A Backward Monte Carlo Method for Simulation of Electron Quantum Kinetics in Semiconductors

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A backward Monte Carlo approach for solving a quantum kinetic equation which accounts for the memory character of the electron-phonon interaction is proposed. The equation derived from the one-band model [1] for femtosecond relaxation of optically excited carriers, appears as a zero electric field differential form of the Barker-Ferry equation [2]

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

It differs from the Boltzmann Equation (BE) by the time integration of the scattering operator and the replacement of the energy conserving delta function $\delta(\hbar\Omega_{k,k'})$ by $\Delta(\mathbf{k}',\mathbf{k},t,t') = \exp(-\Gamma_{k',k}(t-t'))\cos(\Omega_{k',k}(t-t'))$, where $\Gamma_{k',k} = \Gamma_{k'} + \Gamma_k$ and Γ_k is the Boltzmann total scattering rate.

The numerical method is based on stochastic algorithms for solving integral equations, applied to different integral representations of (1). The solutions at desired points $\mathbf{k}$ at time t are independently achieved by a backward time evolution of the numerical trajectories. The convergence of the iteration series of the integral equation obviously affects the efficiency of the method. In the first integral form, obtained by direct time integration of (1), the method is efficient only up to 100 fs due to a dramatic increase of the variance with the evolution time [3]. A similar problem is encountered if the BE is treated by a direct time integration [4].

In the present work we explain the variance increase by the build up of the long time limit of the kernel. The limit appears explicitly in the second integral form, obtained from the first by analytical evaluation of one of the time integrals. The term $\Delta(\mathbf{k}',\mathbf{k},t,t')$ gives rise to a Lorenzian $L_{k',k} = \Gamma_{k',k}/(\Gamma_{k',k}^2 + \Omega_{k',k}^2)$ and an oscillating, exponentially damped function of time [5]. The remedy in the Boltzmann case is in the path integral form of the equation. Thus we explore a third integral form of (1) proposed by Barker and Ferry. We modify the original approach [2], by replacing the self-scattering constant Γ_0, with a positive function λ_k, which allows more flexibility in reducing the $L_{k,k'}$ component of the kernel. A condition can be formulated, such that λ_k cancels the term with the out-scattering Lorenzian $L_{k,k'}$.

Numerical experiments for the case of $\lambda_k = \Gamma_k$ under the same physical conditions as in [3] are presented. We observe a significant improvement of the efficiency of the method, which is explained with the improved convergence of the iteration series, due to the analytical evaluation of the λ fraction of $L_{k,k'}$ giving rise of the effective exponential damping. Now the 300 fs solution can be provided in a reasonable CPU time - one hour per point is required on a 400 MHz PC. Along with the quantum solutions we also present on the figures 1 and 2 the corresponding solutions of a Boltzmann-like equation with kernel equal to $L_{k',k}$ Lorenzian component. It is seen that in the regions of higher densities the Lorezian dominates the electron kinetics.

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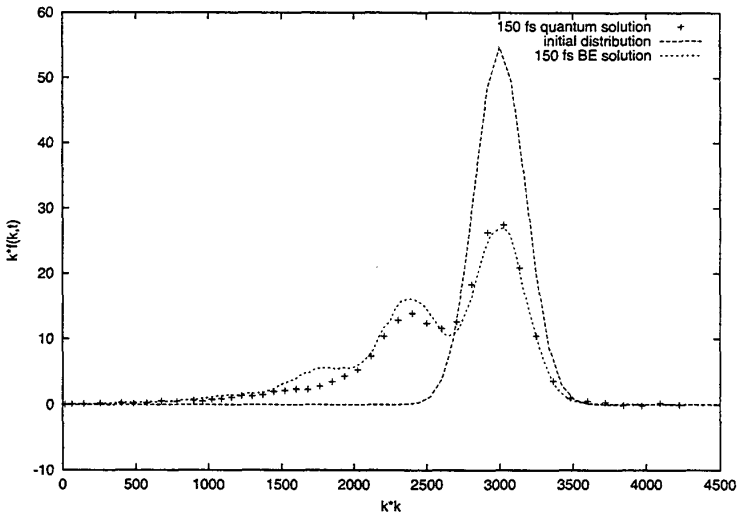

Figure 1: Quantum and Boltzmann equation solutions versus the squared wave vector after 150 femtoseconds evolution of the initial distribution for GaAs at zero lattice temperature

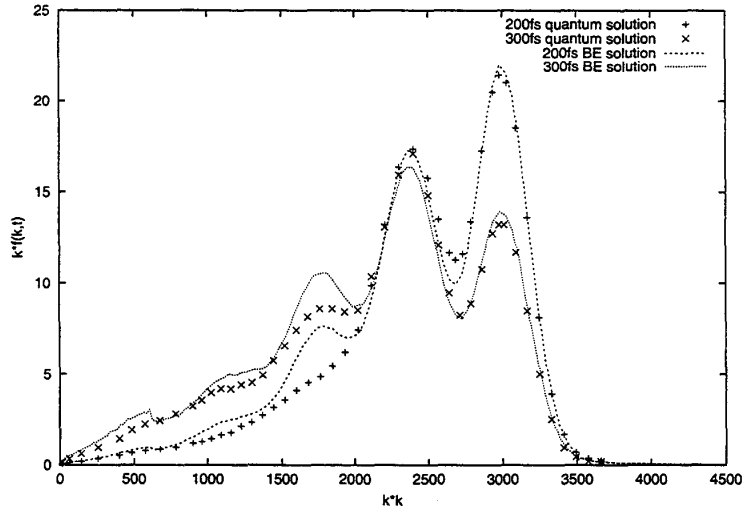

Figure 2: Quantum and Boltzmann equation solutions versus the squared wave vector after 200 and 300 femtoseconds evolution of the initial distribution for GaAs at zero lattice temperature