Transient model for terminal current noise

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The condition of a stationary transport process is a common origin for the approaches for terminal
current noise. Based on a recently-proposed stationary model and the integral form of the
Boltzmann equation, we derive a transient stochastic process whose autocovariance function
characterizes the terminal current noise. The properties and the domain of application of this
transient model and its stationary counterpart are investigated. Numerical experiments are presented
which support the conclusions drawn for the two models. © 2002 American Institute of Physics.
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The current fluctuations in semiconductor devices are entirely characterized by the autocovariance function \( C_i \) of the
current signal \( i(t) \). For a general time dependence \( C_i \) is
defined as:

\[
C_i(t, \tau) = \langle (i(t))^2 \rangle - \langle i(t) \rangle \langle i(t+\tau) \rangle,
\]

where the brackets denote ensemble averages. For a stationary
process the mean value of the current \( \langle i(t) \rangle \) is constant and the
autocovariance does not depend on time \( t \). Furthermore, the ergodicity of the transport process allows to replace the
ensemble average by a time average:

\[
C_i(\tau) = \frac{1}{T} \int_0^T i(t) i(t+\tau) dt - \langle i(t) \rangle^2.
\]

The physical and numerical complexity of transport in modern
devices stimulates a mutual development of basic models and appearance of novel models for the evaluation of the
autocovariance function. Fundamental is the ensemble Monte Carlo (EMC) method which provides both a model and a
numerical approach to the phenomena. The method is based on the notion that a direct emulation of the stochastic
processes underlying the transport phenomena provides along with the physical mean also values their fluctuations. If the
transport process is emulated and the current \( i(t) \) is recorded in the averaging interval \((0,T)\), the autocovariance function
is retrieved from the second equality in Eq. (2). The stationary current is ensured by the physical boundary
conditions (BC). The carriers are injected into the device contacts according to the carrier distribution in the leads. The
carrier number inside the device is kept constant by re-injection of the leaving carriers. It has been recognized that this
physically transparent boundary conditions require thermal equilibrium between the leads and the contacts. When this is
not fulfilled as it is, e.g., in the case of resistors, the EMC model is evolved to a complicated algorithm.2

Recently an alternative model for the current noise has been proposed3,4 in the framework of the stationary definition
given by the first equality in Eq. (2). The autocovariance function has been obtained as a statistical average:

\[
C_i(\tau) = \langle i(t) \rangle \int d\mathbf{k} \int_L d\xi(\mathbf{k},x) g(\mathbf{k},x,\tau) \langle i(t+\tau) \rangle - \langle i(t) \rangle^2;
\]

\[
\langle i(t) \rangle = \int d\mathbf{k} \int_L d\xi(\mathbf{k},x) f_s(\mathbf{k},x).
\]

The space coordinate \( x \) is for a one-dimensional device with a
length \( L \) and \( \mathbf{k} \) denotes the wave vector. Here \( i(\mathbf{k},x) \) is the
current contribution from a particle in the particular phase space point according to the Ramo–Shockley theorem. \( g \) is
an effective distribution function, i.e., the solution of the time dependent Boltzmann equation for an initial condition:

\[
g_0(\mathbf{k},x) = i(\mathbf{k},x)f_s(\mathbf{k},x)/\langle i(t) \rangle,
\]

where \( f_s \) is the stationary solution of the equation. In Ref. 4 the model has been applied to a bulk semiconductor using a
deterministic method. To apply the model (3) for devices, it is convenient to use a stochastic method for solving the
Boltzmann equation. We note that a Monte Carlo (MC) approach in this case simulates an evolution of the effective
distribution function in contrast to the direct emulation of the current fluctuations by the EMC.

The boundary conditions for Eq. (3) are deduced from the limit \( C_i \rightarrow 0 \) when \( \tau \rightarrow \infty \). The effective distribution \( g \) must evolve from \( g_0 \) to \( f_s \) in this limit. The stationary solution \( f_s \) of the Boltzmann equation is ensured by the boundary
conditions imposed. Hence, the same physical boundary conditions utilized by the EMC method must be applied. This
brings the same requirements for equilibrium between leads and contacts also for the alternative model Eq. (3).

We propose the following transformation of Eq. (3). \( C_i \) contains as an integrand the difference \( \phi(\mathbf{k},x,\tau) = g(\mathbf{k},x,\tau) - f_s(\mathbf{k},x) \). Both, \( g \) and \( f_s \) satisfy the Boltzmann equation which has the following integral form:

\[
f(\mathbf{k},x,\tau) = \int_0^\tau dt' \int d\mathbf{k}' f(\mathbf{k}',x,t') \delta(\mathbf{k}' - \mathbf{k})
\times e^{-\int_0^\tau dt'' \phi(\mathbf{k}(t'') \mathbf{k}(t''))} + f_0(\mathbf{k}(0),x(0)) e^{-\int_0^\tau dt'' \phi(\mathbf{k}(t''))}

+ f_b(\mathbf{k}(t_f),x(t_f)) e^{-\int_{t_f}^\tau dt'' \phi(\mathbf{k}(t''))}
\]

with a trajectory determined by the electric force \( F \) and velocity \( v \).

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\[ k(t') = k - \int_{t'}^{x(t')} F(x(y)) dy \]
\[ x(t') = x - \int_{t'}^{x(t')} v_x[k(y)] dy. \]

(6)

The initial condition \( f_0 \) and the boundary conditions \( f_b \) participate explicitly in the integral form [Eq. (6)]. \( f_b \) is zero inside the device and is specified only on the boundaries, while \( f_0 \) is zero if \( x(0) \) is placed outside the device. The time \( t_b \) is determined from the position where the Newton trajectory (6) crosses the device boundary \( x(t_b) = x_b \). \( f_s \) is a solution of Eq. (6) for the initial condition given by \( f_0 = f_s \), while for the function \( g \) the initial condition is given by \( f_0 = g_0 \). Both \( f_s \) and \( g \) utilize the same boundary conditions given by the term \( f_b \). It follows that the equation for \( \phi \) does not contain \( f_b \):

\[ \phi(k, x, \tau) = \int_0^\tau dt' \int L dki' \phi[k', x(t'), t'] \delta[k', k(t')]
\]
\[ \times e^{-\int_{t'}^{x(t')} dv_x[k(y)] + g_0[k(0), x(0)]}
\]
\[ \times e^{-\int_{0}^{x(0)} dv_x[k(y)] - f_s[k(0), x(0)]}
\]
\[ \times e^{-\int_{0}^{x(0)} dv_x[k(y)]}. \]

This equation describes a purely transient problem, where two ensembles with initial conditions \( g_0 \) and \( f_s \) evolve in time as \( \phi_0(k, x, \tau) \) and \( \phi_s(k, x, \tau) \) and give the solution as the difference \( \phi = \phi_0 - \phi_s \). The boundaries absorb all particles that leave the device without reinsertion. The autocovariance Eq. (3) becomes:

\[ C_s(\tau) = \langle i \rangle \int L dki \int L dx_i(k, x) [\phi_0(k, x, \tau) - \phi_s(k, x, \tau)]
\]
\[ = \int L dki \int L dx_i(k, x) i[k(0), x(0)] \phi_s(k, x, \tau)
\]
\[ - \langle i \rangle (\tau) \langle i \rangle (0). \]

(7)

The last equality does not follow in a trivial way from the equality on the previous line. For the derivation we have used Eq. (4) and the Neumann expansion of the Boltzmann equation, written for the function \( \phi_0 \). The brackets define the ensemble average

\[ \langle i(\tau) \rangle = \int L dki \int L dx_i(k, x) \phi_s(k, x, \tau) \]
\[ = \langle i \rangle (0) = \langle i \rangle, \]

where Eq. (7) resembles the definition (1) of the autocovariance function of a transient process of initial time \( t = 0 \). It is obtained that the autocovariance function Eq. (3) of the terminal current fluctuations is the same as the autocovariance function of the following transient process. An ensemble of particles which is initially (at time zero) distributed according to the stationary distribution \( f_s \) in the device evolves with time. The particles follow the natural evolution of the semiconductor carriers and give instant contribution \( i(k, x) \) to the current according to the Ramo–Shockley theorem. The contribution of a particle absorbed by the boundaries vanishes since there is no reinsertion. The current fluctuations are described by the ensemble averages in Eq. (7). Currently, the mean current \( \langle i \rangle (\tau) \) is time dependent in contrast to the stationary case, since particles leaving the device are not reinserted. The role of the boundary conditions is to ensure the stationary solution \( f_s \) in the device. They are switched off in the subsequent evolution of the ensemble and thus do not influence the autocovariance function. In this way the physical conditions in leads and contacts become insignificant for the applicability of Eq. (7). We conclude that the transient model obtained is more universal as compared to its stationary counterpart (3). In the following, the two models are distinguished by the corresponding absorbing or injecting boundary conditions.

A MC approach has been developed for the two models.\(^5\)

The purpose is to check the consistency of the models and to investigate the case when the thermal equilibrium between the leads and the device contacts is violated. The stochastic approach consists of alternative MC algorithms which account for the initial condition, simulate the evolution process, and obey the boundary conditions. The main feature is that a one-particle MC simulation is used to obtain the stationary distribution \( f_s \) inside the device. The latter gives rise
to initial points of an ensemble of particles, whose evolution provides the current autocovariance function.

In the numerical experiments we consider an $n^+nn^+$ diode under bias conditions required by Eq. (3) and a resistor. The silicon diode has a length of each segment of 0.2 μm and doping concentration $10^{17}:10^{16}$ cm$^{-3}$, the resistor $n$ is with the same total length 0.6 μm. The autocovariance functions obtained are normalized as $C_i(\tau)/C_i(0)$ and plotted up to 4 ps evolution time for a better resolution. We note that the decay time for such structures is one order of magnitude higher.\(^6\)

In Fig. 1 the curves for the absorbing and the injecting boundary conditions obtained for 0 and 1 V overlap each other as predicted by the theory. However, this is not true for the resistor considered in Fig. 2. At equilibrium the results of the two models still coincide. At 0.25 V there is already a difference in the corresponding curves. We assign this to the influence of the leads on the autocovariance function during the process of re-injection: the hot fraction of the leaving carriers are injected back thermalized. This is supported by the increase of the effect with the increase of the voltage. At 1 V, Fig. 3, the curve for the absorbing BC relaxes to zero, while the curve for the injecting BC remains well above zero. Additional experiments show a decrease of the effect when the length of the structure increases under a constant electric field inside. In this case the portion of the leaving carriers decreases with respect to the total number of particles in the resistor. Another experiment is shown in Fig. 4. The simulated structure is formed by two tiny highly doped 0.05 μm regions attached on both sides of the resistor which cool the exiting carries. The curves corresponding to the two models overlap again.

We conclude that the stationary model can be applied if the contact regions thermalize the carriers before they leave the device. Otherwise an extra correlation between leads and device contacts is introduced by the model. The absorbing BC model is universal and physically more transparent since it refers to the dwelling time of the particles in the device.

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