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

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Abstract

The femtosecond relaxation of initially excited electrons which interact with phonons in presence of an applied electric field is studied numerically. The evolution at such 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 solution of the equation is investigated for quantum effects introduced by the electric field. The numerical treatment of the original formulation of the Barker-Ferry equation becomes difficult since coordinates and time variables are coupled by the field. Thus no general time independent integration domain in the phase space can be specified. 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.

Simulation results are obtained for $GaAs$ material at different evolution times. Effects of collisional broadening and retardation are observed already in the field-less 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 the structure and the properties of the model equation.

Keywords:
Barker-Ferry equation, intracollisional field effect, collisional broadening.

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1 The integral equation

The Barker-Ferry (B-F) equation Ref. [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 Ref. [2]. Here we explore the transient transport regime - the early time evolution of an initially excited electron distribution ϕ. Experimentally, such a process can be investigated by ultrafast spectroscopy, where the relaxation of electrons is explored during the first femtoseconds after an optical excitation.

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

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

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

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 Eq. (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):

$$f(\mathbf{k},t) = \phi(\mathbf{k}) + \int_0^t dt' \int_0^{t'} dt'' \int d\mathbf{k}' \left\{S(\mathbf{k}',\mathbf{k},t',t'')f(\mathbf{k}',t'') - S(\mathbf{k},\mathbf{k}',t',t'')f(\mathbf{k},t'')\right\} \tag{2}$$

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,θ) 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 $((r-r')^2 + (k'-k)^2)^{-\frac{1}{2}}$ and

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

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 ξ_{l_ε}:

$$f(x_0,t_0) \simeq \frac{1}{N}\sum_{i=1}^{N}(\xi_{l_\varepsilon}[x_0,t_0])_i; \quad \xi_{l_\varepsilon}[x_0,t_0] = \phi(x_0) + \sum_{j=1}^{l_\varepsilon} W_j^\alpha \phi_\alpha(x_j), \qquad (4)$$

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

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 related to the choice of one of the kernels. l_ε determines the precision for truncation of the Neumann series of the solution. The estimators ν_α 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: $p(x,x') = C((r-r')^2 + (k-k')^2)^{-\frac{1}{2}}$. 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 material parameters taken from Ref. [3]. The phonon frequency is a constant, ω, and the initial condition is a Gaussian function of the energy. 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 $10^{14}m^{-2}$, 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. This 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 Ref. [4]. The electric field introduces important effects in the quantum kinetics. The first replica peak of the $12kV/cm$ 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 effects 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 ϕ. The cosine in Eq. (3) has permanent contribution to the solution if the pre factor of $(t' - t'')$ is around zero. Important become states with k' to the left of the k region of the first peak. 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 in 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 pre factor 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 pre factor 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 the experiments, this effects 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 $6kV/cm$. 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 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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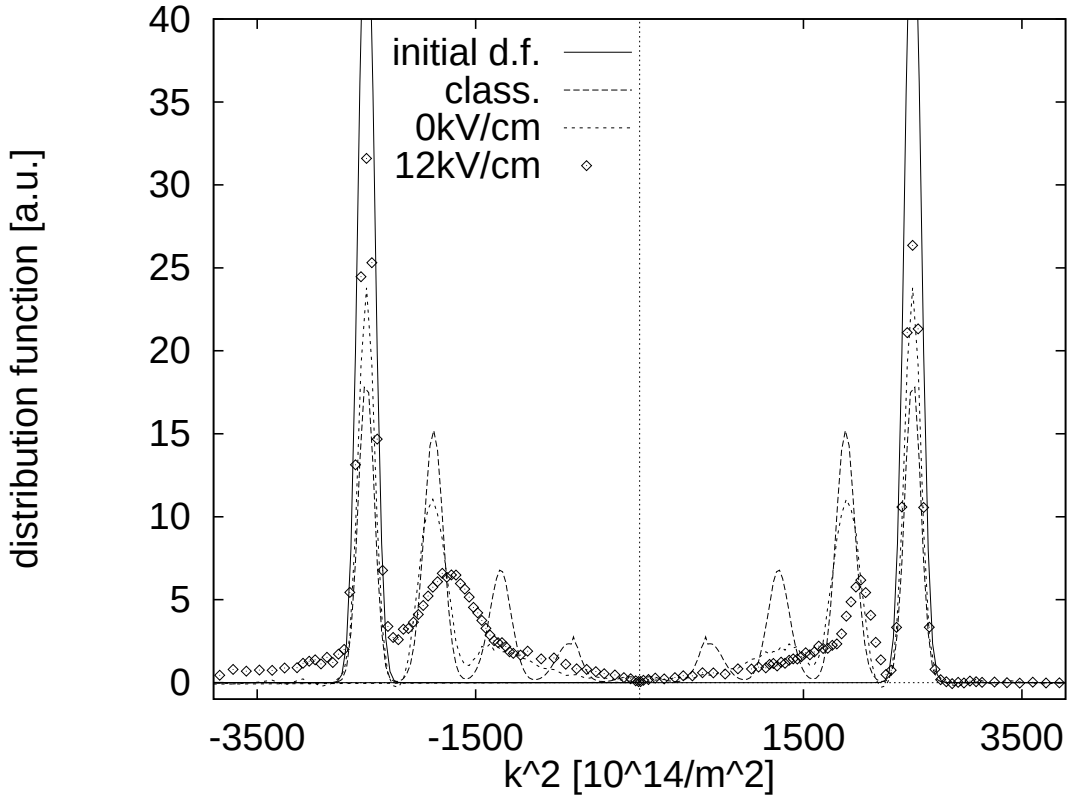
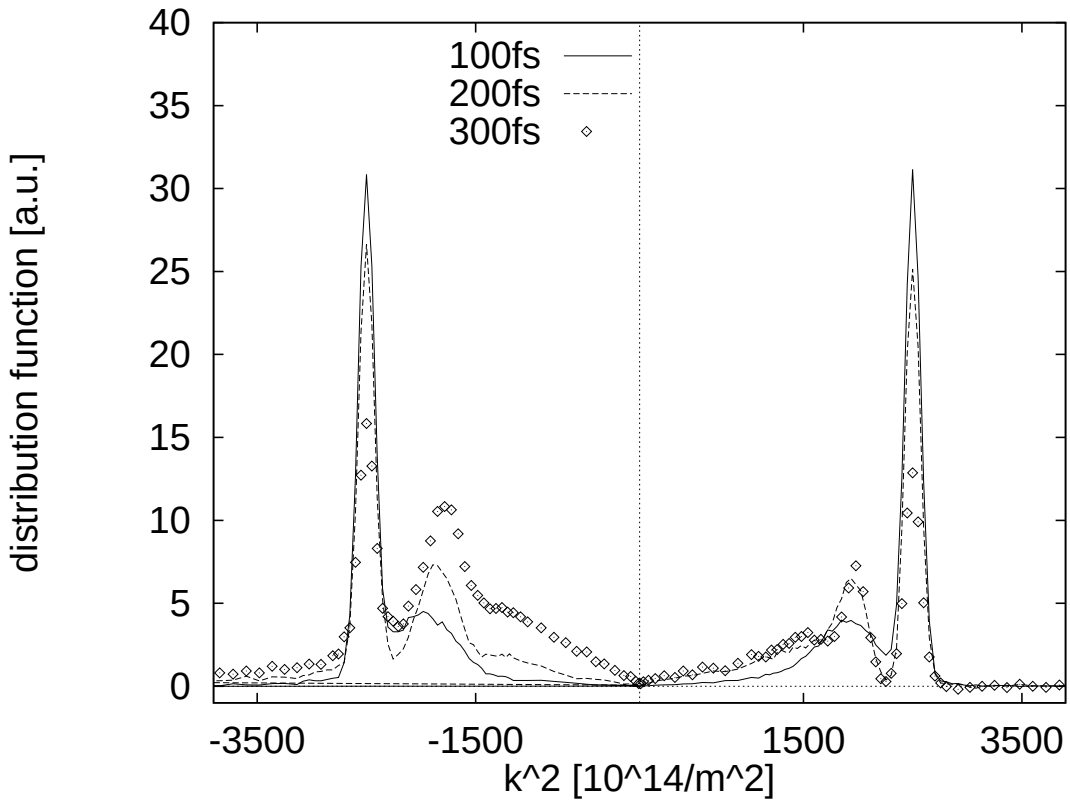


Fig. 1 Classical and quantum solutions at 200 femtoseconds evolution time. The electric field is $0kV/cm$ and $12kV/cm$.

Fig. 2 Quantum solutions at 100, 200 and 300 femtoseconds evolution times. The electric field is $6kV/cm$.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distribution function [a.u.]
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