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## Approach to study the noise properties in nanoscale electronic devices

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An approach to study the noise characteristics in mesoscopic devices is presented. It extends, via quantum trajectories, the classical particle Monte Carlo techniques to devices where quantum nonlocal effects are important. As a numerical example, the fluctuations of the electron current through single-tunnel barriers are compared with the standard Landauer–Buttiker results, showing an excellent agreement. © 2001 American Institute of Physics. [DOI: 10.1063/1.1402651]

The generation of electronic devices in the nanometer scale [such as metal–oxide–semiconductor (MOS) transistors with channel lengths as small as 10 nm] is now being actively studied, both, theoretically and experimentally.<sup>1</sup> The electrical characteristics of these devices are determined by an interesting interplay between quantum-mechanical (QM) and classical theories. In particular, the study of current fluctuations due to the discreteness of the electron charge has become a very active field of research where quantum and classical knowledge merge together. In mesoscopic devices where phase coherence is preserved, the Landauer–Buttiker scattering approach provides a transparent description of electron transport, both for the average current values,  $\langle I \rangle$ , due to Landauer<sup>2</sup> and for the spectral power of current fluctuations,  $S_I(\omega)$ , mainly due to Buttiker:<sup>3</sup>

$$S_I(\omega=0) = \frac{q^2}{\pi\hbar} \int_0^\infty \{T(E)\{f_L(1-f_R) + f_R(1-f_L)\} - T(E)^2(f_L - f_R)^2\} dE, \quad (1)$$

where  $q$  is the absolute value of the electron charge,  $T(E)$  is the transmission coefficient as a function of the total electron energy  $E$  and  $f_{L/R}$  are the Fermi–Dirac occupation functions at the left (right) reservoir (for simplicity, a one-dimensional system is considered). On the other hand, when phase coherence does not play an essential role, a classical particle description has been used by several authors<sup>4–7</sup> to study fluctuations in mesoscopic systems. In this framework, the use of classical Monte Carlo (MC) simulations has been particularly useful because it has the additional advantage of including long-range Coulomb interaction between carriers by considering *self-consistent* potential profiles governed by the Poisson equation.

In this letter, we present an approach to study noise in mesoscopic devices based on quantum trajectories. Our work extends the previous classical MC technique to devices where QM phase-coherent effects (such as tunneling through a potential barrier) are of prime importance. In particular, we will use Bohm trajectories to describe the electron's paths. Bohm's formulation provides exactly the same average results as the standard QM theory and implicitly takes into account the discrete nature of electrons.<sup>8</sup> As a numerical ex-

ample, we study the fluctuations of the electron current through single-tunnel barriers.

Hereafter, we present a brief description of our formulation. In particular, we will discuss the computation of Bohm trajectories, the injection of carriers, and the algorithm used to compute spectral noise power. Full account of the derivations will be presented elsewhere. In order to compute Bohm trajectories, first the time evolution of a wave packet  $\Psi(x,t)$  (i.e., the solution of the time-dependent Schrödinger equation), must be known. Then, according to the Bohm approach,<sup>8</sup> the instantaneous velocity  $v(x,t)$  for an electron located at position  $x$  and time  $t$  is given by

$$v(x,t) = \frac{1}{q} \frac{J(x,t)}{|\Psi(x,t)|^2}, \quad (2)$$

where  $J(x,t)$  is the quantum-mechanical current density. The electron causal trajectory,  $x = x(x_0, t)$ , is determined by integrating Eq. (2) after fixing its initial position  $x_0$ . This initial position accounts for the unavoidable uncertainty in QM and is randomly selected according to the probability  $|\Psi(x_0, 0)|^2$ . An introduction of Bohm trajectories for MC simulators can be found in our previous works.<sup>9</sup> The main difference between a classical MC scheme and our proposal lies in the expression used to compute electron velocity: in the former, the velocity is proportional to the local electric field, while in our approach, the electron velocity takes into account the QM nonlocal effects via  $\Psi(x,t)$ .

When dealing with mesoscopic device simulations, the modeling of carrier injection from thermal reservoirs is a delicate problem. According to Levitov and co-workers,<sup>10</sup> under degenerate conditions one should use a binomial distribution. An injection model for MC particles using a binomial distribution has been developed by Gonzalez *et al.*<sup>5</sup> showing its accuracy to describe either nondegenerate or completely degenerate conditions in one-dimensional mesoscopic conductors. In our quantum MC simulator, we will use an injection scheme based on this model. The probability of injecting a wave packet with a positive central momentum  $k_c$  depends on the probability of being occupied in the left reservoir,  $f_L$ , and also on the probability that there is no wave packet with the same central momentum  $k_c$  at the right contact,  $1 - f_R$  (differently from Gonzalez's model that deals with point particles, we have considered a spatial size of the wave packet,  $\sigma_x$ , much longer than the sample length). Our algorithm to inject particles from the left contact with veloc-

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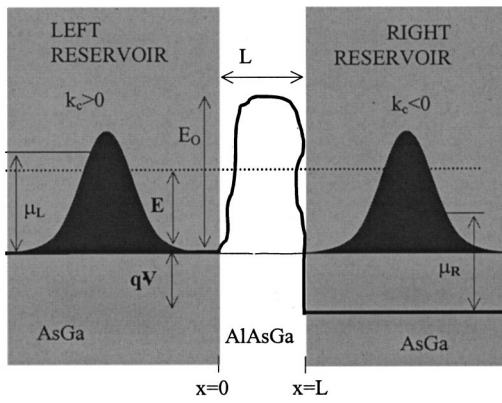


FIG. 1. Schematic potential profile considered in this work. Electrons are described by Bohm trajectories along the whole simulating box that includes the sample and the two reservoirs. A constant bias  $V$  is applied only along sample length  $L$ .

ity  $v_k$  is the following: at each time  $\xi_k$  (inversely proportional to  $v_k$ ) an attempt to introduce an electron takes place. Then, a random number  $r$  uniformly distributed between 0 and 1 is generated, and the attempt is considered successful only if  $r < f_L(1 - f_R)$ . Similar arguments are used to inject electrons from the right reservoir.

Since in our approach we deal with causal trajectories, noise properties can be computed from the classical techniques. In particular, according to the extension of the Ramo–Shockley theorem to semiconductor devices,<sup>11</sup> the total instantaneous current  $I(t)$  through each cross-sectional area of the device, consisting of conduction and displacement current, is computed by

$$I(t) = \frac{q}{L} \sum_{i=1}^{N(t)} v_i(x, t), \quad (3)$$

where  $L$  is the length of the device,  $N(t)$  is the total number of carriers which are instantaneously inside the device, and  $v_i(x, t)$  is the value of the Bohm velocity at time  $t$  and position  $x$ . Level  $i$  identifies each electron, and only those within  $0 < x < L$  are considered (see Fig. 1). The current, neglecting the initial transient, is recorded during the whole simulation time on a time grid of step size  $\Delta T$ . Then, by defining the time length in which the correlation function should be calculated as  $m\Delta T$ , with  $m$  an integer, the current correlation function,  $C_I(t)$ , is obtained from the algorithm<sup>12</sup>

$$C_I(j\Delta T) = \frac{1}{M-m} \sum_{i=1}^{M-m} I(i\Delta T)I[(i+j)\Delta T] - \left( \frac{1}{M} \sum_{i=1}^M I(i\Delta T) \right)^2, \quad (4)$$

where ergodicity is implicitly assumed, and  $j=0, 1, \dots, m$ ,  $M > m$ . The values in the present case are  $M=200\,000$  and  $m=256$ . The corresponding spectral density  $S_I(\omega)$  is determined by Fourier transforming the above correlation function.

At this point, we give two numerical examples of our proposal. We will consider ballistic electronic transport in a one-dimensional tunnel barrier that roughly corresponds, for example, to a scanning tunneling microscopy (STM) tip separated from a metallic surface. Our example, schemati-

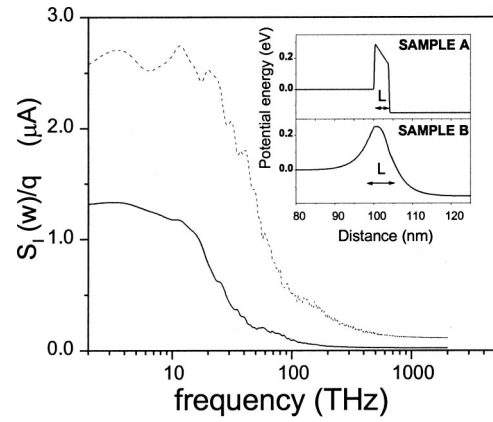


FIG. 2. One-side noise spectral power density  $S_I(\omega)$  for sample A (dashed line) and sample B (solid line) when  $V=0.15$  V and  $\mu_R=\mu_L=0.2$  eV. The insets represent the energy potential profiles associated with each sample.

cally described in Fig. 1, consists of two highly doped layers of AsGa separated by a potential barrier of  $\text{Al}_x\text{AsGa}_{1-x}$ . We assume that applied bias  $V$  falls only in the barrier region without voltage fluctuations. The two AsGa layers are considered large enough to be characterized as perfect reservoirs with the Fermi–Dirac distribution  $f_{L/R}$  at 300 K with the chemical potentials related by  $\mu_L=\mu_R+qV$ . We consider injection from both reservoirs, left and right, but from a unique energy. In this regard, we define two wave packets with the same central energy,  $E=0.15$  eV, but different initial central positions and opposite central wave vectors. At time  $t=0$ , the initial probability presence of each wave packet corresponds to a Gaussian wave packet with a spatial dispersion  $\sigma_x=130$  Å. The wave packet evolution is known by solving the Schrödinger equation along a simulating box of 2048 Å, which includes the sample and the two reservoirs. Every time that an electron is injected into the simulating box, its initial position is selected according to the initial probability presence.<sup>13</sup> In order to compare our numerical results with the Buttiker formalism, the potential profile is considered to be time independent without Poisson *self-consistency*. We will consider two samples: sample A of  $L=40$  Å, consisting of an abrupt rectangular barrier of  $E_0=0.3$  eV height; and a sample B of  $L=76$  Å, which includes a potential barrier described by  $E(x)=E_0 \text{sech}(ax)$  with  $E_0=0.3$  and  $a=0.065$  (see the insets in Fig. 2).

In Fig. 2, according to Eq. (4), the simulated values of spectral noise power, obtained from a total simulation time of 50 ps and  $\Delta T=0.25$  fs, are represented for the two samples with an applied bias of 0.15 V. For low-frequency, it takes a constant value and decreases down to a frequency related to the electron transit time across the sample. The cutoff frequency in sample B is lower than in sample A because electrons have a slower velocity. In Fig. 3, the zero-frequency noise power is computed as a function of the applied bias, and compared with the analytical results obtained from the Buttiker formalism. The analytical results are computed from Eq. (1) considering a monoenergetic system where  $T(E)$  is defined as the average transmission coefficient of the wave packets.<sup>13</sup> The comparison of the noise characteristics is carried out in terms of Fano factor  $F$ , defined by  $S_I(0)=F2q(I)$ . For low bias, the transmittance through the barrier is so low that  $F$  tends to diverge. On the

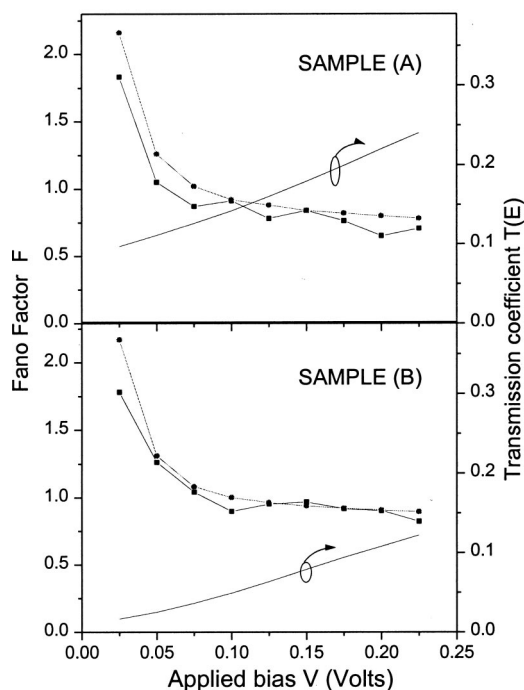


FIG. 3. Fano factor  $F$  as a function of the applied bias computed within our model (squares) and within the Büttiker formalism (circles) for samples A and B. The transmission coefficients are also depicted by the solid line.

other hand, for high voltages only the injection from the left reservoir must be considered, but since the transmission coefficient of the barrier is moderately high, shot noise following a binomial partition process appears. Hence, the expected Fano factor approximates  $F = 1 - f_L T(E)$ . From Fig. 3 we show that the Büttiker results can be perfectly reproduced within the Bohm approach. The Bohm trajectories are used, not only to compute quantum average results, but quantum fluctuations. Our approach provides additional information that cannot be easily accessible from classical or standard quantum formalisms [see the high-frequency features of  $S_I(\omega)$  due to the Bohm dynamics in Fig. 2].

In conclusion, we have developed a MC simulator for phase-coherent mesoscopic devices by means of Bohm trajectories to describe an electron's paths. Our approach is

based on two fundamental characteristics of Bohm's approach:<sup>8</sup> the average QM results (such as average current or transmission coefficient) are perfectly reproduced in terms of Bohm trajectories; and the discrete nature of electrons is explicitly considered in Bohm's formulation (allowing noise computation using classical techniques). In this regard, this work follows the path opened by Landauer,<sup>14</sup> who deduced Büttiker formalism within a simple wave packet framework. The main potentialities of our approach are related to its capability to include a Poisson solver to obtain self-consistent potential profiles and noise spectra at high frequencies. These conditions are not easily accounted for in present phase-coherent noise theories and drastically modify noise characteristics.<sup>4</sup> Future work will follow this direction.

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