

# Coupled maximum entropy: Monte Carlo Estimation of microwave, millimeter-wave and submillimeter-wave spectrum of velocity fluctuations in GaAs

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The maximum entropy method is presented in this letter as a highly interesting procedure for the investigation of high frequency noise properties of bulk semiconductors and electron devices at microscopic level. A Monte Carlo simulation of the hot electron velocity fluctuations in bulk GaAs has been performed to illustrate the efficiency and usefulness of this procedure. Comparisons with the most popular techniques presently used in Monte Carlo simulations of noise have also been performed. © 1998 American Institute of Physics. [S0003-6951(98)04702-0]

Monte Carlo techniques have largely demonstrated their unique usefulness in providing a valuable insight into the physical origin of high frequency noise in semiconductors and devices.<sup>1–6</sup> However, the convergence of electron velocity fluctuation demands for a significant amount of computing time, and this fact has forced the need for using powerful machines specialized in intensive computing tasks such as workstations and parallel-processing computers. This need becomes obviously crucial when the noise of a device is simulated, since the use of self-consistent procedures to obtain the position-dependent electron distributions together with temperature considerably increases the computing time.<sup>7</sup>

The most popular procedures presently used for the calculation of the spectral density of high frequency noise in stationary processes are based on the Wiener–Khinchine theorem. We have not found any Monte Carlo simulation of high frequency noise that makes use of the maximum entropy method (MEM) in previous works, although this technique is well known and widely used in other branches of Physics.<sup>8</sup> The purpose of this letter is to present the results of our investigations on the potential capabilities of MEM in the calculation of noise at the microscopic level. Although we will focus our attention on the simulation of bulk GaAs, the main ideas presented here may also be helpful in the investigation of other materials as well as electron devices.

The noise properties of bulk semiconductors at high frequencies may be characterized in terms of the spectral density  $S_v$  of velocity fluctuations. In stationary processes, the Wiener–Khinchine (WK) theorem provides the most usual way to calculate  $S_v$ :

$$\begin{aligned} S_v(f) &= 2 \int_{-\infty}^{\infty} C(t) \exp(-j\omega t) dt \\ &= 4 \int_0^{\infty} C(t) \cos(\omega t) dt, \end{aligned} \quad (1)$$

where  $C(t)$  is the autocorrelation function of velocity fluctuations given by

$$C(t) = \overline{\delta v(t') \delta v(t+t')}. \quad (2)$$

The spectral density of velocity fluctuations gives a full characterization of the noise properties of a homogeneous material in which the fluctuation of the number of carriers may be neglected. This is the case investigated here, which is applicable to a unipolar semiconductor in which mechanisms such as generation–recombination, traps, and defects are not significant. Neglect of the fluctuations in the number of carriers is also valid when the frequencies under investigation are much higher than the inverse of the time constants associated with these mechanisms.

It is generally accepted that windowing or tapering techniques are necessary in the estimation of the spectrum. These techniques are based on the attenuation of the amplitude of the autocorrelation tail with different functions in order to smooth the time domain truncation. This truncation leads to inaccuracies of the spectrum at the lowest frequencies that are difficult to estimate. The MEM offers an interesting alternative to these procedures.<sup>9</sup> A temporal sequence of a generic variable  $x(t)$  contains information that has an associated entropy  $H$  given by its power spectral density  $S_x(f)$ ,

$$H = \frac{1}{4W} \int_{-W}^W \ln[S_x(f)] df, \quad (3)$$

where  $W$  is the highest frequency at which  $S_x$  has a non-negligible value. In a stationary process, the Wiener–Khinchine theorem provides an additional constraint that must be taken into account when imposing the condition of maximum entropy. This constraint leads to an autoregressive spectrum,<sup>10</sup> i.e.,

$$S_x(f) = \frac{G}{|1 + \sum_{i=1}^M b_i \exp(j\omega i \Delta t)|^2}, \quad (4)$$

where  $M$ , the series number of poles, is a finite integer, and  $\Delta t$  is the rate at which the variable was sampled.  $G$ , the gain factor, and  $b_i$ , the prediction coefficients, may be obtained from a set of equations. The stability of the solution to this set is the main difficulty that must be addressed. We have found that the algorithm proposed by Haykin,<sup>10</sup> which is based on the recursive method of Levinson, provides a good

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TABLE I. Sampling parameters.

	Subintervals ( $N'$ )	Sampling rate ( $\Delta t$ )	Subinterval length ( $N$ )	Resolution ( $\Delta f$ )
WK	500–3000	2 fs	8192	10 GHz
MEM	40	5 fs	60 000	10 GHz

compromise between stability and efficiency. A simple implementation of this algorithm was found in Ref. 11.

A number of practical noise spectra have a Lorentzian shape. In these cases, a very important feature of MEM estimators is the fact that they are able to give an excellent estimation of the spectrum with a very few number of poles. In fact, just the first order series may provide a spectrum which is very close to a Lorentzian in a fairly wide frequency band,

$$S_v(f)|_{M=1} = \frac{G}{|1 + b_1 \exp(j\omega\Delta t)|^2}, \quad (5)$$

$$\omega\Delta t \ll 1 \Rightarrow S_v(f) \approx \frac{G}{(1 + b_1)^2 + (b_1\omega\Delta t)^2}.$$

In typical Monte Carlo simulations, the product  $\omega\Delta t$  is below 0.01 at frequencies up to several hundred GHz. Thanks to this important feature it is possible to achieve a degree of convergence in Lorentzian spectra that would not be obtained with other spectral estimators.

In order to compare the MEM estimator with the conventional procedure based on the Wiener–Khinchine theorem, we have selected a well known example of hot electrons in low doped GaAs. A simple monoparticle Monte Carlo simulator has been developed which includes the following scattering mechanisms:<sup>12</sup> (1) impurity scattering in the Conwell–Weisskopf formalism; (2) polar optical phonon scattering with the Frölich Hamiltonian; (3) acoustic phonon scattering; and (4) piezoelectric interaction.

Alternative impurity scattering models based on the screened Brooks–Herring potential with different refinements have been thoroughly investigated, but we have chosen the Conwell–Weisskopf model since it is more efficient and has recently demonstrated an excellent accuracy even in heavily doped material.<sup>13</sup> The electric field has been selected low enough to enable the neglect of intervalley scattering. Nonparabolicity has been considered in all the mechanisms. The simulation has been performed at 300 K and with an electric field of 0.5 kV/cm. The ionized impurity concentration is  $10^{15} \text{ cm}^{-3}$ .

The spectral density of velocity fluctuations has been obtained by using two different procedures. In the first one, the spectrum was calculated by direct integration of the autocorrelation function. The total time during which the particle is simulated is divided into subintervals. Then, the autocorrelation function is calculated at each subinterval with a double discrete fast Fourier transform. An attenuation that follows a Hann function is applied to each autocorrelation function tail, starting at 1 ps. Finally, all the autocorrelations are averaged, and the spectrum of velocity fluctuations is obtained by direct integration of the mean autocorrelation function.

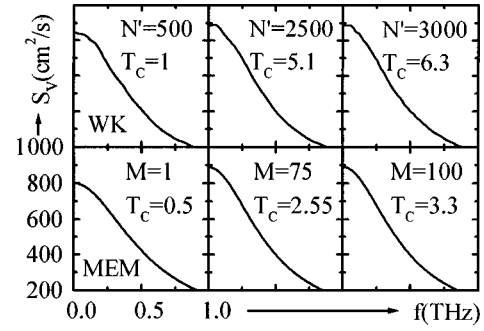


FIG. 1. Convergence of the spectral estimators.  $T_c$ : total simulation time in minutes.

The second procedure was implemented in a similar way. The total time during which the particle is simulated is also divided into subintervals, and the prediction coefficients and the gain factor are obtained at each subinterval. At the end of the simulation both prediction coefficients and gain factor are averaged, and the autoregressive spectrum is calculated at the same frequency resolution as the one used in the first procedure.

The simulations were performed on a personal computer with a 200 MHz microprocessor. The choice of the sampling parameters was made in both procedures by making different estimations with orders of magnitude typical of Monte Carlo simulations encountered in other references.<sup>14–16</sup> The parameters that gave us the best compromise between accuracy and efficiency for each case are shown in Table I. For the WK simulation, an increase of  $N$  or  $\Delta t$  reduces the efficiency of the window, making the spectrum noisier. In the case of the MEM estimation, a reduction of the sampling rate forces the use of higher values of the number of poles to achieve the same accuracy, thus reducing the efficiency. Figure 1 shows the convergence of the spectrum using both estimators and the resulting total simulation times. The calculated longitudinal diffusion coefficient is  $225 \text{ cm}^2/\text{s}$ , as is shown in Fig. 2. The spectrum is in good agreement with previous simulations,<sup>17</sup> but the WK simulation makes a slight underestimation of the diffusion coefficient due to the truncation of the autocorrelation tail. In addition, MEM also provides an analytical expression for the spectrum, which was not available with the conventional procedure.

If higher frequency resolutions were used, increased differences in the simulation times of the two spectral estimators would be obtained. Once the prediction coefficients are

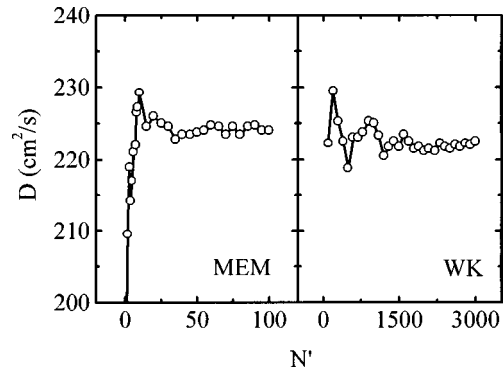


FIG. 2. Convergence of the diffusion coefficient, taken as  $S_{v0}/4$ .

known, the calculation of the autoregressive series is noticeably faster than the integration of the autocorrelation function. This integration may be substituted by a discrete fast Fourier transform if the desired frequency resolution is high enough, and if one accepts the constraints imposed by the fast Fourier transform algorithm to the frequencies at which the spectrum is calculated. This may improve the efficiency of the WK estimator. However, the main difference in terms of computing time is found in the higher amount of scattering events that are simulated in the first estimator. The computing times of the WK estimation demonstrate this fact: they are almost exactly proportional to  $N'$ .

In addition, the availability of two different spectral estimators may be useful to test the accuracy of a given spectrum. When windowing techniques are used it is difficult to know to what extent the low frequency part of the spectrum has been altered. In this sense, a comparison of two spectra that have been obtained by two rather different procedures makes the estimations more accurate.

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