tau_0])_i \approx f(\kappa_0,\tau_0).$$

For the biased estimator of order ε we have (see [14]):

$$|E\Theta_l[\kappa_0,\tau_0] - f(\kappa_0,\tau_0)|^2 \leq c_1\varepsilon^2$$

where c_1 is a positive constant. Now following [14] the root mean square deviation is defined by the relation

$$E(\Theta_l[\kappa_0,\tau_0] - f(\kappa_0,\tau_0))^2 = Var(\Theta_l[\kappa_0,\tau_0]) + (f(\kappa_0,\tau_0) - E\Theta_l[\kappa_0,\tau_0])^2.$$

Hence

$$\begin{aligned}E(\overline{\Theta}_l[\kappa_0,\tau_0] - f(\kappa_0,\tau_0))^2 &= \frac{Var(\Theta_l[\kappa_0,\tau_0])}{N} + (f(\kappa_0,\tau_0) - E\Theta_l[\kappa_0,\tau_0])^2\\ &\leq \frac{d_0}{N} + c_1\varepsilon^2 = \mu^2,\end{aligned} \tag{18}$$

where μ is the desired error and d_0 is an upper bound of the variance. Therefore, in order to obtain the error of order μ the optimal order of the quantities N and ε must be

$$N = O(\mu^{-2}), \quad \varepsilon = O(\mu).$$

The inequality (18) will be clear if we prove the variance is bounded. For this goal it is enough to prove that the second moment of the estimator (17) is bounded.

Lemma 2 *Let us choose the probabilities and the transition density functions in the following way:*

$$p_\alpha = \frac{|K_\alpha(\mathbf{k}, t, \mathbf{k}', t'')|}{|K_1(\mathbf{k}, t, \mathbf{k}', t'')| + |K_2(\mathbf{k}, t, \mathbf{k}', t'')|}, \quad \alpha = 1, 2, \tag{19}$$

$$r_\alpha(\mathbf{k}, t, \mathbf{k}', t'') = \frac{|K_\alpha(\mathbf{k}, t, \mathbf{k}', t'')|}{\int_0^t dt'' \int_G dk' |K_\alpha(\mathbf{k}, t, \mathbf{k}', t'')|}, \quad \alpha = 1, 2. \tag{20}$$

Then the following estimate holds

$$E\Theta_l^2[\kappa_0, \tau_0] < 2\|\phi\|^2 e^{(2Mt)^2}. \tag{21}$$

Proof: First, let us prove the inequality

$$E(\nu_j^{\alpha_1, \ldots, \alpha_j})^2 \le \|\phi\|^2 \frac{(2M^2t^2)^j}{(2j-1)!!} \tag{22}$$

using again induction. For $j = 0$ it is true, $E(\nu_0)^2 \le \|\phi\|^2$. For $j = 1$ we have

$$E(\nu_1^{\alpha_1})^2 = \int_0^{\tau_0 = t} d\tau_1 \int_G d\kappa_1 (\nu_1^{\alpha_1})^2 p_{\alpha_1} r_{\alpha_1}(\kappa_0, \tau_0, \kappa_1, \tau_1)$$

$$= \int_0^t d\tau_1 \int_G d\kappa_1 \frac{K_{\alpha_1}^2(\kappa_0, \tau_0, \kappa_1, \tau_1) \phi^2(\kappa_1^{\alpha_1})}{p_{\alpha_1} r_{\alpha_1}(\kappa_0, \tau_0, \kappa_1, \tau_1)}$$

$$= \int_0^t d\tau_1 \int_G d\kappa_1 \left(|K_1(\kappa_0, \tau_0, \kappa_1, \tau_1)| + |K_2(\kappa_0, \tau_0, \kappa_1, \tau_1)|\right) \phi^2(\kappa_1^{\alpha_1}) \int_0^t d\tau_1 \int_G d\kappa_1 |K_{\alpha_1}(\kappa_0, \tau_0, \kappa_1, \tau_1)|$$

$$\le \|\phi\|^2 \left(M \int_0^t d\tau_1 + M \int_0^t d\tau_1 \right) M \int_0^t d\tau_1 = \|\phi\|^2 2M^2 t^2.$$

Assume that inequality (22) holds for $j = l$. Therefore for $j = l + 1$ we obtain

$$E(\nu_{l+1}^{\alpha_1 \ldots \alpha_{l+1}})^2$$

$$= \int_0^{\tau_0 = t} d\tau_1 \int_G d\kappa_1 \ldots \int_0^{\tau_l} d\tau_{l+1} \int_G d\kappa_{l+1} (\nu_{l+1}^{\alpha_1 \ldots \alpha_{l+1}})^2 p_{\alpha_1} r_{\alpha_1}(\kappa_0, \tau_0, \kappa_1, \tau_1) \ldots p_{\alpha_{l+1}} r_{\alpha_{l+1}}(\kappa_l, \tau_l, \kappa_{l+1}, \tau_{l+1})$$

$$= \int_0^t d\tau_1 \int_G d\kappa_1 \frac{K^2_{\alpha_1}(\kappa_0,\tau_0,\kappa_1,\tau_1)}{p_{\alpha_1} r_{\alpha_1}(\kappa_0,\tau_0,\kappa_1,\tau_1)} \dots \int_0^{\tau_l} d\tau_{l+1} \int_G d\kappa_{l+1} \frac{K^2_{\alpha_{l+1}}(\kappa_l,\tau,\kappa_{l+1},\tau_{l+1})\phi^2(\kappa_{l+1}^{\alpha_{l+1}})}{p_{\alpha_{l+1}} r_{\alpha_{l+1}}(\kappa_l,\tau_l,\kappa_{l+1},\tau_{l+1})}$$

$$= \int_0^t d\tau_1 \int_G d\kappa_1 \frac{K^2_{\alpha_1}(\kappa_0,\tau_0,\kappa_1,\tau_1)}{p_{\alpha_1} r_{\alpha_1}(\kappa_0,\tau_0,\kappa_1,\tau_1)} E(\nu_l^{\alpha_2\dots\alpha_{l+1}})^2$$

$$\le \int_0^t d\tau_1 \int_G d\kappa_1 \left[(|K_1(\kappa_0,\tau_0,\kappa_1,\tau_1)| + |K_2(\kappa_0,\tau_0,\kappa_1,\tau_1)|) \right.$$

$$\left. \times \|\phi\|^2 \frac{(2M^2\tau_1^2)^j}{(2j-1)!!} \right] \int_0^t d\tau_1 \int_G d\kappa_1 |K_{\alpha_1}(\kappa_0,\tau_0,\kappa_1,\tau_1)|$$

$$\le \|\phi\|^2 \left(2M \int_0^t d\tau_1 \frac{(2M^2\tau_1^2)^j}{(2j-1)!!} \right) M \int_0^t d\tau_1$$

$$= \|\phi\|^2 2M^2 t \frac{(2M^2)^j}{(2j-1)!!} \frac{t^{2j+1}}{(2j+1)} = \|\phi\|^2 \frac{(2M^2t^2)^{j+1}}{(2j+1)!!}.$$

On the other hand

$$\Theta_l^2[\kappa_0,\tau_0] = \left(\nu_0 + \sum_{j=1}^{l} \nu_j^{\alpha_1\dots\alpha_j} \right)^2 \le \left(\sum_{j=0}^{\infty} |\nu_j^{\alpha_1\dots\alpha_j}| \right)^2 = |\Theta_\infty[\kappa_0,\tau_0]|^2 .$$

Further

$$|\Theta_\infty[\kappa_0,\tau_0]|^2 = \left(\sum_{j=0}^{\infty} |\nu_j^{\alpha_1\dots\alpha_j}| \right)^2 \le \sum_{i,j=0}^{\infty} |\nu_i^{\alpha_1\dots\alpha_i}| \, |\nu_j^{\alpha_1\dots\alpha_j}|.$$

The last inequality can be written in the form

$$|\Theta_\infty[\kappa_0,\tau_0]|^2 \le \sum_{i,j=0}^{\infty} a^{i+j} (|\nu_i^{\alpha_0\dots\alpha_i}| a^{-i}) \, (|\nu_j^{\alpha_0\dots\alpha_j}| a^{-j}),$$

where $a \in (0,\, 1)$. Using inequality $(2uv \le u^2 + v^2)$ we have

$$|\Theta_\infty[\kappa_0,\tau_0]|^2 \le \frac{1}{2} \sum_{i,j=0}^{\infty} a^{i+j} \left(\frac{(\nu_i^{\alpha_1\dots\alpha_i})^2}{a^{2i}} + \frac{(\nu_j^{\alpha_1\dots\alpha_j})^2}{a^{2j}} \right)$$

$$= \sum_{j=0}^{\infty} a^{-j} (\nu_j^{\alpha_1\dots\alpha_j})^2 \sum_{i=0}^{\infty} a^i = \frac{1}{1-a} \left((\nu_0)^2 + \sum_{j=1}^{\infty} a^{-j} (\nu_j^{\alpha_1\dots\alpha_j})^2 \right).$$

Finally

$$E\Theta_l^2[\kappa_0,\tau_0] \le \frac{1}{1-a} \left(E(\nu_0)^2 + \sum_{j=1}^{\infty} a^{-j} E(\nu_j^{\alpha_1\dots\alpha_j})^2 \right)$$

$$\le \frac{1}{1-a} \left(\|\phi\|^2 + \|\phi\|^2 \sum_{j=1}^{\infty} a^{-j} \frac{(2M^2t^2)^j}{(2j-1)!!} \right) < \frac{\|\phi\|^2}{(1-a)} e^{2M^2t^2/a}.$$

If we choose $a = 1/2$ then we obtain (21). This completes the proof. $\square$

Taking into account that the kernel can be presented as equation (13) we can note that estimate (21) holds for tolerant transiton density functions of the kind

$$r_\alpha(\mathbf{k}, t, \mathbf{k}', t'') = A\frac{\lambda_\alpha(\mathbf{k}, t, \mathbf{k}', t'')}{|\mathbf{k}' - \mathbf{k}|^2}, \quad \alpha = 1, 2, \tag{23}$$

where $\lambda_\alpha(\mathbf{k}, t, \mathbf{k}', t'')$ are arbitrary continuous functions in the domain $\overline{G} \times \overline{G} \times [0, t]$ and A is the normalized constant. In this case only the constant M will be different in estimate (21).

Let us note that the above choice (20) of the transiton density function to be proportional to the kernel leads to a reduction of the variance and such density functions are called "almost optimal" densities (see [2]). Thus if the functions $\lambda_\alpha(\mathbf{k}, t, \mathbf{k}', t'')$, $(\alpha = 1, 2)$ are chosen to be proportional to the contribution from the kernels then the corresponding transiton density functions (23) will lead to a reduction of the variance, too. The choice of the probabilities (19) can be done on the other way, too, for example, using any norm of the kernels.

4 A Backward Monte Carlo algorithm

Before we describe the algorithm let us present equation (12) in a simpler form using spherical coordinates. Thus, we consider an one-dimensional integral equation concerning momentum $\mathbf{k}$.

Suppose that the domain G is a sphere with radius Q. Denote with k and k' the norm of the corresponding vectors $\mathbf{k}$ and $\mathbf{k}'$. Let θ be the angle between this two vectors and k'_z axis be oriented along $\mathbf{k}$. Using spherical coordinates we have $d^3\mathbf{k}' = k'^2 \sin\theta dk' d\theta d\xi$, $\theta \in (0, \pi)$, $\xi \in (0, 2\pi)$.

Taking into account that

$$\int_0^{2\pi} d\xi = 2\pi, \qquad \int_0^{\pi} d\theta \left(\frac{k'^2 \sin\theta}{k'^2 + k^2 - 2kk'\cos\theta}\right) = \frac{k'}{k} \ln\left(\frac{k + k'}{|k - k'|}\right)$$

equation (12) and the kernel (11) can be rewritten in the form

$$f(k, t) = \int_0^t dt'' \int_0^Q dk' \{K_1(k, t, k', t'') f(k', t'')\} \tag{24}$$

$$+\int_0^t dt'' \int_0^Q dk' \{K_2(k,t,k',t'') f(k,t'')\} + \phi(k),$$

where

$$K_1(k,t,k',t'') = k'^2 \mathcal{K}(k',k,t-t''), \quad K_2(k,t,k',t'') = -k'^2 \mathcal{K}(k,k',t-t'')$$

and

$$\mathcal{K}(k',k,t-t'') = \frac{q^2\omega}{\pi\hbar} \left| \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s} \right| \frac{1}{k'k} \ln\left(\frac{k+k'}{|k-k'|}\right)$$

$$\times \left((n+1) L_{k',k} \left[1 + \left(\frac{\Omega_{k',k}}{\Gamma_{k',k}} sin(\Omega_{k',k}(t-t'')) - cos(\Omega_{k',k}(t-t'')) \right) e^{-\Gamma_{k',k}(t-t'')} \right] \right.$$

$$\left. + n L_{k,k'} \left[1 + \left(\frac{\Omega_{k,k'}}{\Gamma_{k,k'}} sin(\Omega_{k,k'}(t-t'')) - cos(\Omega_{k,k'}(t-t'')) \right) e^{-\Gamma_{k,k'}(t-t'')} \right] \right).$$

To complete substitution of the variables we have to rewrite equation (8) in spherical coordinates, namely

$$\Gamma_k = \int_0^{2\pi} d\xi \int_0^{\pi} d\theta \int_0^Q dk' \left(\frac{k'^2 \sin\theta}{k'^2 + k^2 - 2kk'\cos\theta} \right) \frac{q^2\omega}{4\pi} \left| \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s} \right|$$

$$\times \left[\delta\left(\frac{\hbar^2}{2m}(k'^2 - k^2) + \hbar\omega \right)(n+1) + \delta\left(\frac{\hbar^2}{2m}(k'^2 - k^2) - \hbar\omega \right) n \right].$$

In addition using the following properties of the Dirac delta function [26],

$$\delta(ax \pm b) = \frac{1}{a}\delta(x \pm \frac{b}{a}) \text{ and } \int dx \delta(x - x_0) F(x) = F(x_0)$$

with $a = \hbar^2/2m$ and $b = \hbar\omega$, we get

$$\Gamma_k = \begin{cases} \frac{c_2(n+1)}{k} \ln\left(\frac{k+\sqrt{k^2-\omega_1}}{\sqrt{\omega_1}} \right) + \frac{c_2 n}{k} \ln\left(\frac{k+\sqrt{k^2+\omega_1}}{\sqrt{\omega_1}} \right), & \text{if } k^2 \geq \omega_1 \\ \frac{c_2 n}{k} \ln\left(\frac{k+\sqrt{k^2+\omega_1}}{\sqrt{\omega_1}} \right), & \text{if } k^2 < \omega_1, \end{cases}$$

where $\omega_1 = 2m\omega/\hbar$, and $c_2 = (mq^2\omega/\hbar^2)|1/\epsilon_\infty - 1/\epsilon_s|$.

In order to describe a concrete realization of the backward MC algorithm for the estimator (17) we have to know how to model the transition $(k,t) \to (k',t'')$ in the Markov chain. In other words, we must specify sampling rules using a transition density function which is tolerant to the kernels under consideration.

Let us choose the transition density function in the following way

$$r_\alpha(k,t,k',t'') = r(k,k') r(t,t''/k,k'), \quad \alpha = 1,2,$$

where

$$r(k,k') = \overline{C}\frac{k'}{k}\ln\left(\frac{k+k'}{|k-k'|}\right) \tag{25}$$

is a normalized probability density function ($\overline{C}$ is the normalized constant) and

$$r(t,t''/k,k') = \frac{\Gamma_{k,k'}e^{-\Gamma_{k,k'}(t-t'')}}{1-e^{-\Gamma_{k,k'}t}} \tag{26}$$

is a normalized conditional probability density function. The transition $k \to k'$ can be modeled using a decomposition MC technique. For this goal the function (25) can be expressed as an infinite weighted sum of other density functions.

Since,

$$\frac{k'}{k}\ln\left(\frac{k+k'}{|k-k'|}\right) = \begin{cases} 2\sum_{i=0}^{\infty}\frac{(k')^{2i+2}}{(2i+1)k^{2i+2}}, & \text{if } \ 0 \le k' < k \\ 2\sum_{i=0}^{\infty}\frac{k^{2i}}{(2i+1)(k')^{2i}}, & \text{if } \ k < k' \le Q \end{cases} \tag{27}$$

and substituting

$$\overline{C}_i = \begin{cases} \frac{2}{(2i+1)(2i+3)}, & \text{if } \ 0 \le k' < k \\ \frac{\frac{4k^2}{(4i^2-1)}\left(1-(\frac{k}{Q})^{2i-1}\right)}{(Q-k)\left[2k+(Q+k)\ln\left(\frac{Q+k}{Q-k}\right)\right]}, & \text{if } \ k < k' \le Q \end{cases}$$

$$r_i(k,k') = \begin{cases} (2i+3)\frac{(k')^{2i+2}}{k^{2i+3}}, & \text{if } \ 0 \le k' < k \\ (2i-1)\left[\frac{(Qk)^{2i-1}}{Q^{2i-1}-k^{2i-1}}\frac{1}{(k')^{2i}}\right], & \text{if } \ k < k' \le Q \end{cases}$$

the density function (25) can be written

$$r(k,k') = \sum_{i=0}^{\infty}\overline{C}_i r_i(k,k'), \ \text{ where } \ \overline{C}_i \ge 0, \quad \sum_{i=0}^{\infty}\overline{C}_i = 1, \tag{28}$$

where the $r_i(k,k')$ $(i = 0,1,\ldots,)$ are density functions, too. Now we need three uniformly distributed numbers, $\beta_1, \beta_2, \beta_3 \in (0,\ 1)$ to model the transition $k \to k'$. The first two numbers are used to choose the series from (27) and to determine the number "i" and $r_i(k,k')$ from (28). Finally the new momentum

k' in the Markov chain is calculated by formulas

$$k' = \begin{cases} k(\beta_3)^{\frac{1}{2i+1}}, & \text{if } 0 \le k' < k \\ \dfrac{k}{[1-\beta_3(1-(k/Q)^{2i-1})]^{\frac{1}{2i-1}}}, & \text{if } k < k' \le Q \end{cases}$$

In practice, decomposition MC techniques are applied for finate number terms in the series (28).

To complete the transition $(k,t) \to (k',t'')$ we need again an uniformly distributed number $\beta \in (0,\,1)$. The new time $t'' \in (0,\,t)$ can be found by applying the inverse-transformation technique for (26). Thus we get

$$t'' = \frac{1}{\Gamma_{k,k'}} \ln\left(\beta(e^{\Gamma_{k,k'}t} - 1) + 1\right).$$

The backward MC algorithm for finding a solution in a fixed point (k,t) of the equation (24) is as follows:

1. **Choose** any positive small number ε.

2. **Simulate** N independent random paths

$$(\kappa_0^{(i)}, \tau_0^{(i)}) \to \ldots \to (\kappa_j^{(i)}, \tau_j^{(i)}) \to \ldots \to (\kappa_l^{(i)}, \tau_l^{(i)}), \quad i = 1, \ldots, N,$$

of the Markov chain (16) with starting points $(\kappa_0^{(i)}, \tau_0^{(i)}) = (k,t)$ in accordance with the transition density functions (25) and (26). The random paths terminate when $\tau_l^{(i)} < \varepsilon$.

3. **Find**

$$(\Theta_l[\kappa_0, \tau_0])_i = (\nu_0)_i + \sum_{j=1}^{l} (\nu_j^{\alpha_1,\ldots,\alpha_j})_i, \quad i = 1, \ldots, N,$$

where $(\nu_0)_i = \phi(\kappa_0^{(i)})$ and

$$(\nu_j^{\alpha_1,\ldots,\alpha_j})_{(i)}$$

$$= \frac{K_{\alpha_1}(\kappa_0^{(i)}, \tau_0^{(i)}, \kappa_1^{(i)}, \tau_1^{(i)}) \ldots K_{\alpha_j}(\kappa_{j-1}^{(i)}, \tau_{j-1}^{(i)}, \kappa_j^{(i)}, \tau_j^{(i)}) \;\; \phi^{(i)}(\kappa_j^{\alpha_j})}{p_{\alpha_1}^{(i)} r(\kappa_0^{(i)}, \kappa_1^{(i)})\, r(\tau_0^{(i)}, \tau_1^{(i)}/\kappa_0^{(i)}, \kappa_1^{(i)}) \ldots p_{\alpha_j}^{(i)} r(\kappa_{j-1}^{(i)}, \kappa_j^{(i)})\, r(\tau_{j-1}^{(i)}, \tau_j^{(i)}/\kappa_{j-1}^{(i)}, \kappa_j^{(i)})},$$
$$j = 1, 2, \ldots, l, \quad \alpha_s = 1, 2, \quad s = 1, \ldots, j.$$

The probabilities $p_{\alpha_j}^{(i)}$, $(\alpha_j = 1, 2)$ are chosen in accordance with equation (19).

4. **Calculate**

$$\overline{\Theta}_l[\kappa_0, \tau_0] = \frac{1}{N} \sum_{i=0}^{N} (\Theta_l[\kappa_0, \tau_0])_i$$

which estimates the solution $f(k,t)$.

The computational complexity of the presented algorithm can be measured by the quantity

$$F(N,t_0,l) = N \times t_0 \times E(l),$$

where N is the number of the random paths followed; $E(l)$ is the mathematical expectation of the number of transitions in the Markov chain (16) and t_0 is the mean time for modeling one transition.According to (18) N and $E(l)$ are connecting with stochastic and systemtic errors. The time, t_0, depends on the complexity of the transition density function and the choosing of the random number generator (r.n.g.). When the r.n.g. has good random properties such as uniformly distributed, uncorrelated, have a large period of repetition and can be generated rapidly using limited computer memory, then the computational cost of the MC algorithm can be decreased and the accuracy of the MC solution can be improved. It is strongly recommended that all simulations be done with two or more different generators, and the results compared to check whether the random number generator is introducing a bias.

The backward MC algorithm under consideration is realized using two generators that are recommended by many authors for large-scale scientific computations. The first r.n.g. is a combined linear congruential generator (CLCG) with parameters recommended by P. L'Ecuyer [4,5]. He suggests for combining the following two generators:

$$x_s = 40014 x_{s-1} \bmod 2147483563, \qquad y_s = 40692 y_{s-1} \bmod 2147483399.$$

This would produce

$$w_s = (x_s - y_s) \bmod 2147483562.$$

This CLCG generator has a period 2.306×10^{18} and its structural properties are investigated in [5].

The second r.n.g., the Scalable Parallel Random Number Generator (SPRNG) Library is a lagged Fibonacci generator using addition and it provides parallelized independent sequences [13,24].

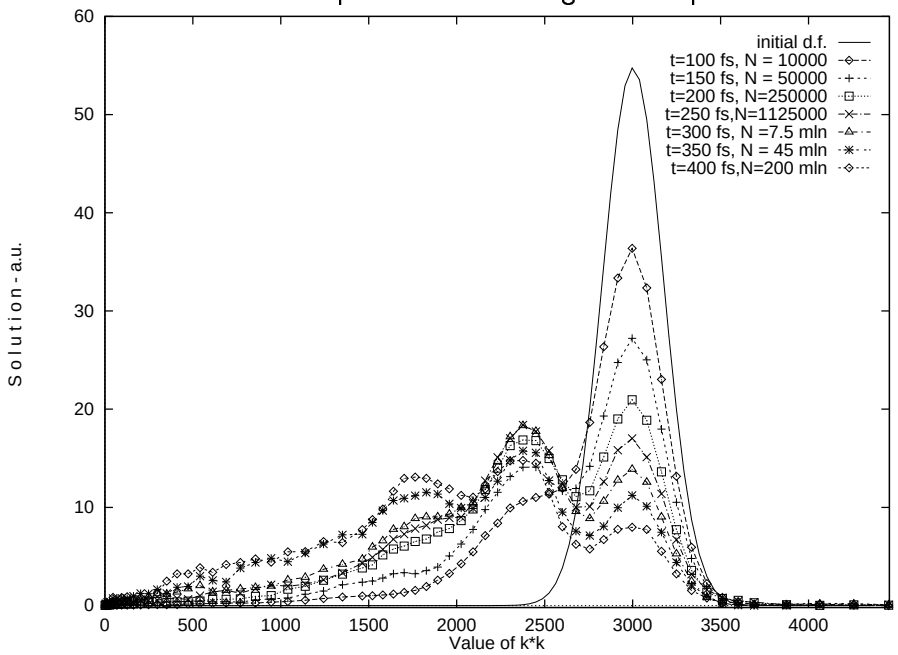
In fact, we need four uniformly distributed numbers between 0 and 1 to model the transition $(k,t) \to (k',t'')$ and one uniformly distributed number to choose the probability (19) in order to construct the estimator in step 3 of the algorithm. Therefore we can use five independent sequences from the SPRNG Library.

The results obtained for computational cost of the MC algotithm and accuracy of the MC solution using CLCG and SPRNG generators are compared in the next section.

5 Numerical results

The results discussed in the following have been obtained by the backward Monte Carlo algorithm under consideration for equation (24). Material parameters for $GaAs$ have been used: the electron effective mass is 0.063, the optimal phonon energy is $36meV$, the static and optical dielectric constants in the Fröhlich coupling are $\varepsilon_s = 10.92$ and $\varepsilon_\infty = 12.9$. The lattice temperature is zero. The initial condition at $t = 0$ is given by a function which is Gaussian in energy and corresponds to a $87fs$ laser pulse with an excess energy of $180meV$, scaled in a way to ensure peak value equal to unity. The quantity presented on the y-axes in Figs. 1–8 is $k * f(k,t)$, i.e. it is proportional to the distribution function multiplied by the density of states. It is given in arbitrary units. The quantity $k * k$, given on the x-axes in units $10^{14}/m^2$, is proportional to the electron energy. The backward MC algorithm was imple-

Fig. 1. The electron energy distribution $k * f(k,t)$ versus $k * k$ for long evolution times. The relaxation leads to a time-dependent broadening of the replicas. $\varepsilon = 0.0001$.



mented in C and compiled with the "cc" compiler at optimization level "-fast". Numerical tests on Sun Ultra Enterprise 4000 with 14 Ultra-SPARC, 250 MHz CPUs running Solaris were performed. Fig.1 shows the electron distribution at long evolution times (until 400 fs) The simulation domain is between 0 and $Q = 66 \times 10^7/m$. The product $k * f(k,t)$ is calculated in 60 points.

The electron energy distribution for short evolution times is presented on Fig.2. Here the simulation domain is between 0 and $Q = 100 \times 10^7/m$. The product $k * f(k,t)$ is calculated in 100 points. The solutions for $t = 10fs, t = 20fs, t = 30fs, t = 40fs$ and $t = 50fs$ is calculated for $\varepsilon = 0.0001$ and

Fig. 2. The electron energy distribution $k*f(k,t)$ versus $k*k$ for short evolution times. Electrons appear in the semiclassically forbidden region above the initial condition. $N = 50000,\ \varepsilon = 0.0001$.

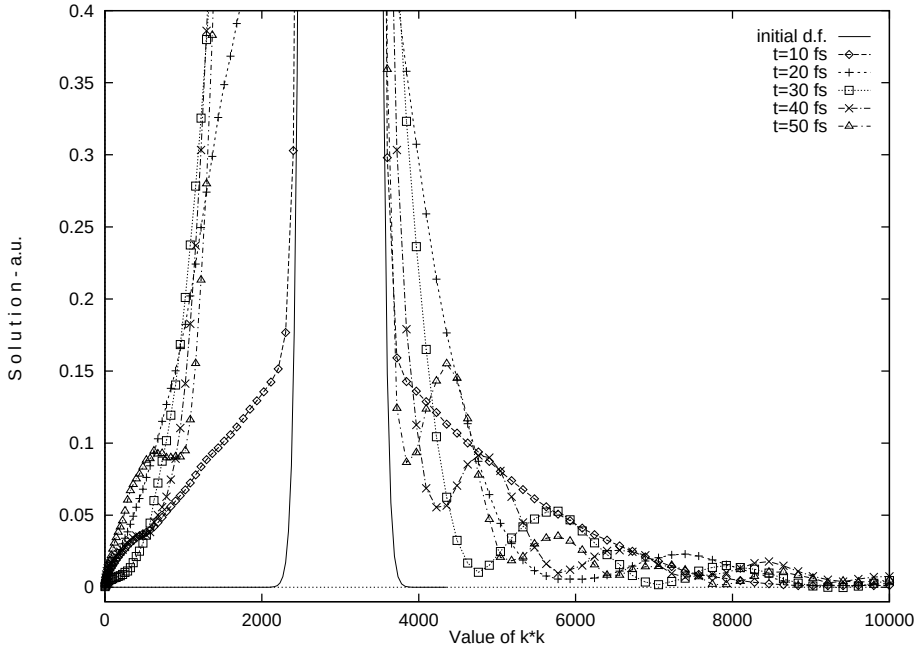
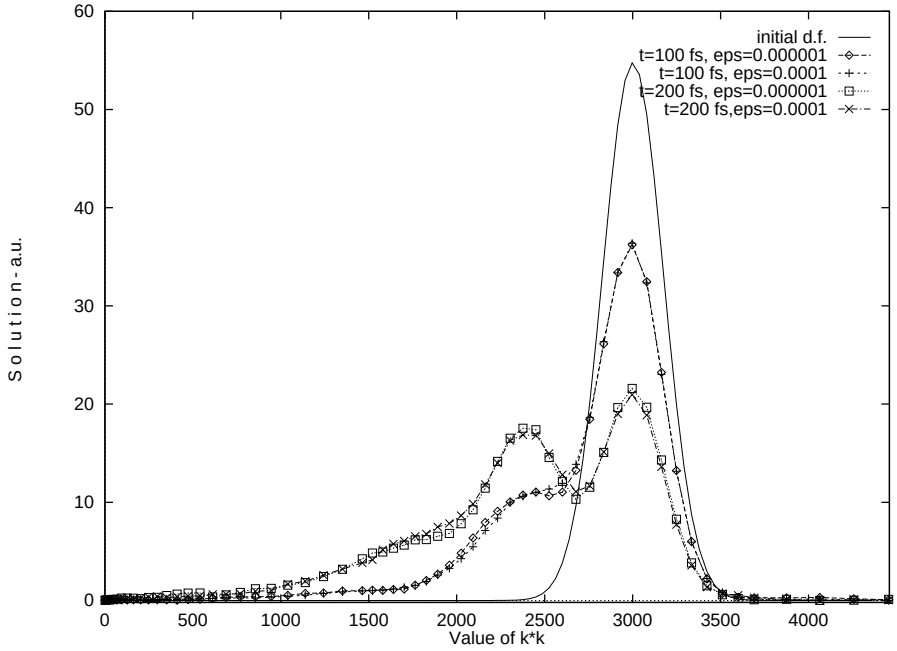
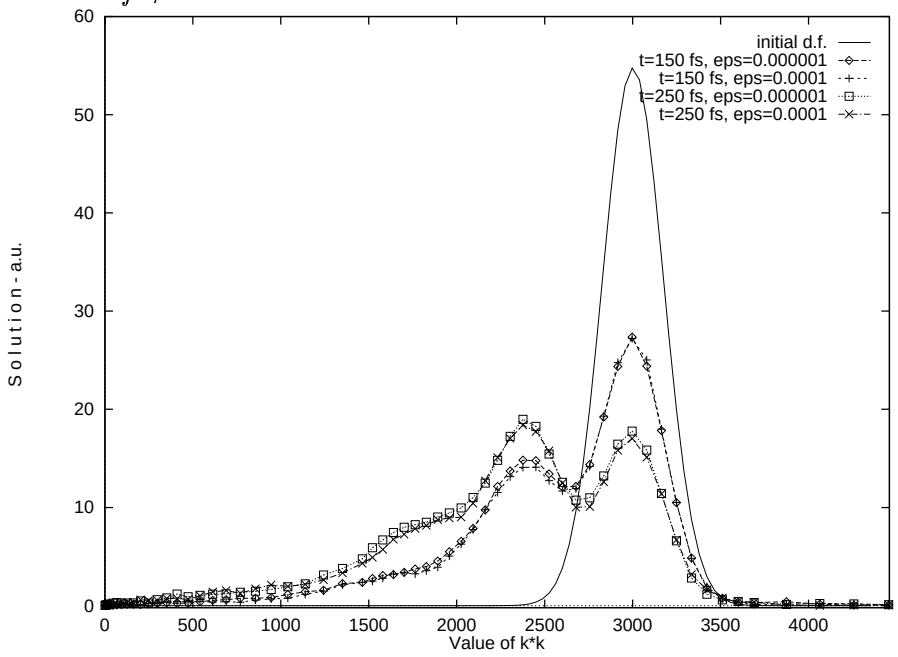


Fig. 3. Comparison of the electron energy distribution $k*f(k,t)$ versus $k*k$ obtained by two different ε-criteria for termination the Markov chain. For $t = 100fs,\ N = 10000$ and for $t = 200fs,\ N = 250000$.



$N = 50000$. The mean computational cost for our algorithm is better than the computational cost of the MC algorithm presented in [17]. Let us note that the number of the realizations for the MC estimator in [17] is $N = 1000000$. The obtained results show that electron appear in the semiclassically forbidden

Fig. 4. Comparison of the electron energy distribution $k * f(k,t)$ versus $k * k$ obtained by two different ε-criteria for termination the Markov chain. For $t = 150fs$, $N = 50000$ and for $t = 250fs$, $N = 1250000$.



region above the initial condition.

Figs. 3-4 shows dependence of the solution for the electron distribution when $\varepsilon = 0.0001$ and $\varepsilon = 0.000001$. The evolution times for the solutions on Fig.3 are $t = 100fs, t = 200fs$ and the realizations of the MC estimator are $N = 10000, N = 250000$, respectively. Results for $t = 150fs, t = 250fs$ and $N = 50000, N = 1250000$, respectively are plotted on Fig 4. Comparing the MC solutions for the electron distribution using the above ε-criteria we see that they approximately coincide. In fact, these comparisons show that we have good balance between the stochastic and systematic errors and we don't need to decrease ε.

Let us consider the results for the computational cost ($CPUtime$ per point) of the backward MC algorithm in Table 1. Here,

$$\sigma_N = \frac{1}{60}\sqrt{\frac{1}{N}\left(\sum_{i=1}^{N}\Theta_l[k,t]\right) - \overline{\Theta}_l[k,t]}$$

is the estimate for the standard deviation $\sigma = \sqrt{Var(\Theta_l[k,t])}$ which is calculated over all 60 points. The results show that the average number of transitions in the Markov chain increases very slowly when ε decreases. Also, the standard deviation (or the variance) increases exponentially when the evolution time increases, while the rate of convergence of the iteration process (or El) is changed very slowly. This results are in accordance with the theo-

retical result in Lemma 1. Therefore, the computational effort increases for long evolution time, because we need more realizations of the MC estimator in order to improve the statistical error. The dependence of the MC solution

Fig. 5. Comparison of the electron energy distribution $k * f(k,t)$ versus $k * k$ obtained by using of SPRNG and CLCG random number generators when the number of the random paths in the Markov chain is fixed. $N = 250000, t = 200fs, \varepsilon = 0.0001$.

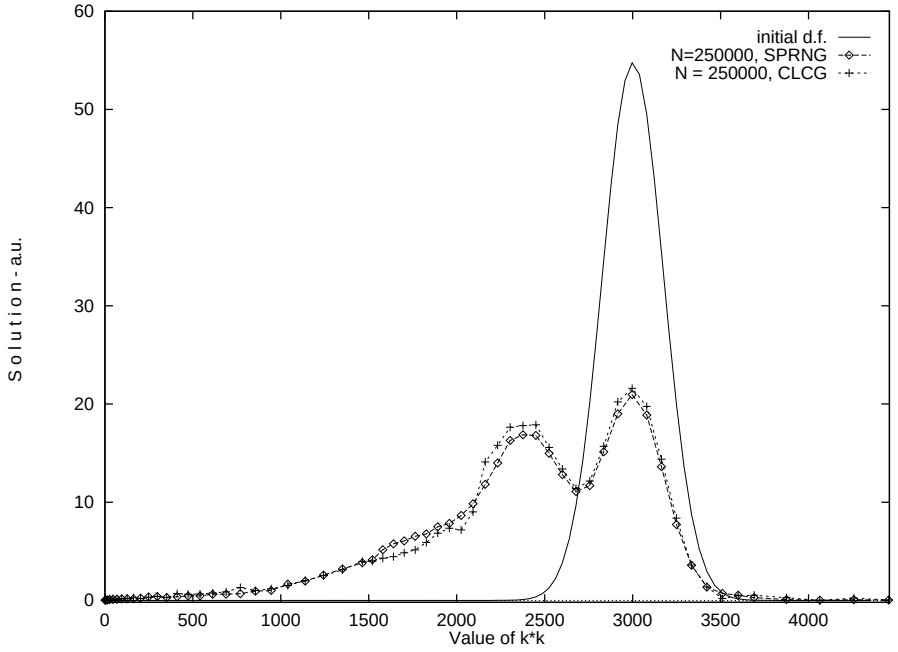
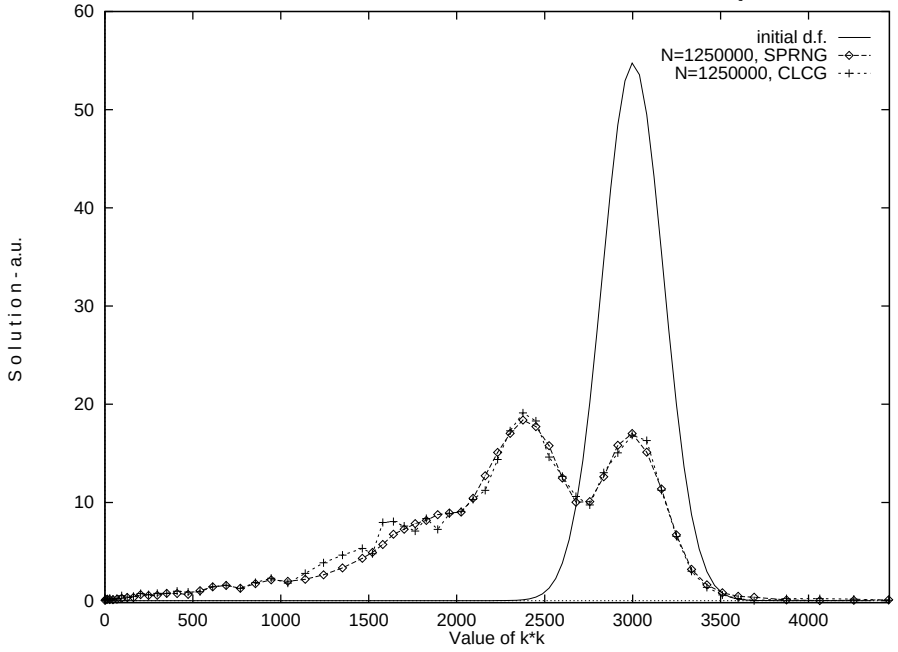


Fig. 6. Comparison of the electron energy distribution $k * f(k,t)$ versus $k * k$ obtained by using of SPRNG and CLCG random number generators when the number of the random paths in the Markov chain is fixed. $N = 1250000, t = 250fs, \varepsilon = 0.0001$.



on the SPRNG and CLCG random number generators is shown on Figs. 5–8 when $\varepsilon = 0.0001$. While the computational cost ($CPU\,time$ for all 60 points)

Fig. 7. Comparison of the distribution $k * f(k,t)$ versus $k * k$ obtained by using of SPRNG and CLCG generators for approximately one and the same computational cost ($CPUtime$). $N = 250000$ and $N = 300000$, respectively. $t = 200fs, \varepsilon = 0.0001$.

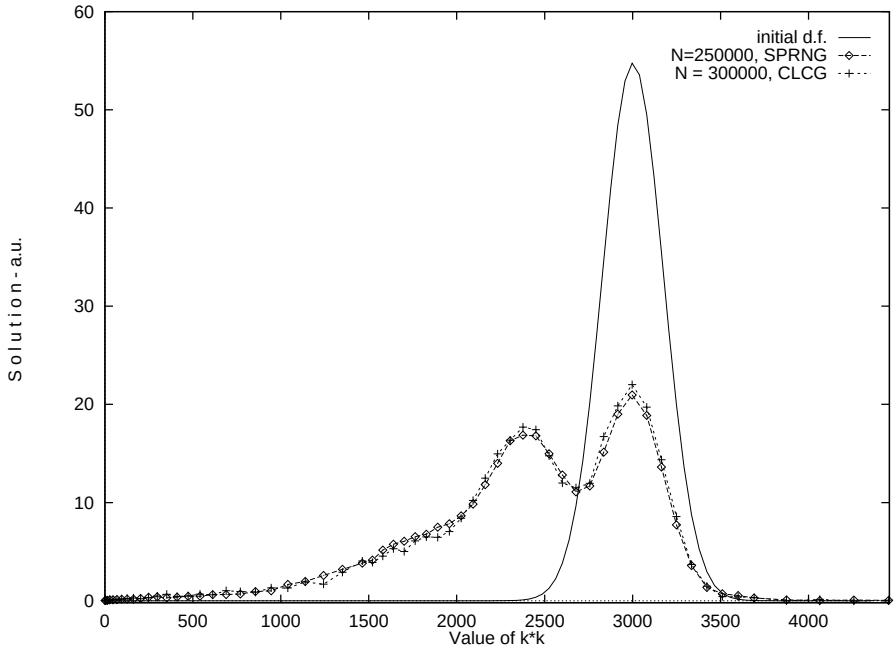
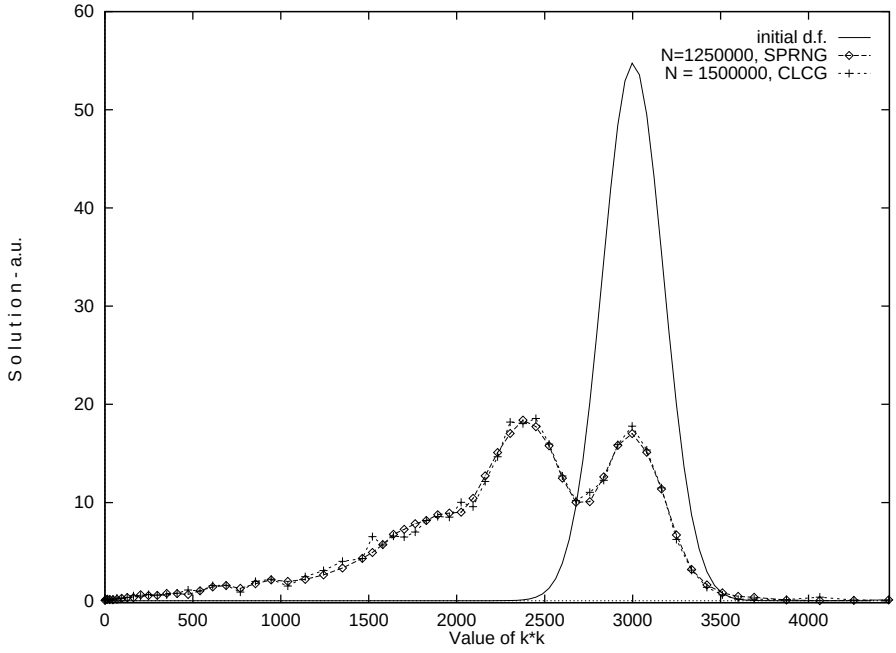


Fig. 8. Comparison of the distribution $k * f(k,t)$ versus $k * k$ obtained by using of SPRNG and CLCG generators for approximately one and the same computational cost ($CPUtime$). $N = 1250000$ and $N = 1500000$, respectively. $t = 250fs, \varepsilon = 0.0001$.



of the MC algorithm using the same generators is presented in Table 2. The

curves that are plotted on the Figs. 5 and 6 are cases when the number of the realizations N is fixed and $t = 200fs$ and $t = 250fs$, respectively.

Table 1
Computational complexity per one point at long evolution times.

		$\varepsilon = 0.0001$			$\varepsilon = 0.000001$		
t	N	El	σ_N	$CPUtime$	El	σ_N	$CPUtime$
$100fs$	10000	14.9876	0.48796	2.50s	19.5855	0.46879	3.43s
$150fs$	50000	15.5150	1.38206	13.04s	20.1182	1.40232	17.30s
$200fs$	250000	15.9040	3.87776	1m07.99s	20.5107	3.84575	1m24.59s
$250fs$	1250000	16.2287	10.7811	5m46.17s	20.8338	11.2736	7m10.20s
$300fs$	7500000	16.5263	31.3913	35m36.24s	21.1318	33.3502	38m59.63s
$350fs$	45 mln	16.8282	100.645	3h37m07.61s	21.3427	106.4081	4h32m05.74s
$400fs$	200 mln	17.1659	330.064	16h27m9.92s	-	-	-

The results show the "noise" in the MC solution is more when the CLCG generator is used, but the computational cost is less, (see Table 2).

Figs. 7 and 8 show the dependence of the solution on the SPRNG and CLCG generators for approximately the same computational complexity of the algorithm, (see Table 2).

Table 2
The computational complexity of the algorithm using SPRNG and CLCG generators.

	SPRNG		CLCG		CLCG	
t	N	$CPUtime$	N	$CPUtime$	N	$CPUtime$
$200fs$	250000	1h07m39.67s	250000	57m08.25s	300000	1h07m 41.58s
$250fs$	1250000	5h46m10.08s	1250000	4h50m55.81s	1500000	5h49m 37.81s

It is clear that the "noise" decreases when the CLCG generator is used with more replications, but it still exists. The solution is more smooth when the SPRNG is used. Therefore, the SPRNG generator is preferable to the one by L'Ecuyer for solving this problem.

6 Conclusion

An efficient backward Monte Carlo estimator and a corresponding algorithm for solving a Voltera-Fredholm integral equation describing a quantum-kinetic

model to the carrier dynamics in photoexcited semiconductors have been proposed and studied. The equation has been reduced from the two time-dimentions to one time-dimention integral form and convergence of the corresponding Neumann series has been proved. It is clear that rate of convergence is better than rate of convergence for the two time-dimensions integral form presented in [17].

The random estimator has been constructed by using backward time evolution of the numerical trajectories. It has been proved that the variance of this estimator has been bounded.

The transition density function in the Markov chain has been chosen to be proportional to the contribution from the integral kernel and the conditional MC aproach has been applied to it. It is well know that this choice reduces the variance of the estimator. A backward MC algorithm has been presented and decomposition and inverse-transformation techniques are used for calculating the sequence of points in the Markov chain. The algorithm has been tested for the GaAs material parameters using SPRNG and CLCG generators.

Numerical results for the electron energy distribution at long and short evolution times has been obtained. Computational complexity of the algorithm has been investigated, too. The results for computational cost and for the accuracy of the MC solution show that SPRNG generator is preferable than CLCG generator. The advantages of the studied algorithm lie in the direct valuation of the functional value in fixed phase space points without being necessary to solve the equation in the whole simulation region.

Finally we would like to mention that the future research of the quantum-kinetic problem under consideration could be developed in the following directions: 1. Consideration of the more realistic physics model with a non-zero electric field; 2. Investigation of a nonlinear electron quantum transport in one-band semiconductor for long evolution times and comparison with the obtained results in the linear case; 3. Creation of parallel Monte Carlo algorithms and investigation of the sensitiveness of the solution using various random number generators.

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