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Self-consistent simulation of quantum shot noise in nanoscale electron devices

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An approach for studying shot noise in mesoscopic systems that explicitly includes the Coulomb interaction among electrons, by self-consistently solving the Poisson equation, is presented. As a test, current fluctuations on a standard resonant tunneling diode are simulated in agreement with previous predictions and experimental results. The present approach opens a new path for the simulation of nanoscale electron devices, where pure quantum mechanical and Coulomb blockade phenomena coexist. © *2004 American Institute of Physics*. [DOI: 10.1063/1.1806546]

The time-dependent fluctuations of the electron current in mesoscopic systems, i.e., the shot noise, are a direct consequence of the quantum mechanical (QM) wave-particle duality.[1] Following this idea, we have recently developed an approach[2,3] to study shot noise in QM systems showing that it can be *naturally* understood within the de Broglie–Bohm (dBB) interpretation of the quantum theory.[4,5] In particular, we have shown that our approach[2] provides identical predictions as the ones obtained within the second quantization framework[1,6] for simple mesoscopic systems. In recent years, shot noise approaches for phase-coherent devices, mainly based on the second quantization formalism, have been greatly developed in the literature.[1,6–8] In these approaches, the (nontrivial) electron–electron interaction has been only considered through the assumption of a linear relationship (i.e., a capacitance) between the charge and the voltage.[7,8] The goal of the present letter is to show that our previous approach[2,3] can be generalized to study Coulomb interaction among electrons by self-consistently solving the Poisson equation.

Now, let us explain how the dynamics of N interacting electrons in a mesoscopic system are described within the dBB formalism using a self-consistent solution of the Poisson equation. In principle, electrons are described by a general wave function, $\Psi(x_1,x_2,\ldots x_N,t)$, solution of the many particle time-dependent Schrödinger equation that explicitly contains the Coulomb interaction in its Hamiltonian. By construction, once the many-particle wave function is known, all QM observable can be perfectly reproduced within the dBB formalism.[5] However, the practical computation of such wave function is far from being trivial and some kind of approximation is mandatory. In this regard, first, we consider that the dynamics of each x_i electron can be described from t to $t+dt$ by assuming that the rest of the electrons remain at fixed positions. Thus, each i-electron is associated to a wave function, $\Psi_i(x_i,t)$, solution of a single-particle Schrödinger equation:[9]

$$i\hbar\frac{\partial\Psi_i(x_i,t)}{\partial t}=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2}+V(x_i)+\frac{1}{2}\sum_{\substack{k=1\\k\neq i}}^{N}\frac{1}{4\pi\varepsilon}\frac{q^2}{|x_i-x_k|}\right)\times\Psi_i(x_i,t), \tag{1}$$

where, ε is the dielectric constant, m is the electron effective mass, q is its charge, and $V(x_i)$ takes into account the external electric potential. Each wave function, $\Psi_i(x_i,t)$, does not depend explicitly on other electron positions, x_k, but (this is the crucial point) a correlation between the wave functions (i.e., between all electron dynamics) is contained in Eq. (1), because the last term of the potential energy depends on all electron positions. The dBB formalism has the technical advantage that the Schrödinger equations have to be solved only for the particular points where Bohm trajectories $\{x_1(t),x_2(t),\ldots x_N(t)\}$ are defined,[10] and not for all configurations points $\{x_1,x_2,\ldots x_N,t\}$. In order to further simplify the computational burden associated with solving N Schrödinger equations, second, we assume that the potential energy, $E_c(x,t)$, is roughly identical for all electrons as defined by expression (2b) [i.e., we neglect the condition $k\neq i$ in Eq. (1)]. Therefore, the three self-consistent equations that we solve in our approach are the following:

$$i\hbar\frac{\partial\Psi_i(x,t)}{\partial t}=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+E_c(x,t)\right)\Psi_i(x,t), \tag{2a}$$

$$\frac{\partial^2E_c(x,t)}{\partial x^2}=\frac{q^2}{\varepsilon\cdot A}\sum_{k=1}^{N}\delta(x-x_k(t)), \tag{2b}$$

$$v_i(t)=\left.\frac{J_i(x,t)}{|\Psi_i(x,t)|^2}\right|_{x=x_i(t)}. \tag{2c}$$

Expression (2a) is the single-particle Schrödinger equation, similar to Eq. (1) but with a unique time-dependent potential, Eq. (2b) is just the Poisson equation (A is the lateral area of the device)[11] and Eq. (2c) is the Bohm velocity[4,5] [defined as the ratio between the QM particle current density, $J_i(x,t)$, and the wave packet probability presence density] that determines the electron trajectory, $x_i(t)$, by integration. Each i-electron has its own particular boundary conditions for solving the set of Eqs. (2a)–(2c) and, therefore, its own wave function $\Psi_i(x_i,t)$ and its own Bohm trajectory $x_i(t)$. In summary, regarding the goal of the present letter, the dBB for-

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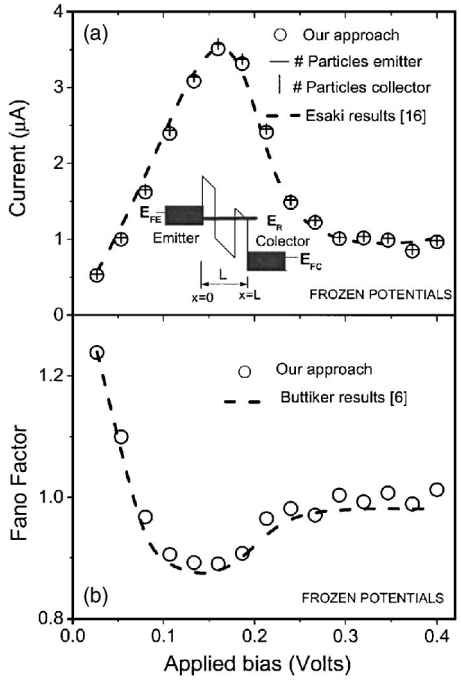

FIG. 1. (a) Current–voltage characteristic for a standard $Al_xGa_{1-x}As$ 2 nm/6 nm/2 nm RTD. The inset shows the static (frozen) potential profile. The excellent agreement between the four different calculations of the average current shows a satisfactory test of the technical implementation of our approach. In dashed line, results obtained from the Esaki (see Ref. 16) expression. (b) In circles, numerical values of the Fano factor for each bias point computed from our approach. In dashed line, results obtained from the Buttiker (see Ref. 6) expression.

malism provides a simulation framework where: (i) all pure QM phenomena, as tunneling, are perfectly reproduced in terms of quantum trajectories,[5] and (ii) the Coulomb interaction can be treated self-consistently via the Poisson equation as in the standard classical-device Monte Carlo technique.

Now, let us emphasize the capabilities of our proposal for dealing with the Poisson equation in a QM framework by providing a numerical example. We study the current through a resonant tunneling diode (RTD) which is a quantum-based device that has been exhaustively investigated, both, from theoretical[8,12,13] and experimental[12–14] points of view. We assume a standard GaAs/AlAs heterostructure system with $m=0.067\ m_o$ (m_o being the free electron mass). We use room temperature, 300 K, for all numerical simulations. The particular heterostructure considered here is a 6 nm intrinsic GaAs quantum well, sandwiched between two $Al_xGa_{1-x}As$ barriers of 2 nm width and 0.3 eV height. At each time step, electrons are injected from emitter/collector contacts into the simulating region according to model presented in Ref. 2. Each *i*-electron of energy *E*, injected into the device, is associated with an initial Gaussian wave packet (with central wave-vector $k=\sqrt{2mE}/\hbar$ and spatial dispersion $\sigma=16$ nm) defined deep inside the emitter or collector contacts, under flat potential profiles.[2,3]

In order to be able to distinguish the effects originated by the electron–electron interaction, first, we consider frozen potentials [i.e, without using Eq. (2b) for self-consistence]. As depicted in the inset of Fig. 1(a), a linear potential profile is assumed along the whole device region at any time. The instantaneous current, $I(t)$, is computed from the extension to semiconductors, due to Pellegrini,[15] of the Ramo–Shockley theorem:

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

where L is the length of the active device region, $N(t)$ is the total number of electrons which is instantaneously inside the device, and $v_i(t)$ is the value of the Bohm velocity defined by Eq. (2c). The time-averaged current, $\langle I(t)\rangle$, for each applied bias is depicted in circles in Fig. 1(a). In the same picture, we have also plotted the dc current obtained by time averaging the net number of Bohm trajectories crossing the emitter (vertical line) or the collector (horizontal line). Moreover, we have also plotted the dc current computed from the well-known Esaki formula.[16] Let us just mention that the excellent agreement between the four different calculations provides a satisfactory test of the technical implementation of our formalism. In addition, within our approach, the total power spectral density of the current fluctuations, $S(f)$, is obtained from the instantaneous current $I(t)$ by simply using the standard numerical technique.[17] The comparison of the noise characteristics is carried out in terms of the Fano factor, F, defined by $S(0)=F\cdot 2\cdot q\cdot\langle I(t)\rangle$. It is well known that the explanation of Fig. 1(b) is based on an interplay between two different sources of noise: (i) The partition noise introduced by the barriers, and (ii) the thermal noise due to the injecting statistics. For low bias, $\langle I(t)\rangle$ tends to zero since it is computed by subtracting the (almost identical) emitter and collector currents, but $S(0)$ is obtained by summing the fluctuations of both currents. Therefore, F tends to diverge. For higher voltages, the transmission coefficient of the barrier is moderately high, and partition and thermal noises are manifested in the value of the Fano factor. Hence, since these sources of noise are described by a Binomial process,[3] the Fano factor approximates 1-*D* (where *D* is the total probability, proportional to the transmission coefficient and occupation function, that an electron can effectively cross the RTD). Thus, the Fano factor, as a function of the applied bias, has the same shape of the average current when flipped vertically (upside down) as seen in Figs. 1(a) and 1(b). For voltages higher than 0.3 V, the transmission coefficient is so low that (even for high temperature) the total probability of traversing the RTD is transformed from a binomial (probability *D* close to 1.0) into a Poisson process (probability *D* close to zero) and a Fano factor roughly equal to 1.0 is obtained. Let us mention that highly doped emitter/collector regions (the emitter/collector Fermi levels, E_{FE}/E_{FC}, are 0.05 eV above their conduction-band minimum) are considered to assume degenerate injection statistics. As an additional test, we have plotted in Fig. 1(b) the Fano factor obtained from the original expression provided by Buttiker[6] in 1992 to describe partition and thermal noise in "frozen" mesoscopic systems (dashed line).

In any case, we are interested in using our approach to study how the Coulomb interaction among electrons can modify the noise properties. The results depicted in Fig. 2 are obtained by self-consistently solving Eqs. (2a)–(2c) for the same RTD considered in Fig. 1. For simplicity, the self-consistence is taken into account inside the $0<x<L$ region [see inset in Fig. 1(a)]. For low doping conditions, the consideration of the Coulomb interaction in the emitter/collector region could modify the present results.[18] The details on the calculation will be explained elsewhere.[10] In Fig. 2(a), we have plotted $\langle I(t)\rangle$ obtained within our approach with circles.

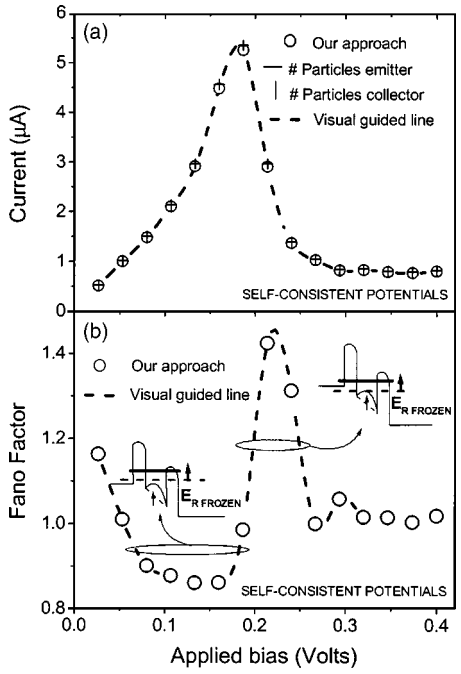

FIG. 2. (a) Current–voltage characteristic for the RTD described in Fig. 1 when the Poisson equation is solved self-consistently with the time-dependent Schrödinger equation. (b) Fano factor for each bias point computed within our approach. The insets show the effect of the time-dependent variations of energy potential profile (due to the presence of an electron at the quantum well) on the QM transmission of other electrons, before and after the resonant voltage.

Again, the horizontal and vertical lines correspond to the dc current obtained from the net number of trajectories traversing the emitter and collector contact, respectively. The effect of the Coulomb correlation between electrons is clearly manifested in the Fano factor depicted in Fig. 1(b). Just after the resonant voltage (when the resonant energy, E_R, is below the conduction band at the emitter contact), the presence of one electron inside the quantum well raises E_R [see inset of Fig. 2(b)]. Thus, the QM transmission for the next electron is highly enhanced. Roughly speaking, the Coulomb interaction affects the electron dynamics by trying to regroup the electrons and providing a Fano factor higher than one. In fact, the previous mechanism also modifies the resonant voltage and the number of transmitted particles. For example, when E_R is just above the conduction band at the emitter contact [see inset of Fig. 2(b)], the presence of an electron inside the quantum well, raises E_R making the probability of transmission for the next electron more difficult (less electrons with this higher resonant energy are available). Consequently, at low bias, the average current values in Fig. 2(a) are lower than in Fig. 1(a). Finally, let us mention that the average current and the Fano factor observed in Fig. 2 are in good agreement with the experimental results obtained by several different groups, with different resonant heterostructures.[12–14] Let us mention that scattering (apart from the electron–electron interaction) is not considered here and it can modify present results. In principle, our approach can accurately deal with additional scattering mechanisms by introducing their interaction/potential directly into the Hamiltonian [Eq. (1)].

In conclusion, we have shown that our previous approach[2,3] for studying shot noise in terms of Bohm trajectories can be generalized to include the Coulomb interaction among electrons via the self-consistent solution of the Poisson equation. On the contrary, most QM noise approaches do only take into account dynamical aspects of the Coulomb (i.e., electron–electron) interaction through a simple linear capacitance relationship. As a test, we have applied our approach to study current fluctuations on standard RTD and our numerical results are in good agreement with previous predictions[8,12,13] and experimental results.[12–14] We believe that the present approach opens a new path for the simulation of electron devices of nanometric dimensions. At such dimensions, pure QM effects (like tunneling or quantization) coexist[19,20] with classical electrostatic phenomena (such as Coulomb blockade), and the ancient Poisson equation becomes as meaningful as the prevalent Schrödinger equation for the correct understanding of actual mesoscopic devices.

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