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ПЛИСКА

БЪЛГАРСКИ МАТЕМАТИЧЕСКИ СТУДИИ

A STOCHASTIC APPROACH FOR INVESTIGATION ULTRAFAST PHENOMENA IN SEMICONDUCTORS

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In this paper a stochastic approach is proposed for investigation the ultrafast evolution of electrons interacting with phonons in the presence of an applied electric field.

The quantum-kinetic equation describing the above ultrafast phenomena contains polynomial non-linearity which allows to use the link between non-stationary iterative processes and the branching stochastic processes.

The considered stochastic approach relies on the numerical Monte Carlo (MC) theory as applied to the integral form of the quantum-kinetic equation and estimates the electron energy distribution using statistical averages over long evolution times.

The numerical tests were performed for $GaAs$ material parameters. The numerical results for the electron energy distribution function in the case of a non-linear electron quantum transport is compared with the obtained results in the linear case.

1. A branching stochastic process and an integral equation with polynomial non-linearity

Consider the following integral equation with polynomial non-linearity

$$f(x,t) \quad =$$

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(1) $$\int_0^t \int_G \mathcal{K}_1(x, x', t, t') f(x', t') dt' dx' + \int_0^t \int_G \mathcal{K}_2(x, x', t, t') f(x, t') dt' dx'$$

$$+ \int_0^t \int_G \mathcal{K}_3(x, x', t, t') f(x', t') f(x, t') dt' dx' + \phi(x).$$

Assume that it has an iterative solution corresponding to the following non-stationary iterative process

$$f_l(x, t) =$$

$$\int_0^t \int_G \mathcal{K}_1(x, x', t, t') f_{l-1}(x', t') dt' dx' + \int_0^t \int_G \mathcal{K}_2(x, x', t, t') f_{l-1}(x, t') dt' dx'$$

(2) $$+ \int_0^t \int_G \mathcal{K}_3(x, x', t, t') f_{l-1}(x', t') f_{l-1}(x, t') dt' dx' + \phi(x),$$

$$f_0(x, t = 0) = \phi(x), \quad l = 1, 2, \dots,$$

The problem is to construct a Monte Carlo estimator for evaluating the functional:

$$J(f) \equiv (g, f) = \int_0^T \int_G g(x, t) f(x, t) dt dx,$$

where the domain $G \subset I\!\!R^d$ and a point $(x, t) \in G \times (0, T)$ is a point in the Euclidean space $I\!\!R^{d+1}$. The functions $f(x, t)$ and $g(x, t)$ belong to any Banach space X and to the adjoint space X^*, respectively, and $f(x, t)$ is an unique solution of the iterative process (2).

The case, when the given function $g(x, t) = \delta(x - x_0, t - t_0)$, is of special interest, because we are interested in calculating the value of f at a fixed point (x_0, t_0).

To solve the problem above we use the link between non-stationary iterative processes and the branching stochastic processes [1]. It is known [1] there is a one-to-one correspondence between the number of the subtrees of the full tree Γ_l of the branching stochastic process with l generations and the number of the terms of the truncated non-stationar iterative process with l iterations.

Let us consider the following branching stochastic process which corresponds to the iterative process Eq.(2). Suppose that any particle distributed with initial density function $p_0(y) \geq 0$ and $\int_{G_1} p_0(y) dy = 1$ is born in the domain $G_1 = G \times (0, T) \in I\!\!R^{d+1}$ in a random point $y = (x, t)$. In the next moment one of the following four events holds:

1. the particle y dies with probability $h(y)$, where $0 \leq h(y) < 1$;

2. y generates a new particle $y' = (x', t')$ with a probability $p_1(y)$ and a transition density $p_1(y, y')$;

3. y generates a new particle $y'' = (x, t')$ with a probability $p_2(y)$ and a transition density $p_2(y, y'')$;

4. y generates new two particles y' and y'' with a probability $p_3(y)$ and a transition density $p_3(y, y', y'')$.

We note that $\sum_{i=1}^{3} p_i(y) = 1 - h(y)$.

The generated particles behave in the next moment as initial one and etc. The traces of such a process are a trees sketched in Picture (1) (up to the first generation).

a)   **b)**   **c)**   **d)**
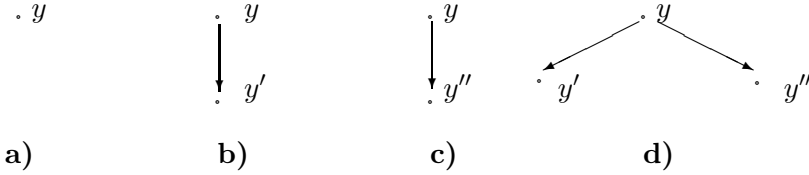
Picture 1.

When we construct the branching stochastic process above we receive arbitrary trees γ. Thus we can associate to every one of these trees the MC estimator $\Theta_{[g]}(\gamma/\Gamma_l)$ depends on the full tree Γ_l in the following way: if the tree consists of the initial point y, then

$$\Theta_{[g]}(\gamma/\Gamma_l) = \frac{g(y)}{p_0(y)} \frac{\phi(y)}{h(y)}.$$

If the tree consists of other points, then $\Theta_{[g]}(\gamma/\Gamma_l)$ is constructed simultaneously with the construction of the tree γ. If the point $y_{\gamma[s]}$ from the s-th generation generates a new point $y'_{\gamma[s]}$ or $y''_{\gamma[s]}$ then $\Theta_{[g]}(\gamma/\Gamma_l)$ is multiplied by

$$\frac{\mathcal{K}_1(y_{\gamma[s]}, y'_{\gamma[s]})}{p_1(y_{\gamma[s]})p_1(y_{\gamma[s]}, y'_{\gamma[s]})} \quad \text{or} \quad \frac{\mathcal{K}_2(y_{\gamma[s]}, y''_{\gamma[s]})}{p_2(y_{\gamma[s]})p_2(y_{\gamma[s]}, y''_{\gamma[s]})}.$$

If the point $y_{\gamma[s]}$ generates new two points $y'_{\gamma[s]}$ and $y''_{\gamma[s]}$ then $\Theta_{[g]}(\gamma/\Gamma_l)$ is multiplied by

$$\frac{\mathcal{K}_3(y_{\gamma[s]}, y'_{\gamma[s]}, y''_{\gamma[s]})}{p_3(y_{\gamma[s]})p_3(y_{\gamma[s]}, y'_{\gamma[s]}, y''_{\gamma[s]})}.$$

Finally, if the random point $y_{\gamma[m]}$ from the m-th generation dies then $\Theta_{[g]}(\gamma/\Gamma_l)$ is multiplied by $\frac{\phi(y_{\gamma[m]})}{h(y_{\gamma[m]})}$.

Thus, the MC estimator $\Theta_{[g]}(\gamma/\Gamma_l)$ has the following form:

$$(3) \qquad \Theta_{[g]}(\gamma/\Gamma_l) = \frac{g(y)}{p_0(y)} \times$$

$$\prod_{y_{\gamma[s]} \in A} \frac{\mathcal{K}_1(y_{\gamma[s]}, y'_{\gamma[s]})}{p_1(y_{\gamma[s]})p_1(y_{\gamma[s]}, y'_{\gamma[s]})} \prod_{y_{\gamma[s]} \in A} \frac{\mathcal{K}_2(y_{\gamma[s]}, y''_{\gamma[s]})}{p_2(y_{\gamma[s]})p_2(y_{\gamma[s]}, y''_{\gamma[s]})} \times$$

$$\prod_{y_{\gamma[s]} \in A} \frac{\mathcal{K}_3(y_{\gamma[s]}, y'_{\gamma[s]}, y''_{\gamma[s]})}{p_3(y_{\gamma[s]})p_3(y_{\gamma[s]}, y'_{\gamma[s]}, y''_{\gamma[s]})} \prod_{y_{\gamma[m]} \in B} \frac{\phi(y_{\gamma[m]})}{h(y_{\gamma[m]})},$$

$$1 \le s \le l - 1, \ \ 1 < m \le l, \ \ l = 1, 2, \ldots,$$

where A is the set of all points that generate new points and B is the set of the points that die.

The following statement holds.

Theorem 1. *The mathematical expectation of the MC estimator $\Theta_{[g]}(\gamma/\Gamma_l)$ is equal to the functional $J(f_l)$, i.e. $E\Theta_{[g]}(\gamma/\Gamma_l) = J(f_l) = (g, f_l)$.*

Here f_l is l-th iteration of the iterative process (2). The proof of this theorem is similar to the proof in [2] for general case of integral equations with polynomial non-linearity.

2. An application for ultrafast phenomena in semiconductors

Consider the physics model that includes a femtosecond relaxation process of optically excited carriers in one-band semiconductor [3]. The electron-phonon interaction is switched on after a laser pulse creates an initial electron distribution. The quantum-kinetics equation described the above process appears as a simplified Barker-Ferry (B-F) equation [4] written for the case of a zero electronic field. The original formulation of this equation [5] accounts for the action of the electric field **E** during the process of electron-phonon interaction - the intracollisional field effect. 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 hundreds femtoseconds after an optical excitation [6, 7]. The low density regime is considered, where the interaction with phonons dominates the carrier-carrier interaction [7].

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

$$(4) \qquad \frac{\partial f(\mathbf{k}, t)}{\partial t} + \mathbf{F} \cdot \nabla_{\mathbf{k}} f(\mathbf{k}, t) =$$

$$\int_0^t \int \{S(\mathbf{k}',\mathbf{k},t,t')[f(\mathbf{k}'(t'),t')(1-f(\mathbf{k}(t'),t'))]$$
$$-S(\mathbf{k},\mathbf{k}',t,t')[f(\mathbf{k}(t'),t')(1-f(\mathbf{k}'(t'),t'))]\}dt'd\mathbf{k}'$$

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

where $\mathbf{F}=e\mathbf{E}/\hbar$, $n_\mathbf{q}$ is the Bose function [4], $\omega_\mathbf{q}$ 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. (4):

$$f(\mathbf{k},t) = \phi(\mathbf{k}(0)) +$$
$$\int_0^t \int_0^{t'} \int \{S(\mathbf{k}',\mathbf{k},t',t'')[f(\mathbf{k}'(t''),t'')(1-f(\mathbf{k}(t''),t''))]$$
$$-S(\mathbf{k},\mathbf{k}',t',t'')[f(\mathbf{k}(t''),t'')(1-f(\mathbf{k}'(t''),t''))]\}dt'dt''d\mathbf{k}'$$

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 $0 \le t'' \le t$ and hence no general integration domain can be specified in the phase space. This problem is solved by the transformation described in [8] and it is known as "center of mass transform".

This transformation decouples the phase space and time arguments of the cosine functions in the kernels.

Using the mention transformation, the integral equation becomes:

(5)
$$f(\mathbf{k},t) = \phi(\mathbf{k}) +$$
$$\int_0^t \int_0^{t'} \int \left\{ S(\mathbf{k}',\mathbf{k},t',t'')[f(\mathbf{k}',t'')(1-f(\mathbf{k},t''))] \right.$$
$$\left. -S(\mathbf{k},\mathbf{k}',t',t'')[f(\mathbf{k},t'')(1-f(\mathbf{k}',t''))] \right\} dt'dt''d\mathbf{k}'$$

It can be proved that Eq. (5) has an iterative solution in case when $|f(\mathbf{k}, t)| \leq 0$ because it is bounded from the linear one. The proof is similar to the proof in [9]. 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. Now we use 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. For zero lattice temperature ($n_{\mathbf{q}} = 0$) the equation obtained reads:

$$(6) \qquad f(x, t) = \phi(x) + \int_0^t \int_G \left[K(x, x') \left\{ \int_{t''}^t S(x', x, t', t'') dt' \right\} \times \right.$$

$$f(x', t'')(1 - f(x, t'')) - \left\{ \int_{t''}^t S(x, x', t', t'') dt' \right\} f(x, t'')(1 - f(x', t'')) \right] dt'' dx'$$

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

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

$$S(x', x, t', t'') = S(r', k', r, k, t', t'') = exp(-\Gamma(t' - t'')) \times$$

$$\cos \left(\left(\frac{\hbar}{2m}(r'^2 + k'^2 - r^2 - k^2) + \omega_q \right) - \frac{\hbar}{2m} F(k' - k)(t' + t'') \right) (t' - t'') \right).$$

The equation (6) can be rewritten in the following form:

$$(7) \quad f(x, t) = \phi(x) + \int_0^t \int_G K(x, x') \left\{ \int_{t''}^t S(x', x, t', t'') dt' \right\} f(x', t'') dt'' dx'$$

$$- \int_0^t \int_G K(x, x') \left\{ \int_{t''}^t S(x, x', t', t'') dt' \right\} f(x, t'') dt'' dx'$$

$$+ \int_0^t \int_G K(x, x') \left\{ \int_{t''}^t (S(x, x', t', t'') - S(x', x, t', t'')) dt' \right\} f(x, t'') f(x', t'') dt'' dx'.$$

The equation (1) is obtained using substitutions

$$\mathcal{K}_1(x, x', t, t'') = K(x, x') \left\{ \int_{t''}^t S(x', x, t', t'') dt' \right\},$$

$$\mathcal{K}_2(x, x', t, t'') = -K(x, x') \left\{ \int_{t''}^t S(x, x', t', t'') dt' \right\}$$

and $\mathcal{K}_3(x, x', t, t'') = -\mathcal{K}_2(x, x', t, t'') - \mathcal{K}_1(x, x', t, t'')$. Thus, the MC estimator (3) can be used to evaluated the solution of Eq. (7).

3. The stochastic algorithm

The equation is solved by a randomized branched Monte Carlo (RBMC) algorithm, namely, during construction of the MC estimator (3), a MC method is used to estimate the integral part in the kernels of the Eq.(7). The solution of the Eq.(7) at the fixed point $y = (x, t)$ is evaluated by N realizations (random trees) of the MC estimator: $f(x, t) \simeq \frac{1}{N} \sum_{i=1}^{N} (\Theta_{[\delta]}(\gamma/\Gamma_l)[x, t])_i$, where $x = (r, k)$ and $g(x, t)$ is the δ- function.

In case, when we construct one random tree the RBMC algorithm is as follows:

1. **Input** *initial data: the MC estimator* $\Theta_{[\delta]}(\gamma/\Gamma_l) := 1$, *the point* $y = (x, t)$, *the positive constant* Q, *the probabilities* $p_1(y), p_2(y), p_3(y)$, *and the probability* $h(y)$.

2. **Sample** *a value* t'' *with a density function* $q(t, t'') = 1/t$.

3. **Sample** *a value* $x' = (r', k')$ *with a density function*

   $p(x, x') = p(r, k, r'k') = C/((r - r')^2 + (k - k')^2)^{\frac{1}{2}}$

   using an acceptance-rejection method (C *is a constant for normalization).*

4. **Estimate** *both intergals* $\int_{t''}^{t} S(x', x, t', t'') dt'$ *and* $\int_{t''}^{t} S(x, x', t', t'') dt'$ *by MC estimators* $\mu_1(x', x, t, t'')$ *and* $\mu_2(x, x', t, t'')$, *respectively.*

5. **Choose** *an independent realization,* α, *of an uniformly distributed random variable in the interval* $(0, 1)$.

6. **If** $(\alpha < h(y))$ **Then** $\Theta_{[\delta]}(\gamma/\Gamma_l) := \Theta_{[\delta]}(\gamma/\Gamma_l)\frac{\phi(y)}{h(y)}$. *In this case we say that the point* $y = (x, t)$ *dies.*

   Else

   6.1. If $(\alpha < h(y) + p_1(y))$ **Then**

   $$\Theta_{[\delta]}(\gamma/\Gamma_l) := \Theta_{[\delta]}(\gamma/\Gamma_l)\frac{K(x, x')\mu_1(x', x, t, t'')}{p_1(y)q(t, t'')p(x, x')} .$$

   Save the point $y' = (x', t'')$ *in the pipeline and go to a step* 7.

   6.2. If $(\alpha < h(y) + p_1(y) + p_2(y))$ **Then**

   $$\Theta_{[\delta]}(\gamma/\Gamma_l) := \Theta_{[\delta]}(\gamma/\Gamma_l)\frac{(-K(x, x')\mu_2(x, x', t, t''))}{p_2(y)q(t, t'')p(x, x')} .$$

   Save the point $y'' = (x, t'')$ *in the pipeline and go to a step* 7.

6.3. If $(\alpha < 1)$ **Then**

$$\Theta_{[\delta]}(\gamma/\Gamma_l) := \Theta_{[\delta]}(\gamma/\Gamma_l)\frac{K(x,x')(\mu_2(x,x',t,t'') - \mu_1(x',x,t,t''))}{p_3(y)q(t,t'')p(x,x')} \ .$$

Save the points $y' = (x',t'')$ *and* $y'' = (x,t'')$ *in the pipeline.*

7. Repeat *steps* $2 - 6$ *for each point of the pipeline.*

8. Stop *the algorithm when all points of the pipeline die.*

The acceptance-rejection method used in the third step is described in [8] for linear case of the Eq. (6). To calculate the MC estimators in the fourth step, N_1 independent random values of t' are sampled with a density function $q_1(t') = 1/(t - t'')$. The probabilities $p_i(y)$, $i = 1, 2, 3$ are chosen to be proportional to the kernels' norm of the Eq. (7). To converge the branching Markov process, the probability $h(y)$ is chosen to be greater then $p_3(y)$. The RBMC algorithm can be generalized for finite temperatures in a straightfoward way.

4.   Numerical results

The simulation results are obtained for $GaAs$ with standard material parameters [8, 10] and effective mass 0.063. The phonon energy is a constant, $\hbar\omega = 36 \ meV$. The coupling $|g_q|^2$ applies to the Frohlich interaction [10]. A value $Q = 66 \cdot 10^7 m^{-1}$ is chosen for the integration domain G. The initial condition at $t = 0$ is given by a function which is Gaussian in energy, $(\phi(k) = exp(-(b_1 k^2 - b_2)^2)$, $b_1 = 96$ and $b_2 = 24$), scaled in a way to ensure, that the peak value is equal to unity. The quantities r^2 and k^2 that are given in units of $10^{14}/m^2$, are proportional to the electron energy. The numerical tests were performed on a PowerPC (G4 w/AltiVec) 450 MHz, running YDL 2.0. The solutions $kf(r = 0, k, t)$ versus k^2 and $rf(r, k = 0, t)$ versus r^2 are calculated in 55 points.

A necessary step is to test the proposed RBMC algorithm by a comparison with the randomized iterative Monte Carlo (RIMC) algorithm discussed in [8]. The probability $p_3(y)$, which generates the contribution of the nonlinear term, is set to be equal to zero. Then the numerical task reduces to the linear case. The probability for death of particles, $h(y)$, is 0.5 and $p_1(y) + p_2(y) = 0.5$. Figure 1 shows the excellent agreement between the solutions provided by both RBMC and RIMC algorithms.

A number of experiments are done, exploring the stability of the RBMC algorithm for different values of the probability for death. Some of them are presented on Figure 2. They show a good agreement between all RBMC solutions.
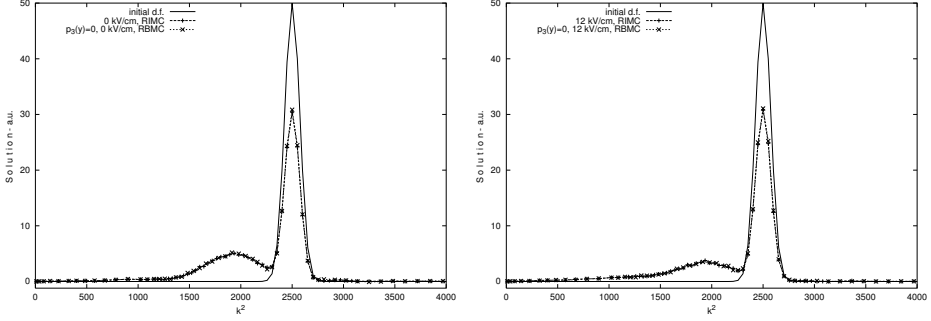
Figure 1: Comparison of both RIMC and RBMC solutions $kf(r, k, t)$ for $r = 0, k \in (0, Q)$ and evolution time $100\ fs$. The probability $p_3(y) = 0$ and the electric field is $0\ kV/cm$ on the left graphics and $12\ kV/cm$ on the right graphics.
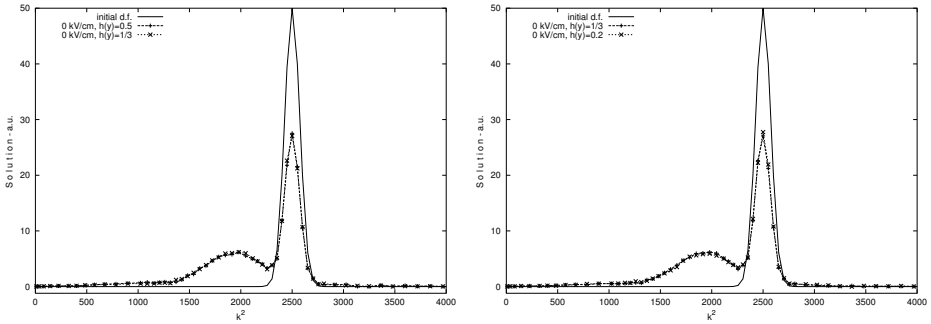

Figure 2: Comparison of RBMC solutions $kf(r, k, t)$ for $r = 0, k \in (0, Q)$ and evolution time $100\ fs$. The electric field is $0\ kV/cm$. The probability $h(y)$ is 0.5 and 1/3 on the left graphics, and 1/3 and 0.2 on the right graphics.
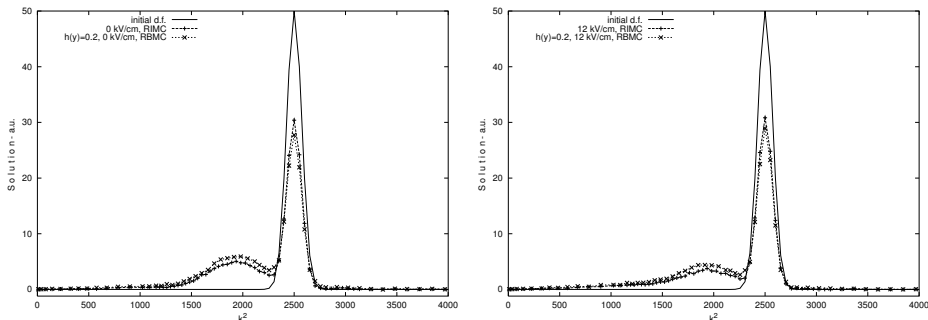
Figure 3: Comparison of both RIMC and RBMC solutions $kf(r, k, t)$ for $r = 0, k \in (0, Q)$ and evolution time $100 \ fs$. The probability $h(y) = 0.2$ and the electric field is $0 \ kV/cm$ on the left graphics, and $12 \ kV/cm$ on the right graphics.

The number of realizations, N, of the random trees is 1 million. The probabilities $p_i(y)$, $i = 1, 2, 3$ are chosen to be proportional to the norm of the kernels and $\sum_{i=1}^{3} p_i(y) + h(y) = 1$.

Figure 3 compares the solutions $kf(r = 0, k, t)$ versus k^2 for $100 \ fs$ evolution time. The effect is in pushing down the RBMC solution around the first peak, under the initial condition, and pulling it up, when the second peak is appeared. We explain this effect with contribution of the nonlinear part of the Eq. (7).

The intracollisional field effect is demonstrated on Figures 4-6. The electric field is 0, $6kV/cm$ and $12kV/cm$ and the evolution time is $150fs$. Here the number of realizations, N, of the random trees is 20 million. The presented solutions are in direction opposite to the field on the Figure 4, along the field on the Figure 5 and normal to the field on the Figure 6, respectively. The replicas are shifted to the left (Figure 4) or the right (Figure 5) by the increasing electric field. On the Figure 4 the solution in the classically forbidden region (on the right of the initial condition) demonstrates enhancement of the electron population with the growth of the field. These effects can be associated with the structure of the integral parts in the kernels, which controls the electron transfer between the states. No shift in the replicas is observed in the normal to the field direction (Figure 6). This is expected from theoretical considerations because of the symmetry of the task.

5. Conclusion

In this work a stochastic approach have been studied for investigation ultrafast phenomena in semiconductors. The solutions obtained with the RBMC algorithm
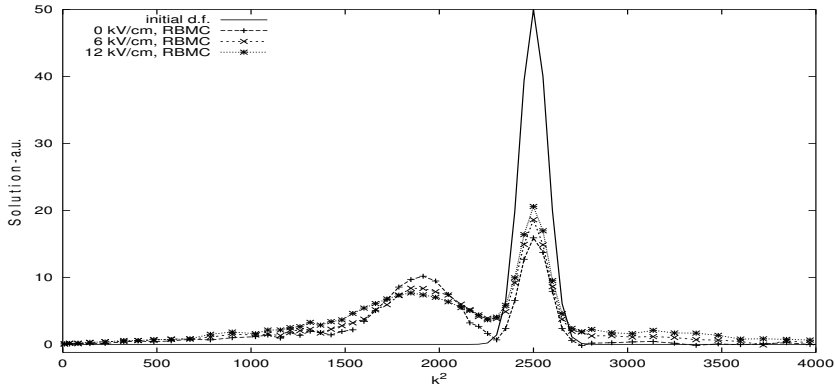
Figure 4: RBMC solutions $|k|f(r, k, t)$ for $r = 0, k \in (0, -Q)$ and evolution time $150\ fs$. The probability $h(y) = 0.5$ and the electric field is $0\ kV/cm$, $6\ kV/cm$, and $12\ kV/cm$.
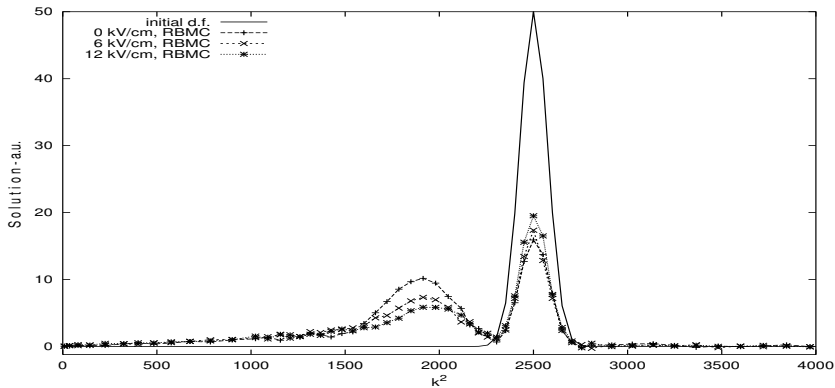

Figure 5: RBMC solutions $kf(r, k, t)$ for $r = 0, k \in (0, Q)$ and evolution time $150\ fs$. The probability $h(y) = 0.5$ and the electric field is $0\ kV/cm$, $6\ kV/cm$, and $12\ kV/cm$.
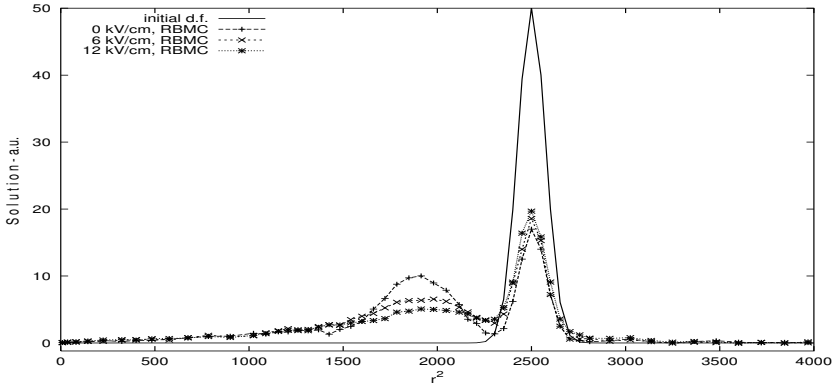
Figure 6: RBMC solutions $rf(r, k, t)$ for $k = 0, r \in (0, Q)$ and evolution time 150 fs. The probability $h(y) = 0.5$ and the electric field is 0 kV/cm, 6 kV/cm, and 12 kV/cm.

under consideration have been compered with the solution obtained with RIMC algorithm for the linear case of the B-F equation [8]. The results show that the proposed algorithm can be effectively applied for investigation of the quantum equation for the non-linear case.

The physical aspect is related to the contribution of the nonlinear part of the equation and the application of the electric field. The intracollisional field effect is well demonstrated as an effective change of the phonon energy, which depends on the field direction and evolution time.

Because of the fast increase of the variance with increasing the evolution time, the use of massively parallel machines is necessary.

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