Statistical Algorithms for Simulation of Electron Quantum Kinetics in Semiconductors - Part II

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Abstract. The applied electrical field destroys the spherical symmetry of the field less Barker-Ferry equation. The dimensionality of the task increases and furthermore no general integration domain can be specified due to the correlation of the phase space and time coordinates. In this part of the work we propose and integral formulation which decouples these coordinates. The equation is solved by the randomized iterative Monte Carlo algorithm introduced in Part I. An analysis of the quantum effects demonstrated by the solutions is presented.

1 Integral Form of the Barker-Ferry Equation

The quantum-kinetic equation, explored in Part I, has been obtained in a framework of a physical model which describes the relaxation of semiconductor electrons initially excited by a laser pulse [1]. The equation appears as a simplified Barker-Ferry (B-F) equation [2] written for the case of zero electric field. The original formulation of the B-F equation accounts for the effect of the electric field on the process of collision - the intra collisional field effect. It is argued that this effect plays a negligible role in the stationary solution of the quantum-kinetic equation [3]. Here we investigate the transient problem, i.e. electron - phonon relaxation of initially excited electrons in the presence of an applied electric field **E**. The B-F equation has the following integro-differential form:

$$\frac{\partial f(\mathbf{k},t)}{\partial t} + \mathbf{F}\cdot\nabla_{\mathbf{k}} f(\mathbf{k},t) = \int_0^t dt' \int d\mathbf{k}' \left\{ S(\mathbf{k}',\mathbf{k},t,t') f(\mathbf{k}'(t'),t') - S(\mathbf{k},\mathbf{k}',t,t') f(\mathbf{k}(t'),t') \right\} \tag{1}$$

$$S(\mathbf{k}',\mathbf{k},t,t') = \frac{2V}{(2\pi)^3\hbar^2} |g_{\mathbf{q}}|^2 \exp(-\Gamma(t-t')) \times \left[(n_{\mathbf{q}}+1)\cos\left(\int_{t'}^t d\tau \Omega(\mathbf{k}(\tau),\mathbf{k}'(\tau)) \right) + n_{\mathbf{q}} \cos\left(\int_{t'}^t d\tau \Omega(\mathbf{k}'(\tau),\mathbf{k}(\tau)) \right) \right],$$

S. Margenov, J. Wasniewski, and P. Yalamov (Eds.): ICLSSC 2001, LNCS 2179, pp. 183–190, 2001.

where $\mathbf{F} = e\mathbf{E}/\hbar$, $n_{\mathbf{q}}$ is the Bose function, $\omega_{\mathbf{q}}$ generally depends on $\mathbf{q} = \mathbf{k}' - \mathbf{k}$,

$$\mathbf{k}(t') = \mathbf{k} - \mathbf{F}(t - t'); \qquad \Omega(\mathbf{k}(\tau), \mathbf{k}'(\tau)) = \frac{\epsilon(\mathbf{k}(\tau)) - \epsilon(\mathbf{k}'(\tau)) + \hbar\omega_{\mathbf{q}}}{\hbar}.$$

The damping factor Γ is considered independent of the electron states $\mathbf{k}$ and $\mathbf{k}'$. This is reasonable since Γ weakly depends on $\mathbf{k}$ and $\mathbf{k}'$ for states in the energy region above the phonon threshold, where the majority of the electrons reside due to the action of the electric field. An application of the method of characteristics leads to the following integral form of (1):

$$f(\mathbf{k}, t) = \phi(\mathbf{k}(0)) + \int_0^t dt' \int_0^{t'} dt'' \int d\mathbf{k}' \left\{ S(\mathbf{k}', \mathbf{k}, t', t'') f(\mathbf{k}'(t''), t'') - S(\mathbf{k}, \mathbf{k}', t', t'') f(\mathbf{k}(t''), t'') \right\}$$

The equation obtained is rather inconvenient for a numerical treatment since the solution for a phase space point $\mathbf{k}$ at instant t is related to the solutions at shifted points $\mathbf{k} - \mathbf{F}(t - t'')$. The shift depends on the electric field and the time interval $0 \leq t'' \leq t$ and hence no general integration domain can be specified in the phase space. This problem can be solved by the following transformation. A new variable k^t and function f^t are introduced such that:

$$\mathbf{k}_1^t = \mathbf{k}_1 - \mathbf{F}t; \qquad \mathbf{k}_1^t(\tau) = \mathbf{k}_1^t + \mathbf{F}\tau; \qquad f(\mathbf{k}, t) = f(\mathbf{k}^t + \mathbf{F}t, t) \stackrel{\text{def}}{=} f^t(\mathbf{k}^t, t),$$

where $\mathbf{k}_1$ stands for $\mathbf{k}$ and $\mathbf{k}'$ respectively. Then

$$f(\mathbf{k}_1(t''), t'') = f(\mathbf{k}_1^t + \mathbf{F}t'', t'') = f^t(\mathbf{k}_1^t, t'').$$

The transformation decouples the phase space and time arguments of the cosine functions in S according to:

$$\epsilon(\mathbf{k}'(\tau)) - \epsilon(\mathbf{k}(\tau)) = \epsilon(\mathbf{k}'^t) - \epsilon(\mathbf{k}^t) + 2\hbar\mathcal{F}(\mathbf{q})\tau; \qquad \mathcal{F}(\mathbf{q}) = \frac{\hbar}{2m}\mathbf{q} \cdot \mathbf{F}.$$

The integral equation becomes (the superscript t is omitted):

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

The symmetry around the direction of the electric field can be used to reduce the number of variables in the equation. In cylindrical coordinates (r, k, θ) with r chosen normal to the field direction, the relevant variables become $x = (r, k)$ where x is a two dimensional point. For zero lattice temperature ($n_{\mathbf{q}} = 0$) the equation obtained reads:

$$f(x, t) = \phi(x) + \int_0^t dt'' \int_G dx' \left[K(x, x') \times \left\{ \int_{t''}^t dt'\, S_1(x, x', t', t'') \right\} f(x', t'') + \left\{ \int_{t''}^t dt'\, S_2(x, x', t', t'') \right\} f(x, t'') \right] \tag{2}$$

where $x \in G = (0, Q) \times (-Q, Q)$, $\mathcal{G}$ is a constant,

$$K(x, x') = K(r, r', k, k') = \frac{\mathcal{G}r'}{\sqrt{((r - r')^2 + (k' - k)^2)((r + r')^2 + (k' - k)^2)}};$$

$$S_1(x, x', t', t'') = -S_2(x', x, t', t'') =$$
$$e^{-\Gamma(t'-t'')} \cos\left(\left(\Omega(x, x') - \frac{\hbar}{2m} F(k' - k)(t' + t'')\right)(t' - t'')\right). \qquad (3)$$

At this temperature the semiclassical solution has a simple behavior, which will be the reference background for exploring the effects imposed by the quantum-kinetic equation. The analysis of the quantum effects is presented in the last section.

Equation (2) is solved by a randomized iterative Monte Carlo algorithm (RIMC) described in the next section. We note that the algorithm can be generalized for finite temperatures in a straightforward way.

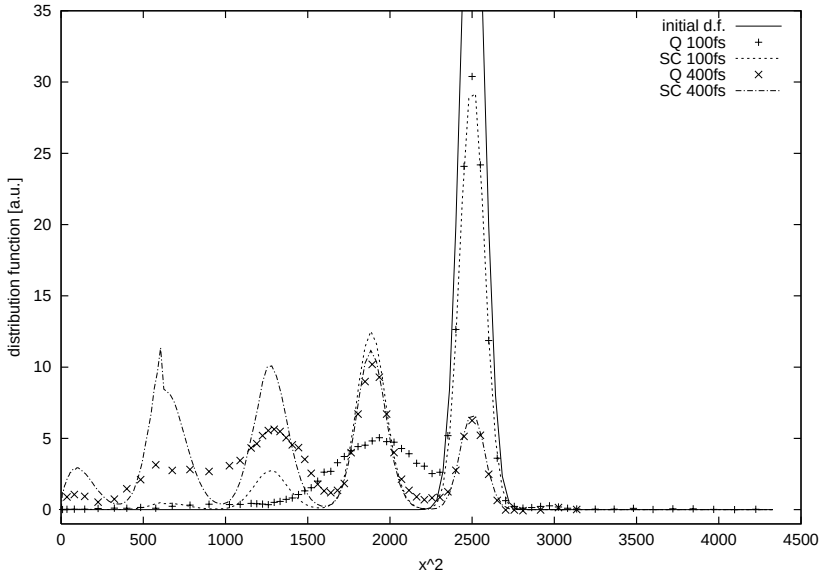

Fig. 1. Semiclassical (SC) and quantum solutions (Q) for zero electric field

2 The RIMC Algorithm

The biased Monte Carlo estimator for the solution of equation (2) at the fixed point $(x_0, t_0) = (r_0, k_0, t_0)$ is defined as follows:

$$\xi_{l_\varepsilon}[x_0, t_0] = \phi(x_0) + \sum_{j=1}^{l_\varepsilon} W_j^\alpha \phi_\alpha(x_j), \tag{4}$$

$$W_j^\alpha = W_{j-1}^\alpha \frac{K(x_{j-1}, x_j)\nu_\alpha(x_{j-1}, x_j, t_{j-1}, t_j)}{p_\alpha p(x_{j-1}, x_j) q(t_j)},\ W_1^\alpha = 1,\ \ j = 0, 1, \ldots, l_\varepsilon$$

Here $\nu_\alpha(x, x', t, t'')$ is the estimator of the integrals $\left\{\int_{t''}^{t} dt' S_\alpha(x, x', t', t'')\right\}$. $q(t'')$ and $p(x, x')$ are transition density functions in the Markov chain and p_α, $(\alpha = 1, 2)$ are probabilities for choosing one of the above integrals. Using N independent samples of the estimator (4) we obtain [4]:

$$\overline{\xi}_{l_\varepsilon}[x_0, t_0] = \frac{1}{N} \sum_{i=1}^{N} (\xi_{l_\varepsilon}[x_0, t_0])_i \approx f(x_0, t_0). \tag{5}$$

The RIMC algorithm for one random walk is given by the following steps:

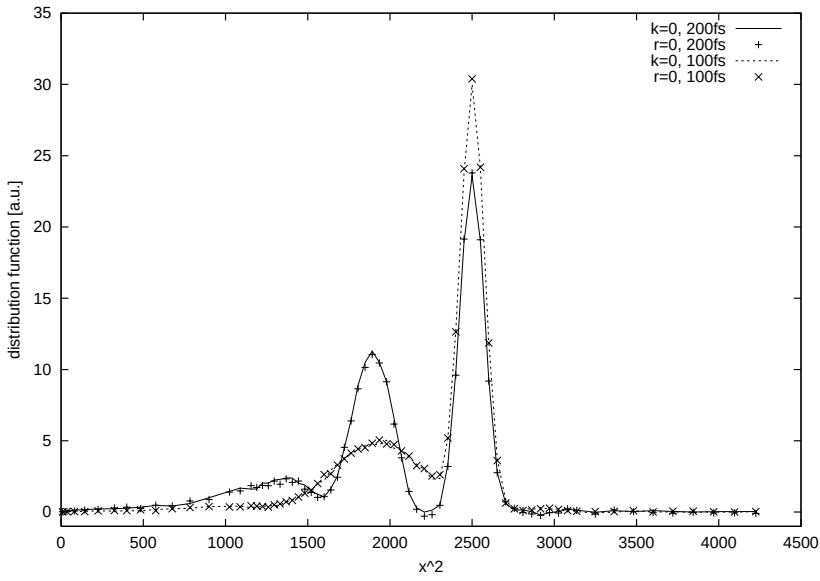

Fig. 2. Comparison of the solutions for the two orthogonal directions at zero electric field for evolution times 100fs and 200fs.

1. **Choose** a positive small number ε and **set** initial values $\xi := \phi(x)$,$W := 1$.
2. **Sample** a value t'' with a density function $q(t'') = 1/t$.
3. **Sample** a value $x' = (r', k')$ with a density function $p(x, x') = C/((r - r')^2 + (k - k')^2)^{\frac{1}{2}}$ using an acceptance-rejection method (C is a constant for normalization).
4. **Sample** N_1 independent random values of t' with a uniform density function $q_1(t') = 1/(t - t'')$.
5. **Calculate** $\overline{\nu}_\alpha = \frac{t-t''}{N_1} \sum_{i=1}^{N_1} S_\alpha(x, x', t'_i, t'')$, $p_\alpha = \frac{|\overline{\nu}_\alpha|}{|\overline{\nu}_1|+|\overline{\nu}_2|}$, $\alpha = 1, 2$.
6. **Choose** a value β, uniformly distributed random variable in $(0, 1)$. **If** $(p_1 \le \beta)$ **then** $W := W \frac{K(x,x')\overline{\nu}_1}{p_1 p(x,x') q(t'')}$, $\xi := \xi + W\phi(x')$, $x := x'$; **else** $W := W \frac{K(x,x')\overline{\nu}_2}{p_2 p(x,x') q(t'')}$, $\xi := \xi + W\phi(x)$.
7. **Set** $t := t''$ and **repeat** from step 2 until $t \le \varepsilon$.

The acceptance-rejection method used in the third step is given below. Using the substitution $u = r - r'$, $v = k - k'$ the domain G is divided into four sub domains $(G_i = (0, a_i) \times (0, b_i))$, $(i = 1, \ldots, 4)$. We can sample in every sub domain G_i with probability C_i/C using density function $p_i(u, v) = C_i/(u^2 + v^2)^{\frac{1}{2}}$. Then:

1. **Choose** values β_1 and β_2, uniformly distributed in the interval $(0, 1)$.
2. **Sample** $u = R_i\beta_1 \cos(\beta_2\pi/2)$ and $v = R_i\beta_1 \sin(\beta_2\pi/2)$, where $R_i^2 = a_i^2 + b_i^2$.
3. **If** $((u \le a_i)\&(v \le b_i))$ accept u and v, **else** repeat from 1.

The empirical results show that the efficiency of the acceptance-rejection algorithm is approximately 56%. The RIMC algorithm can be modified by a choice of alternative transition density function. For example, $\tilde{p}(r, k, r', k') = \tilde{C}r'p(r, k, r', k')$. Such a choice guarantees that the variance of the MC estimator is bounded [5], because the singularity of the kernel of (2) is canceled by the transition density function.

3 Results and Discussions

The simulation results are obtained for $GaAs$ with material parameters taken from [1]. A value $Q = 66 \cdot 10^7 m^{-1}$ has been chosen for the integration domain G. The phonon frequency is a constant, ω. For zero field the symmetry of the task allows the use of spherical coordinates with wave vector amplitude $|k|$. Figure 1 compares semiclassical (inverse hyperbolic cosine [6]) and quantum solutions $|k|f(|k|, t)$ for times $100fs$ 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.

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. This quantum effects

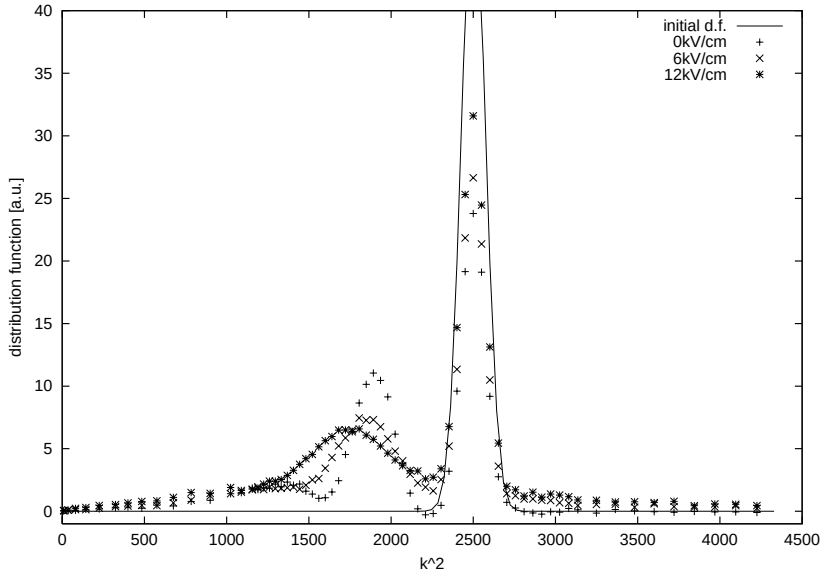

Fig. 3. Solutions $|k|f(r,k,t)$ for $r=0$, $k \in (0,-Q)$ and evolution time $200fs$. The electric field is 0, $6kV/cm$ and $12kV/cm$.

are associated with the memory character of the equation and the fact that the long time limit of the kernel does not recover the semiclassical delta function [6]. At the phonon threshold, $|k|^2 \simeq 600$ the solutions show a theoretically expected discontinuity [6].

The solution of (2) has been investigated for $r=0$, along k, the direction of the applied field, and for $k=0$ along r, the direction normal to the electric field. For zero field the solutions $kf(r=0,k,t)$ versus k^2 and $rf(r,k=0,t)$ versus r^2 must coincide due to the symmetry of the task. This condition has been used to test the numerical approach. Figure 2 compares the corresponding solutions for 100 and 200 femtoseconds evolution time. The electric field introduces important effects in the quantum kinetics. Figure 3 compares the $200fs$ solutions as a function of $k \in (0,-Q)$ for different positive values of the electric force F. The first replica peaks are shifted to the left by the increasing electric field. The solution in the semiclassically forbidden region, above the initial condition, demonstrates enhancement of the electron population with the growth of the field. This effects can be associated with the structure of the S_1 term in the kernel. The cosine has a significant contribution to the solution if the pre factor of $(t'-t'')$ in (3) is around zero. 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 initial condition the energy of the field reduces the phonon energy and thus the electron population in the vicinity of the initial condition increases.

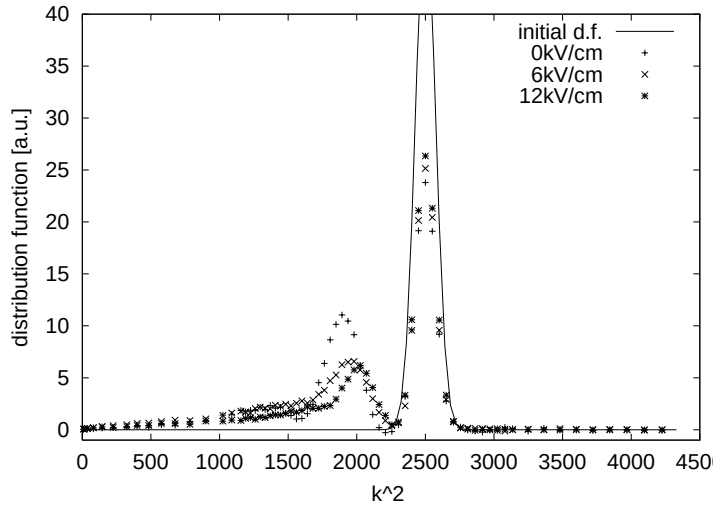

Fig. 4. Solutions $kf(r,k,t)$ for $r=0$, $k \in (0,Q)$ and evolution time $200fs$. The electric field is 0, $6kV/cm$ and $12kV/cm$.

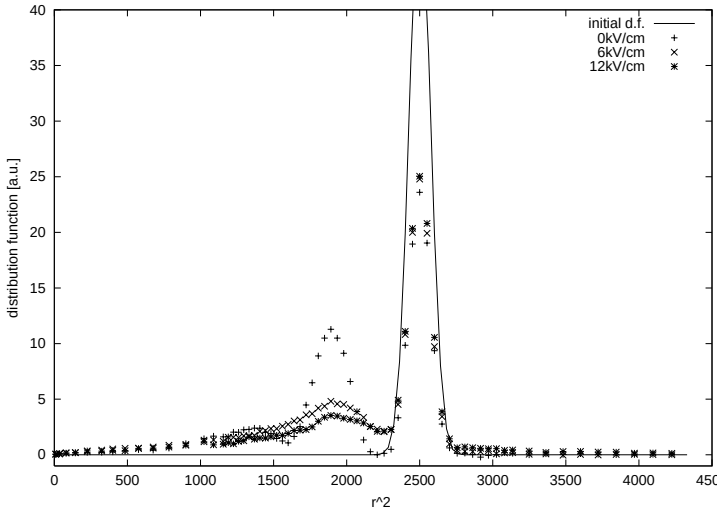

Fig. 5. Solutions $rf(r,k,t)$ for $k=0$, $r \in (0,Q)$ and evolution time $200fs$. The electric field is 0, $6kV/cm$ and $12kV/cm$.

Just the opposite effects must appear in the region of positive k values. This is demonstrated on Figure 4. The first replicas peaks are shifted to the right and there is no enhancement of the electron population above the initial condition.

As should be expected, in the direction normal to the field there is no shift in the replicas as seen from Figure 5.

A comparison of the first replicas and the main peaks under the initial condition on figures 3, 4 and 5 shows that the field has a pronounced influence on the effects of the collisional broadening and the retardation.

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 shift in the replicas, population of the semiclassically forbidden regions and influences the broadening and retardation of the solution.

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