



# Femtosecond relaxation of hot electrons by phonon emission in presence of electric field

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## Abstract

The femtosecond relaxation of an initial distribution of electrons which interact with phonons in presence of applied electric field is studied numerically. The evolution at such a time scale cannot be described in terms of Boltzmann transport. Here, the Barker–Ferry equation is utilized as a quantum-kinetic model of the process. The numerical treatment of the original formulation of the Barker–Ferry equation becomes difficult since coordinates and time variables are coupled by the field. A transformation which decouples coordinates and time variables in the equation is proposed. A randomized iterative Monte Carlo algorithm is developed to solve the transformed equation. The quantum character of the equation is investigated. An instantaneously created initial condition is favored above the physically more adequate generation term in order to point out the quantum effects. Simulation results are obtained for GaAs material at different evolution times. Effects of collisional broadening and retardation are observed already in the fieldless case. The intracollisional field effect is clearly demonstrated as an effective change of the phonon energy, which depends on the field direction and the evolution time. Moreover, the collisional broadening and retardation are affected by the applied field. The observed phenomena are understood from the structure and the properties of the model equation. © 2002 Elsevier Science B.V. All rights reserved.

*Keywords:* Barker–Ferry equation; Intracollisional field effect; Collisional broadening

## 1. The integral equation

The Barker–Ferry (B–F) equation [1] accounts for the action of the electric field  $\mathbf{E}$  during the process of electron–phonon interaction — the intracollisional field effect. It has been shown that the effect plays a negligible role in the regime of stationary transport [2]. Here, we explore the transient transport regime — the early time evolution of an initially excited electron distribution  $\phi$ . Experimentally, such a process can be

investigated by ultrafast spectroscopy, where the relaxation of electrons is explored during the first hundreds femtoseconds after an optical excitation [3,4]. The low-density regime is considered, where the interaction with phonons dominates the carrier–carrier interaction [4].

The B–F equation has the following integro-differential form:

$$\begin{aligned} \frac{\partial f(\mathbf{k}, t)}{\partial t} + \mathbf{F} \cdot \nabla_{\mathbf{k}} f(\mathbf{k}, t) \\ = \int_0^t dt' \int d\mathbf{k}' \{ S(\mathbf{k}', \mathbf{k}, t, t') f(\mathbf{k}'(t'), t') \\ - S(\mathbf{k}, \mathbf{k}', t, t') f(\mathbf{k}(t'), t') \}, \end{aligned} \quad (1)$$

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

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

$$\mathbf{k}(t') = \mathbf{k} - \mathbf{F}(t - t'),$$

$$\Omega(\mathbf{k}(\tau), \mathbf{k}'(\tau)) = \frac{\varepsilon(\mathbf{k}(\tau)) - \varepsilon(\mathbf{k}'(\tau)) + \hbar\omega_{\mathbf{q}}}{\hbar}.$$

The damping factor  $\Gamma$  is considered independent of the electron states  $\mathbf{k}$  and  $\mathbf{k}'$ . This is reasonable since  $\Gamma$  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 Eq. (1):

$$\begin{aligned}
f(\mathbf{k}, t) &= \phi(\mathbf{k}(0)) + \int_0^t dt' \int_0^{t'} dt'' \\
&\times \int d\mathbf{k}' \{ S(\mathbf{k}', \mathbf{k}, t', t'') f(\mathbf{k}'(t''), t'') \\
&- S(\mathbf{k}, \mathbf{k}', t', t'') f(\mathbf{k}(t''), t'') \}.
\end{aligned}$$

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

$$\mathbf{k}_1^t = \mathbf{k}_1 - \mathbf{F}t, \quad \mathbf{k}_1^t(\tau) = \mathbf{k}_1^t + \mathbf{F}\tau,$$

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

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

$$\varepsilon(\mathbf{k}'(\tau)) - \varepsilon(\mathbf{k}(\tau)) = \varepsilon(\mathbf{k}'') - \varepsilon(\mathbf{k}') + 2\hbar\mathcal{F}(\mathbf{q})\tau,$$

$$\mathcal{F}(\mathbf{q}) = \frac{\hbar}{2m} \mathbf{q} \cdot \mathbf{F}.$$

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

$$\begin{aligned}
f(\mathbf{k}, t) &= \phi(\mathbf{k}) + \int_0^t dt' \int_0^{t'} dt'' \\
&\times \int d\mathbf{k}' \{ S(\mathbf{k}', \mathbf{k}, t', t'') f(\mathbf{k}', t'') \\
&- S(\mathbf{k}, \mathbf{k}', t', t'') f(\mathbf{k}, t'') \}.
\end{aligned} \tag{2}$$

The symmetry around the direction of the electric field can be used to reduce the number of variables in the equation. In cylindrical coordinates  $(r, k, \theta)$  with  $r$  chosen normal to the field direction, the relevant variables are  $x = (r, k)$ . For zero lattice temperature,  $S$  becomes a product of two terms:  $S(x', x, t', t'') = K(x, x') S_1(x, x', t', t'')$  where  $K$  contains a polar part proportional to  $((r - r')^2 + (k' - k)^2)^{-1/2}$  and

$$\begin{aligned}
S_1 &= \exp(-\Gamma(t' - t'')) \cos \left( \left( \Omega(x, x') \right. \right. \\
&\left. \left. - \frac{\hbar F}{2m} (k' - k)(t' + t'') \right) (t' - t'') \right).
\end{aligned} \tag{3}$$

At this temperature the classical solution has a simple behavior, which will be the reference background for exploring the effects imposed by the quantum-kinetic equation.

## 2. The stochastic algorithm

The equation is solved by a randomized iterative Monte Carlo algorithm. A preliminary step uses the equality  $\int_0^t dt' \int_0^{t'} dt'' = \int_0^t dt'' \int_{t''}^t dt'$  in order to assign the  $t'$  integral to the kernels. This analytically formal operation increases significantly the efficiency of the algorithm. The solution at the fixed point  $(x_0, t_0)$  is evaluated by  $N$

realizations of the random variable  $\xi_{l_c}$ :

$$f(x_0, t_0) \simeq \frac{1}{N} \sum_{i=1}^N (\xi_{l_c}[x_0, t_0])_i,$$

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

$$W_j^\alpha = W_{j-1}^\alpha \frac{K(x_{j-1}, x_j) v_\alpha(x_{j-1}, x_j, t_{j-1}, t_j)}{p_\alpha p(x_{j-1}, x_j) q(t_j)},$$

$$W_1^\alpha = 1.$$

Here  $v_\alpha(x, x', t, t')$  is the estimator of the integrals  $\{\int_{t'}^t dt' S_\alpha(x, x', t', t'')\}$ .  $q(t'')$  and  $p(x, x')$  are transition density functions in the Markov chain and  $p_\alpha$  ( $\alpha = 1, 2$ ) are probabilities related to the choice of one of the kernels.  $l_c$  determines the precision for truncation of the Neumann series of the solution. The estimators  $v_\alpha$  are evaluated by  $N_1$  random values of  $t'$  sampled with a uniform density in  $(t'', t)$ . An important point is the choice of the transition density  $p$  to be proportional to the polar part of the kernels:  $p(x, x') = C((r - r')^2 + (k - k')^2)^{-1/2}$ . In this way, the variance of the Monte Carlo estimator remains bounded which allows to control the precision of the results. The algorithm can be generalized for finite temperatures in a straightforward way.

### 3. Results and discussions

The simulation results are obtained for GaAs with standard material parameters [5,6] and effective mass 0.063. The PO phonon energy is a constant,  $\hbar\omega = 36$  meV. The finite duration of the initial optical excitation can be taken into account by a generation term. Instead, in order to demonstrate the quantum effects, as an instantaneous initial condition a sharp (corresponding to 200 femtoseconds laser pulse) Gaussian function of the energy is assumed.

Classical electrons can only emit phonons and loose energy equal to a multiple of  $\hbar\omega$ . 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.

Fig. 1 compares classical and quantum solutions on the cutline along the field, ( $r = 0$ ), for 200 femtoseconds evolution time. The quantity  $|k|^2$  is proportional to the electron energy in units  $10^{14} \text{ m}^{-2}$ , where the negative values denote the direction opposite to the field. Collisional broadening and retardation are observed already at zero field. 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. These quantum effects are associated with the memory character of the equation and the fact that the long time limit of the kernel does not recover the classical delta function [6]. The electric field introduces important effects in the quantum kinetics. The first replica peak of the 12 kV/cm solution is shifted in the field direction. For negative states the distance to the initial peak increases. Moreover, the solution in the classically forbidden region, to the left of the initial condition, demonstrates enhancement of the electron population. This effect can be associated with the structure of the first kernel of Eq. (2) which controls the electron transfer between the states. Responsible for the build up of the peak is the first iteration term, obtained from the first integral in Eq. (2) by replacing  $f$  with the initial condition  $\phi$ . The cosine in Eq. (3) has a permanent contribution to the solution if the prefactor of  $(t' - t'')$  is around

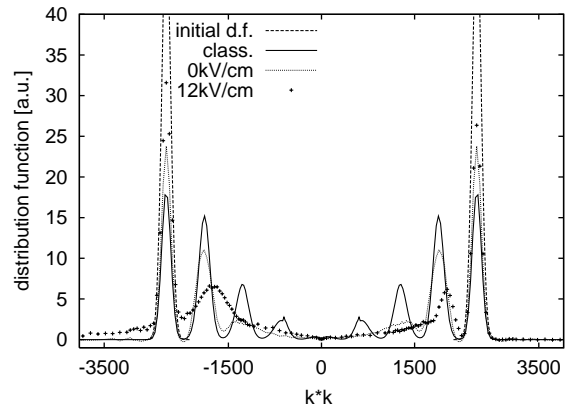


Fig. 1. Classical and quantum solutions at 200 femtoseconds evolution time. The electric field is 0 and 12 kV/cm.

zero. States with  $k'$  to the left of the  $k$  region of the first peak become important. For such states  $k' - k < 0$  and since  $F$  is positive the energy of the field is added to the phonon energy. Accordingly, the solution behaves as if in the presence of a phonon with energy higher than  $\hbar\omega$ ; the distance between the first replica and the initial condition increases. In the classically forbidden region,  $k' - k > 0$ , so that the energy of the field is subtracted from the phonon energy. The prefactor is small for states  $k$  close to the  $k'$  region of the initial condition. Accordingly, the electron population in the vicinity to the left of the initial condition increases. Just the opposite effects must appear in the region of positive  $k$  values. Indeed, the first peaks are shifted to the right since now  $k' - k > 0$  and the energy of the field is subtracted from the phonon energy. In the semiclassically forbidden region, to the right of the initial condition, the prefactor is large and there is no enhancement of the electron population.

A comparison of the first replicas and the main peaks under the initial condition shows that the field has a pronounced influence on the collisional broadening and retardation. As demonstrated by additional numerical experiments, this effect depends on the field strength and direction.

The field term in Eq. (3) depends also on the factor  $(t' + t'')$ . Since the two times are integration variables bounded by  $t$ , the shift of the replicas must depend also on the evolution time  $t$ . Fig. 2 compares quantum solutions for different evolution times. The electric field is 6 kV/cm. This dependence is well demonstrated on the left part of the figure by an increase of the distance to the main peak with the evolution time. On the right part of the figure, for positive  $k$  values, the dependence is suppressed by the retardation effect.

We conclude that the intracollisional field effect is well demonstrated in the early time evolution of

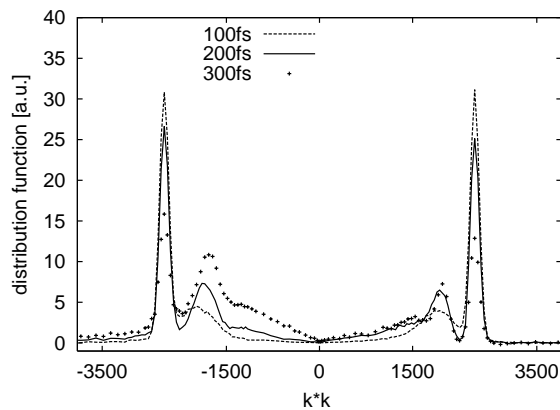


Fig. 2. Quantum solutions at 100, 200 and 300 femtoseconds evolution times. The electric field is 6 kV/cm.

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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