

A Monte-Carlo Method to Analyze the Small Signal Response of the Semiconductor Carriers

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SUMMARY An approach for analysis of the small signal response of the carriers in semiconductors is presented. The integro-differential equation, describing the phenomenon in the time domain is transformed into a Fredholm integral equation of the second kind. The response of the carrier system to a small signal of a general time dependence can be calculated by the knowledge of the response to an impulse signal, defined by a delta function in time. For an impulse signal, the obtained integral equation resembles the basic structure of the integral form of the time dependent (evolution) Boltzmann equation. Due to this similarity a physical model of the impulse response process is developed. The model explains the response to an impulse signal in terms of a relaxation process of two carrier ensembles, governed by a Boltzmann equation. A Monte-Carlo method is developed which consists of algorithms for modeling the initial distribution of the two ensembles. The numerical Monte-Carlo theory for evaluation of integrals is applied. The subsequent relaxation process can be simulated by the standard algorithms for solving the Boltzmann equation. The presented simulation results for Si and GaAs electrons serve as a test of the Monte-Carlo method and demonstrate that the physical model can be used for explanation of the small signal response process.

key words: Monte Carlo method, stochastic algorithms, small signal analysis, kinetic coefficients

1. Introduction

The knowledge of the small signal response functions of the carriers system depending on the frequency ω and the DC electric field \mathbf{E}_s is of significant importance to forecast modern device performance. The differential response functions give the relationship between a small harmonic perturbation $\mathbf{E}_1 e^{i\omega t}$ of the DC field and the induced changes in the mean physical quantities $\langle A \rangle$ (e.g. the mean velocity components or the mean energy) which oscillate with the same frequency ω . The amplitude $\langle A \rangle_1$ of the oscillations around the stationary value $\langle A \rangle_s$ is linearly related to \mathbf{E}_1 : $\langle A \rangle_1(\omega) = K_A(\omega)\mathbf{E}_1$. Accordingly, the differential response function K_A is the gradient of the response $\langle A \rangle_1$ with respect to \mathbf{E}_1 . Of particular interest is the tensor of the differential velocity function (or differential mobility) $K_v = \mu(\omega)$ of the velocity response: $\langle \mathbf{v} \rangle_1(\omega) = \mu(\omega)\mathbf{E}_1$. Often the symmetry properties of the task allow to introduce scalar differential response functions.

Linked by the Fourier transform, analyses in the time and the frequency domains provide equivalent information. Furthermore, the response $\langle A \rangle_1(t)$ to a signal of a general time dependence $\mathbf{E}_1(t)$ can be calculated from the knowledge of the response $\langle A \rangle_i(t)$ to an impulse $\mathbf{E}_i(t) = \delta(t)\mathbf{E}_1$, defined by a delta function in time. Thus the knowledge of the carrier system response to an impulse signal is the main task of the small signal analysis. The advantages of Monte-Carlo simulations have been utilized for more than two decades [1] to explore the phenomenon.

Within the Monte-Carlo method single-particle simulations are popular, supported by the well established theory of correlation functions of the physical characteristics over a steady state trajectory [2], [3]. Another alternative is a transient description, given by the following derivative of the Boltzmann equation:

$$\begin{aligned} \frac{\partial f_1(\mathbf{k}, t)}{\partial t} + \frac{e}{\hbar} \mathbf{E}_s \cdot \nabla f_1(\mathbf{k}, t) \\ = Q[f_1(\mathbf{k}, t)] - \frac{e}{\hbar} \mathbf{E}_1(t) \cdot \nabla f_s(\mathbf{k}) \end{aligned} \quad (1)$$

where

$$Q[f_1(\mathbf{k}, t)] = \int S(\mathbf{k}', \mathbf{k}) f_1(\mathbf{k}', t) d\mathbf{k}' - \lambda(\mathbf{k}) f_1(\mathbf{k}, t)$$

is the common Boltzmann scattering term and f_1 is the correction to the distribution function f around a steady-state value f_s :

$$f(\mathbf{k}, t) = f_s(\mathbf{k}) + f_1(\mathbf{k}, t)$$

Accordingly, the mean of a physical characteristic $A(\mathbf{k})$ is given by

$$\langle A \rangle(t) = \langle A \rangle_s + \langle A \rangle_1(t)$$

With an impulse $\mathbf{E}_i(t)$ on the right hand side (1) cannot be treated numerically. The used stochastic or deterministic methods [2], [4] solve (1) for the case of a step-like signal: $\mathbf{E}_{step}(t) = \theta(t)\mathbf{E}_1$. Then an impulse response characteristic $\langle A \rangle_i(t)$ is obtained by taking the time derivative of the step response $\langle A \rangle_{step}(t)$.

In this work we utilize an integral formulation of (1) for an impulse signal. It suggests a physical model, interpreting the response phenomena as a relaxation process. The model allows to develop new Monte-Carlo algorithms, discussed in Sect. 3. The simulation results presented in Sect. 4 can be considered as a test both of

Manuscript received November 24, 1999.

Manuscript revised February 26, 2000.

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the physical model and the Monte-Carlo method.

The proof that the response to a general signal is obtained from the impulse response is given in the Appendix.

2. The Physical Model

We introduce a phase space trajectory

$$\mathbf{K}(t') = \mathbf{k} - \frac{e}{\hbar} \mathbf{E}_s(t - t') \quad (2)$$

which is initialized by \mathbf{k} at time t , so that $\mathbf{K}(t) = \mathbf{k}$. The left hand side of (1) becomes a total derivative and the equation can be formally written as $\frac{d}{dt}f(t) = -\lambda(t)f(t) + g(t)$. The latter has the solution

$$f(t) = \int_{t_0}^t g(t') e^{-\int_{t'}^t \lambda(y) dy} dt' + f(t_0) e^{-\int_{t_0}^t \lambda(y) dy}$$

with $f(t_0)$ given at some initial time t_0 . This result allows to reformulate (1) as an integral equation. For the case of an impulse at the time origin we obtain:

$$\begin{aligned} f_i(\mathbf{k}, t) &= \int_0^t dt' \int d\mathbf{k}' f_i(\mathbf{k}', t') S(\mathbf{k}', \mathbf{K}(t')) e^{-\int_{t'}^t \lambda(\mathbf{K}(y)) dy} \\ &\quad - \frac{e}{\hbar} \mathbf{E}_1 \cdot (\nabla f_s)(\mathbf{K}(0)) e^{-\int_0^t \lambda(\mathbf{K}(y)) dy} \end{aligned} \quad (3)$$

Here we have used that f_i is zero for negative time, and accounted for the delta function by the time integration. (3) is equivalent to the integral form of the Boltzmann equation [5], [6], with the only difference that the initial distribution function is now replaced by the function $G_i(\mathbf{k}) = -\frac{e}{\hbar} \mathbf{E}_1 \cdot (\nabla f_s)(\mathbf{k})$. Since $\int G_i(\mathbf{k}) d\mathbf{k} = 0$, G_i takes also negative values, obstructing a direct physical interpretation of (3). To continue, we decompose G_i into positive and negative parts $G_i = G_i^+ - G_i^-$, and consider the following set of integral equations:

$$\begin{aligned} f_i^\pm(\mathbf{k}, t) &= \int_0^t dt' \int d\mathbf{k}' f_i^\pm(\mathbf{k}', t') S(\mathbf{k}', \mathbf{K}(t')) e^{-\int_{t'}^t \lambda(\mathbf{K}(y)) dy} \\ &\quad + G_i^\pm(\mathbf{K}(0)) e^{-\int_0^t \lambda(\mathbf{K}(y)) dy} \end{aligned} \quad (4)$$

These are two Boltzmann equations with initial conditions given by $G_i^\pm \geq 0$. (3) is obtained by a subtraction of the two equations such that $f_i(\mathbf{k}, t) = f_i^+(\mathbf{k}, t) - f_i^-(\mathbf{k}, t)$ holds.

Some peculiarities of f_i can be derived from this result. Since $\int G_i(\mathbf{k}) d\mathbf{k} = 0$, the two functions f_i^\pm are equally normalized at the initial time $t = 0$. The Boltzmann equation conserves the normalization for later

times (no generation or recombination processes included). Thus (4) describe the evolution of two ensembles of equal number of particles.

The second conclusion concerns the dependence on the impulse field. Only the free terms in the two equation (4) linearly depend on the impulse field. The latter does not affect the evolution of the ensembles, determined by the kernel in (4). Thus all $\langle A \rangle_i(t)$ appear explicitly linear on the impulse field.

Furthermore, due to this linearity, the response to a general signal can be obtained from the impulse response. The proof is given in the Appendix.

The following physical model can be assigned to the impulse response phenomena.

- The impulse at $t = 0$ creates instantaneously an initial condition G_i , corresponding to two carrier ensembles P and M , initially distributed according to G_i^+ and G_i^- .
- The ensembles are of equal number of particles N , which can be chosen arbitrarily.
- The particles evolve under the action of the stationary field \mathbf{E}_s , Eq. (2).
- The response of a physical quantity A is given by the difference of the two ensembles mean values of A .

$$\langle A \rangle_i(t) = \langle A \rangle_P(t) - \langle A \rangle_M(t)$$

- At large times the ensembles relax to a common steady state corresponding to \mathbf{E}_s and hence:

$$\langle A \rangle_i(t) \rightarrow 0 \quad \text{when} \quad t \rightarrow \infty$$

Actually the relaxation process continues for some characteristic time T , which depends on the physical conditions and the semiconductor and has typical values from a few picoseconds to hundred picoseconds as discussed in Sect. 4.

3. The Monte-Carlo Method

The Monte-Carlo method consists of algorithms providing in a different way the initial condition G . For a general direction of \mathbf{E}_1 one possibility is to approximate the gradient of f_s by a finite difference quotient. The wave vector increment has to be taken colinear to \mathbf{E}_1 . Then the task is to apply algorithms, simulating f_s . If the Ensemble Monte-Carlo is used, the algorithm of Price [1] is particularly obtained. Alternatively, one can sample f_s by a single-particle trajectory. In the important case of colinear DC and perturbation vectors, the steady-state Boltzmann equation is used to obtain:

$$G(\mathbf{k}) = \frac{E_1}{E_s} \left(\lambda(\mathbf{k}) f_s(\mathbf{k}) - \int f_s(\mathbf{k}') S(\mathbf{k}', \mathbf{k}) d\mathbf{k}' \right)$$

This leads to a natural splitting into G^+ and G^- terms. Two algorithms using different factors of the

G terms as probability densities are discussed in what follows. In general, G^+ and G^- are sampled over a main steady state trajectory. N evolution trajectories are started from G^+ , and the same number of trajectories are started from G^- . The chosen probability densities which generate the initial trajectory points, are enclosed below in curly brackets. We note that it is possible to merge the main and the evolution trajectories and to collect the whole information over one trajectory.

Algorithm 1. We use the equalities:

$$G_i^+(\mathbf{k}_0) = \frac{E_1}{E_s} \lambda(\mathbf{k}_0) \{f_s(\mathbf{k}_0)\}$$

$$G_i^-(\mathbf{k}') = \frac{E_1}{E_s} \int \{f_s(\mathbf{k}_0)\} \left\{ \frac{S(\mathbf{k}_0, \mathbf{k}')}{\lambda(\mathbf{k}_0)} \right\} \lambda(\mathbf{k}_0) d\mathbf{k}_0$$

Both terms contain f_s which can be sampled by the standard stationary algorithm, based on a single-particle trajectory simulation. In addition, G_i^- has an extra term in curly brackets, which is the conditional probability density for an after-scattering state \mathbf{k}' provided that \mathbf{k}_0 has been selected. To ensure the normalization to unity, S has been divided by the out-scattering rate λ . In order to conserve the integral value, the integrand has been multiplied by the same λ . Thus the latter must be accounted as a weight factor of the particular M trajectory. The above expressions suggest the following algorithm:

- 1) Choose \mathbf{k}_0 with density f_s , by sampling the main trajectory at constant time steps.
- 2) Realize a scattering event from \mathbf{k}_0 to \mathbf{k}' .
 - a) Start a trajectory from \mathbf{k}_0 and give it the weight $w^+ = \lambda(\mathbf{k}_0)$.
 - b) Start a trajectory from \mathbf{k}' and give it the negative weight $w^- = -w^+$.
- 3) Follow each trajectory in an interval $[0, T]$ and estimate the value of A at desired times t_i (e.g. a constant time step can be used) Add $w^+ A(\mathbf{K}^+(t_i))$ and $w^- A(\mathbf{K}^-(t_i))$ to a histogram ν_i .
- 4) Continue from step 1) by choosing the next value until N successive \mathbf{k}_0 points are selected. At the end calculate

$$\langle A \rangle_i(t_i) = \frac{E_1}{E_s N} \nu_i$$

Algorithm 2. We use the equalities:

$$G_i^+(\mathbf{k}_0) = \frac{E_1}{E_s} \langle \lambda \rangle_s \left\{ \frac{\lambda(\mathbf{k}_0) f_s(\mathbf{k}_0)}{\langle \lambda \rangle_s} \right\}$$

$$G_i^-(\mathbf{k}') = \frac{E_1}{E_s} \langle \lambda \rangle_s \int \left\{ \frac{\lambda(\mathbf{k}_0) f_s(\mathbf{k}_0)}{\langle \lambda \rangle_s} \right\} \left\{ \frac{S(\mathbf{k}_0, \mathbf{k}')}{\lambda(\mathbf{k}_0)} \right\} d\mathbf{k}_0$$

where $\langle \lambda \rangle_s = \int f_s(\mathbf{k}) \lambda(\mathbf{k}) d\mathbf{k}$ appears in the denominators to provide the normalization, and factors the

numerators to conserve the values of G_i^\pm unchanged. $\langle \lambda \rangle_s$ is the inverse of the mean free flight time, [7] as it follows from the 'before-scattering' method. The probability density $\lambda f_s / \langle \lambda \rangle_s$ generates \mathbf{k}_0 according the before-scattering states distribution. Over a single trajectory with this density are distributed the successive (with respect to a constant step l , $l = 1, 2, \dots$ in their occurrence) states just before the next scattering event. The second probability term in G_i^- is interpreted as in the previous algorithm.

The main steps are:

- 1) Choose \mathbf{k}_0 with density $\lambda f_s / \langle \lambda \rangle_s$, by selecting the before-scattering states with a chosen step l .
- 2) Realize a scattering event from \mathbf{k}_0 to \mathbf{k}' .
 - a) Start a trajectory from \mathbf{k}_0 and give it the weight $w^+ = 1$.
 - b) Start a trajectory from \mathbf{k}' and give it the negative weight $w^- = -w^+$.
- 3) Follow each trajectory in an interval $[0, T]$ and estimate the value of A at desired times t_i (e.g. a constant time step can be used) Add $w^+ A(\mathbf{K}^+(t_i))$ and $w^- A(\mathbf{K}^-(t_i))$ to a histogram ν_i .
- 4) Continue from step 1) by choosing the next \mathbf{k}_0 value until N points are selected. At the end calculate

$$\langle A \rangle_i(t_i) = \frac{E_1 \langle \lambda \rangle_s}{E_s N} \nu_i$$

The mean free flight time must be additionally calculated during the simulation.

The value of T must be large enough to allow the response of the quantity A to relax to zero.

4. Results

The simulation results have been obtained by utilizing the second algorithm, since the used Monte Carlo platform is based on the before-scattering method. First, typical conditions for silicon electrons have been considered. Second, a special carrier dynamics feature, the Transit Time Resonance (TTR) effect [7], [8] has been explored for *GaAs* electrons. The effect can be explained in the framework of the physical model.

For silicon electrons the common model [9] with spherical non-parabolic X valleys has been adopted. The DC field is taken along $\langle 100 \rangle$ direction and the temperature is 300 K.

Figure 1 and Fig. 2 show the time response of the differential energy $\partial \langle \epsilon \rangle_i / \partial E_1$ and the differential velocity $\partial \langle v \rangle_i / \partial E_1$ along the electric field for different field values. As predicted by the model, the response characteristics tend to zero when the two ensembles approach the steady state. The relaxation behavior depends on the steady-state field, and for a given field on the concrete physical characteristics. Generally, above a few

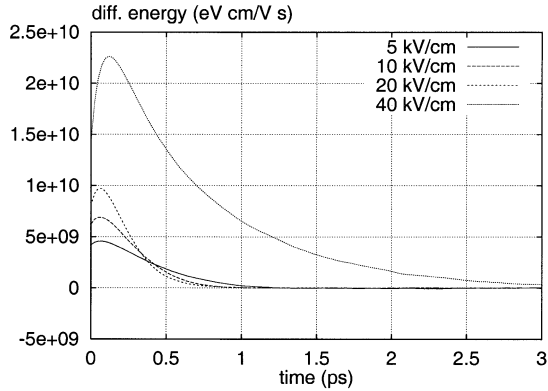


Fig. 1 Impulse response of the differential energy.

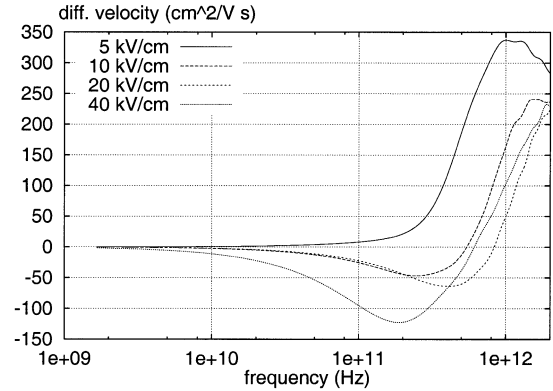


Fig. 4 Imaginary part of the differential velocity spectra.

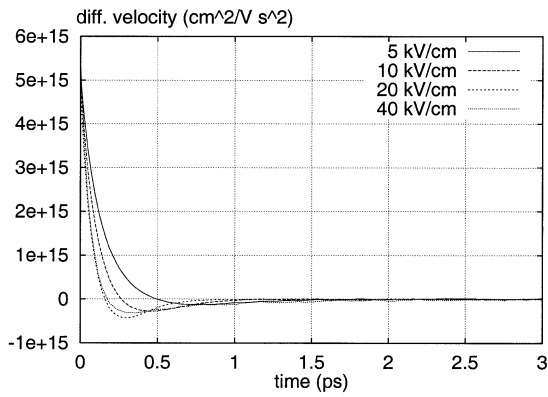


Fig. 2 Impulse response of the differential velocity.

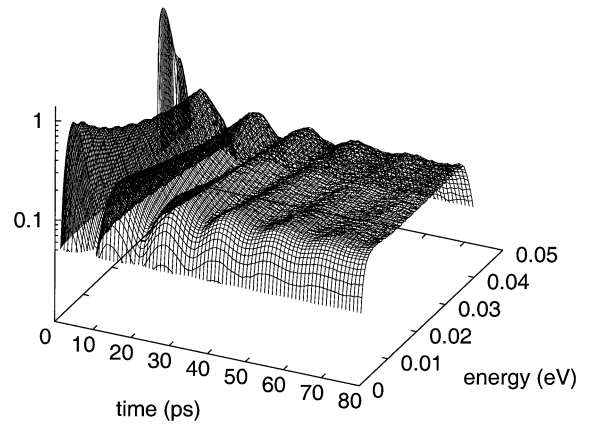


Fig. 5 Evolution of the P ensemble distribution function.

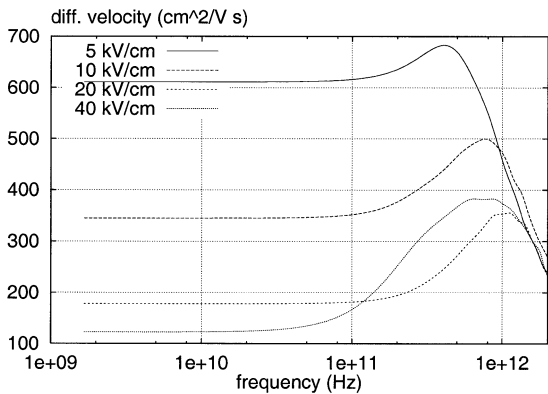


Fig. 3 Real part of the differential velocity spectra.

picoseconds the steady state is reached by the two ensembles.

Figure 3 and Fig. 4 show the spectral dependence of the differential velocity obtained by a Fourier transform of the data shown in Fig. 2. The low frequency limits of the imaginary parts tend to zero, while the real parts tend to the corresponding differential mobility values $\partial\langle v \rangle_s / \partial E_s$.

The *GaAs* electrons are considered at a temperature of 10 K and a steady-state field $E_s = 120$ V/cm.

The physical conditions determine a peculiar behavior of the individual electrons already in the steady-state. All electrons are in the central spherical Γ valley. Since acoustical phonon scattering is low (below one scattering for 100 ps), the electrons are drifted by the field until reaching energies above the energy of the polar optical phonon (0.036 eV). The latter is characterized by a high scattering rate, so that the electrons, penetrating the phonon threshold are intensively scattered back around the zero energy. The carriers mutually repeat the motion cycle of acceleration by the DC field and a subsequent optical phonon emission.

This individual behavior does not change after the impulse is applied, since the physical conditions remain the same. The impulse instantaneously creates at time zero the P and M ensembles. Figure 5 and Fig. 6 show the evolution of the two ensembles. The initial distributions G_i^- and G_i^+ appear as two peaks, placed near the energy bottom and slightly above the phonon threshold respectively. The M ensemble is accelerated by the field towards the phonon threshold. The P ensemble is transferred for less than two picoseconds near the energy bottom and is then accelerated by the electric field. During the evolution, the P ensemble is followed by the M ensemble with some delay. Both ensembles oscillate

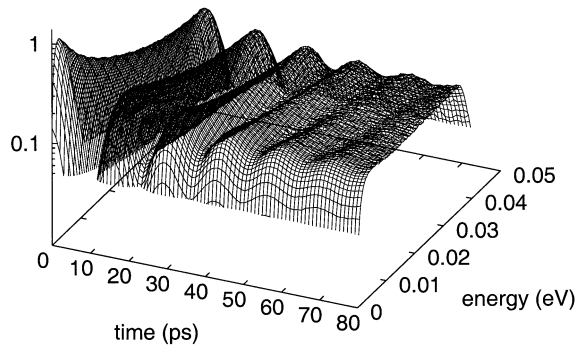


Fig. 6 Evolution of the M ensemble distribution function.

in the energy domain, giving rise to oscillations in the response characteristics $\langle A \rangle_i(t)$. The process continues for above 80 ps, when the initial peaks broaden towards the steady state.

It must be noted that the individual electron behavior is a necessary, but not a sufficient condition for TTR. The latter is also an ensemble dependent phenomenon. Indeed assume that the P and M distributions are equivalent at given time. Then all response characteristics become zero, despite that the two ensembles will oscillate for later times.

Acknowledgments

This work has been supported by the FWF project P13333-TEC, Austria.

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Appendix

For completeness we show that f_1 corresponding to a general time dependent signal is provided by f_i . Without loss of generality we regard time dependent fields $\mathbf{E}_1(t) = \mathbf{E}_1\phi(t)$, whose orientation is determined by \mathbf{E}_1 . The function ϕ is assumed bounded by unity: $|\phi(t)| \leq 1$, so that the small signal conditions are ensured by the magnitude of \mathbf{E}_1 . A generalization for fields with varying in time orientation is obtained by regarding the cases of \mathbf{E}_1 oriented along the three coordinate axes.

We consider the response at time t , caused by an impulse at time t_i . Then the function f_i depends on the time difference $t - t_i$: $f_i(\mathbf{k}, t - t_i)$ and (3) becomes:

$$\begin{aligned}
 f_i(\mathbf{k}, t - t_i) &= \int_{t_i}^t dt' \int d\mathbf{k}' f_i(\mathbf{k}', t' - t_i) \\
 &\quad \cdot S(\mathbf{k}', \mathbf{K}(t')) e^{-\int_{t'}^t \lambda(\mathbf{K}(y)) dy} \\
 &\quad + G_i(\mathbf{K}(t_i)) e^{-\int_{t_i}^t \lambda(\mathbf{K}(y)) dy}
 \end{aligned} \tag{5}$$

We multiply the equation by $\phi(t_i)$, integrate over t_i in the interval $(0, t)$, and introduce the function

$$f_1(\mathbf{k}, t) = \int_0^t dt_i \phi(t_i) f_i(\mathbf{k}, t - t_i) \tag{6}$$

Further a step function $\theta(t' - t_i)$ is used to set the lower bound of the t' integral to 0. This allows to exchange the order of the time integrals to obtain:

$$\begin{aligned}
 f_1(\mathbf{k}, t) &= \int_0^t dt' \int d\mathbf{k}' \left(\int_0^{t'} dt_i \phi(t_i) f_i(\mathbf{k}', t' - t_i) \theta(t' - t_i) \right) \\
 &\quad \cdot S(\mathbf{k}', \mathbf{K}(t')) e^{-\int_{t'}^t \lambda(\mathbf{K}(y)) dy} \\
 &\quad + \int_0^t dt_i \left(-\frac{e}{\hbar} \mathbf{E}_1(t_i) \cdot \nabla_{\mathbf{k}} f_s(\mathbf{K}(t_i)) e^{-\int_{t_i}^t \lambda(\mathbf{K}(y)) dy} \right)
 \end{aligned} \tag{7}$$

The integral in the brackets is $f_1(\mathbf{k}', t')$, as it can be seen from (6). By substituting (2) into (7) and taking the derivative on t we can recover (1).

It follows that if f_i is known, the solution f_1 can be found by evaluating the convolution integral (6).



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