A Parallel Monte Carlo Method for Electron Quantum Kinetic Equation*

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Abstract. We study a parallel Monte Carlo (MC) method for investigation of a quantum kinetic equation which accounts for the action of the electric field during the process of electron-phonon interaction. Optimization of the presented parallel algorithm is done using variance reduction techniques and parallel random sequences from the Scalable Parallel Random Number Generator (SPRNG) library. The developed code written in C is parallelized with MPI and OpenMP codes.
Numerical results for the parallel efficiency of the algorithm are obtained. The dependence of the electron energy distribution on applied electric field is investigated for long evolution times. The distribution function is computed for GaAs material parameters.

1 Introduction

The development and application of the MC methods for quantum transport in semiconductors and semiconductor devices has been initiated during the last decade [1, 2]. The stochastic approach relies on the numerical MC theory as applied to the integral form of the generalized electron-phonon Wigner equation. An equation for reduced electron-phonon Wigner function which accounts for electron-phonon interaction has been recently derived [3].

For a bulk semiconductor with an applied electric field the equation resembles the Levinson equation [4], or equivalently the Barker-Ferry (B-F) equation [5] with infinite electron lifetime. A crude MC method has been proposed to find quantum solutions up to 200 femtoseconds (fs) evolution times of the B-F equation at zero temperature [6]. It is proved [7] that stochastic error has order $O(\exp(ct)/N^{\frac{1}{2}})$, where t is the evolution time, N is the number of samples of the MC estimator, and c is a constant depending on the kernel of the quantum kinetic equation. This estimate shows that when t is fixed and $N \to \infty$ the error decreases, but for N fixed and t large the factor for the error looks ominous. Therefore, the problem of estimating the electron energy distribution function for long evolution times with small stochastic error requires combining both MC variance reduction techniques and distributed or parallel computations.

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In this paper a parallel MC method for solving the B-F equation is studied. The transition density function for the Markov chain is chosen to be proportional to the contribution from the kernels. The integral parts of the kernels are estimated using MC integration. An importance sampling technique is introduced to reduce the variance in the MC quadrature. A new rule for sampling the transition density function of the Markov chain is used to construct the MC estimator. In this way, we avoid the acceptance-rejection techniques used [6]. The parallelisation of the MC algorithm is done using MPI and OpenMP codes. All these improvements in the MC approach lead to a decrease of the computational complexity of the algorithm and allow to estimate the electron energy distribution function for long evolution times.

2 The Quantum Kinetic Equation

The quantum kinetic equation accounting for the electron-phonon interaction in presence of applied electric field can be written in the following integral form [6]:

$$f(\mathbf{k},t) = \phi(\mathbf{k}) + \int_0^t dt'' \int_G d\mathbf{k}' K(\mathbf{k},\mathbf{k}') \times \tag{1}$$
$$\left\{ \int_{t''}^t dt' S_1(\mathbf{k},\mathbf{k}',\mathbf{F},t',t'') f(\mathbf{k}',t'') + \int_{t''}^t dt' S_2(\mathbf{k},\mathbf{k}',\mathbf{F},t',t'') f(\mathbf{k},t'') \right\},$$

where the kernel is separated in two terms:

$$K(\mathbf{k},\mathbf{k}') = \frac{2V}{2\pi^3\hbar^2}|g(\mathbf{q})|^2, \quad \text{and} \tag{2}$$

$$S_1(\mathbf{k},\mathbf{k}',\mathbf{F},t',t'') = -S_2(\mathbf{k}',\mathbf{k},\mathbf{F},t',t'') = exp(-\Gamma(t'-t'')) \times \tag{3}$$
$$\left[(n_\mathbf{q}+1)\cos\left(\frac{\varepsilon(\mathbf{k})-\varepsilon(\mathbf{k}')+\hbar\omega_\mathbf{q}}{\hbar}(t'-t'') - \frac{\hbar}{2m}(\mathbf{k}'-\mathbf{k})\cdot\mathbf{F}(t'^2-t''^2) \right) \right.$$
$$\left. + n_\mathbf{q}\cos\left(\frac{\varepsilon(\mathbf{k})-\varepsilon(\mathbf{k}')-\hbar\omega_\mathbf{q}}{\hbar}(t'-t'') - \frac{\hbar}{2m}(\mathbf{k}'-\mathbf{k})\cdot\mathbf{F}(t'^2-t''^2) \right) \right].$$

Here, $\mathbf{k}$ and t are the momentum and the evolution time, respectively. $f(\mathbf{k},t)$ is the distribution function. $\phi(\mathbf{k})$ is the initial electron distribution function. $\mathbf{F} = e\mathbf{E}/\hbar$, where $\mathbf{E}$ is the applied electric field. $n_\mathbf{q} = 1/(exp(\hbar\omega_\mathbf{q}/\mathcal{K}T)-1)$ is the Bose function, where $\mathcal{K}$ is the Boltzmann constant and T is the temperature of the crystal, corresponds to an equilibrium distributed phonon bath. $\hbar\omega_\mathbf{q}$ is the phonon energy which generally depends on $\mathbf{q} = \mathbf{k}' - \mathbf{k}$, and $\varepsilon(\mathbf{k}) = (\hbar^2\mathbf{k}^2)/2m$ is the electron energy. A Fröhlich coupling is considered

$$g(\mathbf{q}) = -i\left[\frac{2\pi e^2\hbar\omega_\mathbf{q}}{V}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s} \right)\frac{1}{(\mathbf{q})^2} \right]^{\frac{1}{2}},$$

where (ϵ_∞) and (ϵ_s) are the optical and static dielectric constants. 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.

3 Monte Carlo Approach

Consider the problem for evaluating the following functional

$$J_h(f) \equiv (h, f) = \int_0^{\mathcal{T}} \int_G h(\mathbf{k}, t) f(\mathbf{k}, t) d^3\mathbf{k} dt$$

by a MC method. Suppose the distribution function $f(\mathbf{k}, t)$ and the arbitrary function $h(\mathbf{k}, t)$ belong to any Banach space X and the adjoint space X^*, respectively. The wave vector $\mathbf{k}$ belongs to a finite domain $G \in R^3$ and $t \in (0, \mathcal{T})$. The value of f at a fixed point $(\mathbf{k_0}, t_0)$ is provided by the special case $h(\mathbf{k}, t) = \delta(\mathbf{k}-\mathbf{k_0})\delta(t-t_0)$. Since the Neumann series of the integral equation (3) converges [7] the solution $f(\mathbf{k_0}, t_0)$ can be evaluated by a MC method.

Define a terminated Markov chain $(\mathbf{k}_0, t_0) \to \ldots \to (\mathbf{k}_j, t_j) \to \ldots \to (\mathbf{k}_{m_{\varepsilon_1}}, t_{m_{\varepsilon_1}})$, such that $(\mathbf{k}_j, t_j) \in G \times (0, \mathcal{T})$ as $t_j \in (0, t_{j-1})$, $j = 1, 2, \ldots, m_{\varepsilon_1}$ (ε_1 is the truncation parameter). All points are sampled using an arbitrary transition density function $p(\mathbf{k}, \mathbf{k}', t, t'')$ which is tolerant[1] of both kernels in equation (1). The biased backward MC estimator for the solution of (1) at the fixed point $(\mathbf{k}_0, t_0)$ has the following form:

$$\xi_{m_{\varepsilon_1}}[\mathbf{k}_0, t_0] = \phi(\mathbf{k}_0) + \sum_{j=1}^{m_{\varepsilon_1}} W_j^{\alpha} \phi(\mathbf{k}_j^{\alpha}), \tag{4}$$

where

$$\phi(\mathbf{k}_j^{\alpha}) = \begin{cases} \phi(\mathbf{k}_j), & \text{if } \alpha = 1 \\ \phi(\mathbf{k}_{j-1}), & \text{if } \alpha = 2, \end{cases}$$

$$W_j^{\alpha} = W_{j-1}^{\alpha} \frac{K(\mathbf{k}_{j-1}, \mathbf{k}_j) \nu_{\alpha}(\mathbf{k}_{j-1}, \mathbf{k}_j, t_{j-1}, t_j)}{p_{\alpha} p(\mathbf{k}_{j-1}, \mathbf{k}_j, t_{j-1}, t_j)}, \quad j = 1, \ldots, m_{\varepsilon_1}, \qquad W_0^{\alpha} = 1.$$

Here $\nu_{\alpha}(\mathbf{k}_{j-1}, \mathbf{k}_j, t_{j-1}, t_j)$ is a MC estimator for $\int_{t_{j-1}}^{t_j} dt' S_{\alpha}(\mathbf{k}_{j-1}, \mathbf{k}_j, \mathbf{F}, t', t_{j-1})$ in the j-th transition at the Markov chain. The probabilities $p_{\alpha}, (\alpha = 1, 2)$ are chosen to be proportional to the absolute values of the kernels.

Now we can define a Monte Carlo method

$$\frac{1}{N} \sum_{i=1}^{N} (\xi_{m_{\varepsilon_1}}[\mathbf{k}_0, t_0])_i \xrightarrow{P} J_{\delta}(f_{m_{\varepsilon_1}}) \approx f(\mathbf{k}_0, t_0), \tag{5}$$

where $\xrightarrow{P}$ means stochastic convergence as $N \to \infty$; $f_{m_{\varepsilon_1}}$ is the iterative solution obtained by the Neumann series of (1). The relation (5) still does not determine

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

the computational algorithm. The sampling rule, which compute the next point at the Markov chain, has to be specified by using random number generators.

In order to avoid the singularity in (2) the following transition density function is suggested: $p(\mathbf{k},\mathbf{k}',t,t'') = p(\mathbf{k}'/\mathbf{k})p(t,t'')$, where $p(t,t'') = 1/t$. In spherical coordinates (ρ,θ,φ), the function $p(\mathbf{k}'/\mathbf{k})$ is chosen in the following way: $p(\mathbf{k}'/\mathbf{k}) = (4\pi)^{-1}(\rho)^{-2}l(\omega)^{-1}$, where $\omega = (\mathbf{k}'-\mathbf{k})/\rho$, $\rho = |\mathbf{k}'-\mathbf{k}|$ and $l(\omega)$ is distance in the direction of the unit vector ω from $\mathbf{k}$ to the boundary of the domain G. If G is a sphere with radius Q, the function $p(\mathbf{k}'/\mathbf{k})$ satisfies the condition for a transition density. Indeed,

$$\int_G p(\mathbf{k}'/\mathbf{k})d^3\mathbf{k}' = \oint (4\pi)^{-1}d\omega \int_0^{l(\omega)} (r')^{2-2}l(\omega)^{-1}dr' = 1.$$

Suppose the direction of the field $\mathbf{E}$ parallel to the k_z-axis. Then the unit vector ω can be sampled in the xz-plane (or $\sin\varphi = 0$) because of the symmetry of the task around the direction of the field.

Thus, if we know the wave vector $\mathbf{k}$ the next state $\mathbf{k}'$ can be computed by the following sample rule:

Algorithm 1:

1. **Sample** a random unit vector $\omega = (\sin\theta, 0, \cos\theta)$ as $\sin\theta = \sin 2\pi\beta_1$ and $\cos\theta = \cos 2\pi\beta_1$, where β_1 is an uniformly distributed number in (0, 1);
2. **Calculate** $l(\omega) = -\omega\cdot\mathbf{k} + (Q^2 + (\omega\cdot\mathbf{k})^2 - \mathbf{k}^2)^{\frac{1}{2}}$, where $\omega\cdot\mathbf{k}$ means a scalar product between two vectors;
3. **Sample** $\rho = l(\omega)\beta_2$, where β_2 is an uniformly distributed number in (0, 1);
4. **Calculate** $\mathbf{k}' = \mathbf{k} + \rho\omega$.

In order to evaluate $f(\mathbf{k},\mathbf{t})$ in the fixed point $(\mathbf{k_0},t_0))$, N random walks of the MC estimator can be computed by the following algorithm:

Algorithm 2:

1. **Choose** a positive small number ε_1 and **set** initial values $\mathbf{k} := \mathbf{k_0}, t := t_0$, $\xi := \phi(\mathbf{k})$,$\mathbf{W} := \mathbf{1}$;
2. **Sample** a value t'' with a density function $p(t,t'') = 1/t$;
3. **Sample** the next state $\mathbf{k}'$ using **Algorithm 1**;
4. **Sample** N_1 independent random values of t' with a density function

$$q_1(t',t'') = \frac{\Gamma exp(-\Gamma(t'-t''))}{1-exp(-\Gamma(t-t''))};$$

5. **Calculate**

$$\overline{\nu}_\alpha = \frac{1}{N_1}\sum_{i=1}^{N_1}\frac{S_\alpha(\mathbf{k},\mathbf{k}',t_i',t'')}{q_1(t_i',t'')} \quad \text{and} \quad p_\alpha = \frac{|\overline{\nu}_\alpha|}{|\overline{\nu}_1| + |\overline{\nu}_2|}, \quad \alpha = 1,2;$$

6. **Choose** a value β, uniformly distributed random variable in $(0, 1)$;
   If $(\beta \leq p_1)$ **then**

$$W := W\frac{K(\mathbf{k},\mathbf{k}')\,t\,\overline{\nu}_1}{p_1\,p(\mathbf{k}'/\mathbf{k})},\ \ \xi := \xi + W\phi(\mathbf{k}'),\ \ \mathbf{k} := \mathbf{k}';$$

   else

$$W := W\frac{K(\mathbf{k},\mathbf{k}')\,t\,\overline{\nu}_2}{p_2\,p(\mathbf{k}'/\mathbf{k})},\ \ \xi := \xi + W\phi(\mathbf{k});$$

7. **Set** $t := t''$ and **repeat** from step 2 until $t \leq \varepsilon_1$;
8. **Repeat** N times steps $1 - 7$ and **estimate** the electron energy distribution function by Eq.(5).

4 Parallel Implementation and Numerical Results

The computational complexity of the obtained **Algorithm 2** can be measured by the quantity $F = N \times \tau \times E(m_{\varepsilon_1})$. The number of the random walks, N, and the average number of transitions in the Markov chain, $E(m_{\varepsilon_1})$, are connected with stochastic and systematic errors [7]. The mean time for modeling one transition, τ, depends on the complexity of the transition density functions and on the sampling rule, as well as on the choice of the random number generator (rng).

It is well known that the MC algorithms are very convenient for parallel implementations on parallel computer systems [8], because every realization of the MC estimator can be done independently and simultaneously. Although MC algorithms are well suited to parallel computation, there are a number of potential problems. The available computers can run at different speeds; they can have different user loads on them; one or more of them can be down; the rng's that they use can run at different speeds; ets. On the other hand, these rng's must produce independent and non-overlapping random sequences. Thus, the parallel realization of the MC algorithms is not a trivial process on different parallel computer systems.

In our research, the **Algorithm 2** has been implemented in C and has been parallelized using an MPI code. The numerical tests have been performed on Sunfire 6800 SMP system with twenty-four 750 MHz UltraSPARC-III processors located at the Edinburgh Parallel Computer Centre (EPCC). The SPRNG library has been used to produce independent and non-overlapping random sequences [9]. Our aim is to estimate the electron energy distribution function for evolution times greater than 200 fs. That is way, our parallel implementation with n processors includes the following strategy. A master-slave model is used where the master processor delegates work (N/n random walks) to the other processors. The slave processors complete the required work and obtain "local" MC estimates. After that they return the results back to the master processor which produces the "global" MC estimate. Such a parallel strategy is expected to give linear speed-up and high parallel efficiency. The results in Table 1 confirm this assumption in general. In addition, an MPI/OpenMP mixed code has

been developed for parallel implementation of the **Algorithm 2**. Such mixed mode code has been proposed in [10] as a more efficient parallelisation strategy to perform diffusion Monte Carlo calculations for an SMP (Share Memory Programming) cluster.

Table 1. The CPU time (seconds) for all 96 points, the speed-up, and the parallel efficiency for various combination of OpenMP threads and MPI processes. The number of random walks is $N = 9600$. The electric field is $0\,kV/cm$ and the evolution time is $100\,fs$.

Processes ×Threads	CPU Time	Speed-up	Parallel Efficiency	Processes ×Threads	CPU Time	Speed-up	Parallel Efficiency
1×1	567.177			1×1	567.177		
1×2	565.955	1.00216	0.5011	2×1	287.505	1.97276	0.9864
1×4	524.357	1.08167	0.2704	4×1	144.540	3.92401	0.9810
1×6	460.623	1.23133	0.2052	6×1	96.321	5.88840	0.9814
1×8	426.134	1.33098	0.1664	8×1	74.465	7.61669	0.9521
2×2	310.443	1.82699	0.4567	2×2	310.443	1.82699	0.4567
2×3	292.286	1.94049	0.3234	3×2	211.674	2.67948	0.4466
2×4	274.871	2.06343	0.2579	4×2	160.933	3.54094	0.4426

The results in Table 1 demonstrate that this style of programming is not always the most efficient mechanism on SMP systems and cannot be regarded as the ideal programming model for all codes.

The numerical results discussed in Figures 1–4 are obtained for zero temperature and $GaAs$ material parameters: the electron effective mass is 0.063, the optimal phonon energy is $36meV$, the static and optical dielectric constants are $\varepsilon_s = 10.92$ and $\varepsilon_\infty = 12.9$. The initial condition at $t = 0$ is given by a function which is Gaussian in energy, ($\phi(k) = exp(-(b_1k^2 - b_2)^2)$, $b_1 = 96$ and $b_2 = 24$), scaled in a way to ensure, that the peak value is equal to unity. A value $Q = 66 \times 10^7 m^{-1}$ is chosen for a radius of integration domain G. The solution $f(0, 0, k_z, t)$ is estimated in 2×96 points that are symmetrically located on z-axes, the direction of applied field. The truncation parameter $\varepsilon = 0.001$. The quantity presented on the y-axes in all figures is $|\mathbf{k}| * f(0, 0, k_z, t)$, i.e., it is proportional to the distribution function multiplied by the density of states. It is given in arbitrary units. The quantity $\mathbf{k}^2$, given on the x-axes in units of $10^{14}/m^2$, is proportional to the electron energy.

The results for the computational cost of the **Algorithm 2** are obtained and are compared with the algorithm from [6]. To obtain a smooth solution in the case when $t = 200\,fs$, the **Algorithm 2** needs approximately 9 minutes per point on one processor while the algorithm presented in [6] needs approximately 30 minutes. These results and the parallelisation of the **Algorithm 2** allow to estimate the solution of (1) with high accuracy for $300\,fs$ evolution time.

The results for the electron energy distribution are presented on Figures 1-4 for $200fs$ and $300fs$ evolution times. The relaxation leads to a time-dependent

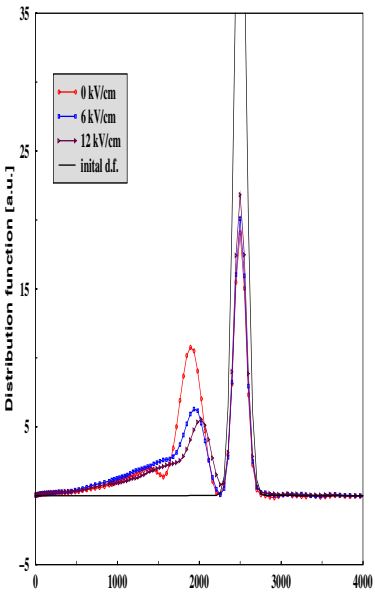

Fig. 1. Solutions $|\mathbf{k}|f(0,0,k_z,t)$ versus $|\mathbf{k}|^2 10^{14} m^{-2}$, at positive direction on the z-axis, and $t = 200\, fs$. The electric field is 0, $6\, kV/cm$, and $12\, kV/cm$ and the number of random walks per point is 1 million.

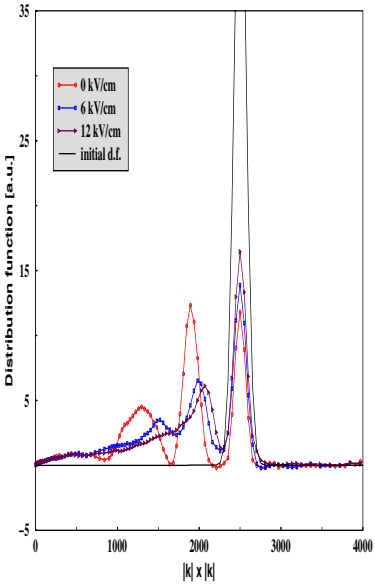

Fig. 2. Solutions $|\mathbf{k}|f(0,0,k_z,t)$ versus $|\mathbf{k}|^2 10^{14} m^{-2}$, at positive direction on the z-axis, and $t = 300\, fs$. The electric field is 0, $6\, kV/cm$, and $12\, kV/cm$ and the number of random walks per point is 24 millions.

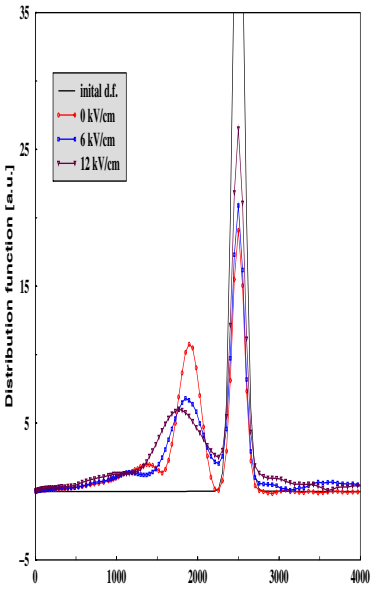

Fig. 3. Solutions $|\mathbf{k}|f(0,0,k_z,t)$ versus $|\mathbf{k}|^2 10^{14} m^{-2}$, at negative direction on the z-axis, and $t = 200\,fs$. The electric field is 0, $6\,kV/cm$, and $12\,kV/cm$ and the number of random walks per point is 1 million.

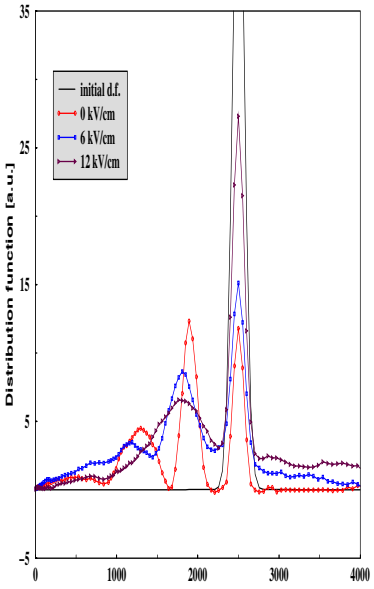

Fig. 4. Solutions $|\mathbf{k}|f(0,0,k_z,t)$ versus $|\mathbf{k}|^2 10^{14} m^{-2}$, at negative direction on the z-axis, and $t = 300\,fs$. The electric field is 0, $6\,kV/cm$, and $12\,kV/cm$ and the number of random walks per point is 24 millions.

broadening of the replicas. The presented solutions on Figures 1 and 2 are along the electric field and the replicas are shifted to the right by the increasing electric field. Figures 3 and 4 show the solutions in direction opposite to the field and the replicas are shifted to the left. Also, we see on Figures 2 and 4 that second peak is appeared on the left of the initial condition and the replicas begin to shift at the same way with the increase of the electric field. The solution in the classically forbidden region (see Figures 3 and 4), on the right of the initial condition, demonstrates enhancement of the electron population with the growth of electric field. The numerical results show that the intra-collisional field effect is well demonstrated for $300fs$ evolution time of the electron-phonon relaxation.

Conclusions. A parallel MC algorithm for solving the B-F equation in presence of applied electric field is presented. A new transition density for the Markov chain and an algorithm described the sample rule are suggested. The MC algorithm has low complexity in comparison with the algorithm from [6]. MPI/OpenMP mixed mode code is developed and is compared with pure MPI performance. The numerical results show that the pure MPI performance is preferable for large-scale MC simulations in order to investigate the quantum kinetic equation under consideration.

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