Enhanced shot noise in carbon nanotube FETs due to electron-hole interaction

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***Abstract*—We predict the possibility of shot noise enhancement in defect-free Carbon Nanotube Field Effect Transistors, through a numerical investigation based on Monte Carlo simulations of randomly injected electrons from the reservoirs and the self-consistent solution of the Poisson and Scrödinger equations within the non-equilibrium Green's functions formalism. Such enhancement can be explained by a positive correlation between holes trapped in quasi-bound states in the channel valence band and thermionic electrons injected from the source and can yield a remarkable Fano factor at room temperature equal to 1.22.**

I. Introduction

The electrical behaviour of nanoscale one-dimensional Field Effect Transistors (FETs) is heavily affected by carrier fluctuations, due to the small amount of mobile charge in the channel [1]. Noise is then an important aspect to be taken into account when investigating device electrical behavior, since it represents a precious source of information on electron-electron interaction [2]. Indeed, it is well-known that the Pauli exclusion principle and Coulomb repulsion among electrons affect current fluctuations by limiting the occupancy of injected states from the reservoirs and by inducing fluctuations of the potential profile in the device region.

In most cases, electron-electron correlations lead to sub-poissonian noise. This issue has been widely investigated in carbon-based electron devices [3], [4], [5]. However, in few cases, super-poissonian noise can be obtained. In particular, noise enhancement has been observed in resonant tunneling diodes [6], [7], due to the positive correlation between electrons tunneling into the quantum well.

As of now, noise enhancement has not been yet observed in Carbon NanoTubes (CNTs). Here we provide numerical investigation, highlighting a shot noise enhancement in CNT-FETs, due to the modulation of current injected from the source by holes injected from the drain and trapped in the channel. Such results have been obtained by means of an ad hoc method, based on the self-consistent solution of the 3D Poisson and Schrödinger equations within the Non-Equilibrium Green's Functions (NEGF) formalism by exploiting our open-source simulator NanoTCAD ViDES [8] and on Monte Carlo simulations of randomly injected electrons from the reservoirs [9].

Shot noise is commonly described by means of the noise current spectral density at zero frequency $S(0)$, which has been calculated by exploiting a recently developed statistical approach, which extends Landauer-Buttiker's approach by including the effect of Coulomb interaction on noise. Such approach is described in detail in Refs. [5] and [9].

Correlations among electrons are usually described in terms of the Fano Factor, defined as $F = S(0)/(2qI)$, where $2qI$ is the Poissonian noise, q is the electron charge and I is the mean current. F can be further decomposed in the injection and partition contributions, $F_{PN} = S_{PN}(0)/(2qI)$ and $F_{IN} = S_{IN}(0)/2qI$, respectively. If $S_{LB}(0)$ is the Landauer and Büttiker noise power spectrum, where the effect of Coulomb repulsion on noise is neglected, we can in a similar way define $F_{LB} = S_{LB}(0)/(2qI)$.

We consider a double gate (DG) CNT-FET: the nanotube is a 2 nm-diameter zig-zag (25,0) CNT with band gap E_{gap}=0.39 eV. The oxide thickness is 1 nm, the channel is undoped and has a length L of 10 nm. Source and drain extensions are 10 nm long and doped with a molar fraction f=5 $\times$ 10^3. For comparison purposes, we also consider a (13,0) CNT-FET, with E_{gap} = 0.75 eV and the same device geometry and doping profile [5], [9]. In Fig. 1b the tunneling current component and the total current are reported as a function of the gate overdrive $V_{GS} - V_{th}$ for a (25,0) CNT-FET ($V_{th} = 0.36$ V). As can be observed, the tunneling component is at least two orders of magnitude smaller than the total current, which therefore is almost equal to the thermionic component.

The Fano factors for a (25,0) and a (13,0) zig-zag CNT are plotted as a function of gate overdrive in Figs. 2a-b. Noise enhancement occurs only in the case of the (25,0) CNT. The whole shaded area in Fig. 2a indicates that shot noise enhancement in (25,0) CNT is entirely due to the Coulomb interaction: indeed when it is not considered, the Fano factor reduces to $F_{LB} < 1$. Unlike (25,0) CNT, in (13,0) CNT Coulomb repulsion among electrons instead suppresses noise below the value predicted by only including Pauli exclusion principle.

Shot noise enhancement in the (25,0) CNT-FET can be explained with the help of Fig. 3. E_C and E_V are the conduction and valence band edge profiles in the channel, respectively, whereas E_{CS} (E_{CD}) is the conduction band edge at the source (drain), and E_{BS} is the energy level of the quasibound state in the valence band. When the drain Fermi level E_{FD} roughly aligns with E_{BS}, holes in the conduction band in correspondence of the drain can tunnel into the bound state, shifting downwards E_C in the channel (Fig. 3a). As a result, thermionic electrons injected from the source can more easily overcome the barrier (Fig. 3b). Instead, when a hole leaves the bound state, the barrier increases by the same amount, reducing thermionic injection. The noise

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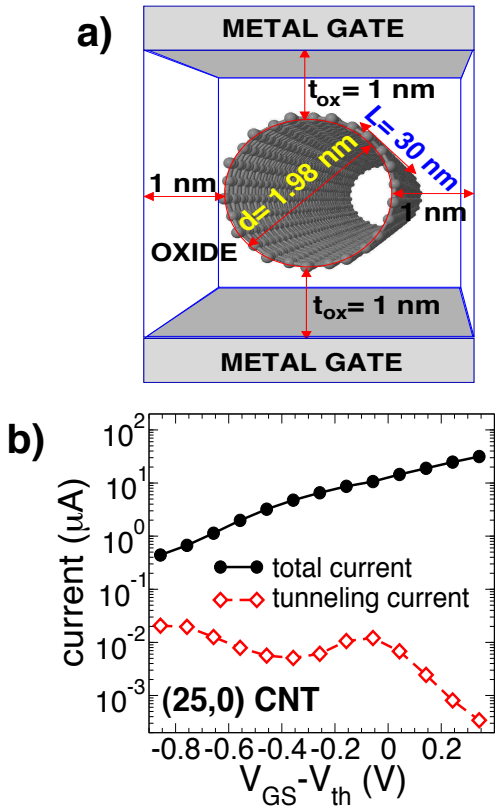

Fig. 1. (a) Sketch of the simulated (25,0) DG-CNT Field Effect Transistor. (b) Transfer characteristics and tunneling current for (25,0) CNT-FETs.

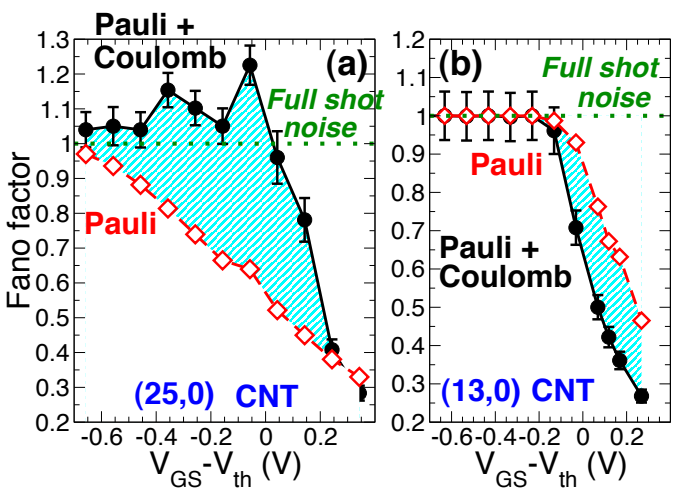

Fig. 2. a) Fano factor as a function of the gate overdrive for a (25,0) and b) (13,0) CNT-FETs for V_{DS}=0.5 V. The threshold voltage V_{th} is 0.43 V for the (13,0) CNT-FET, and 0.36 V for the (25,0) CNT-FET.

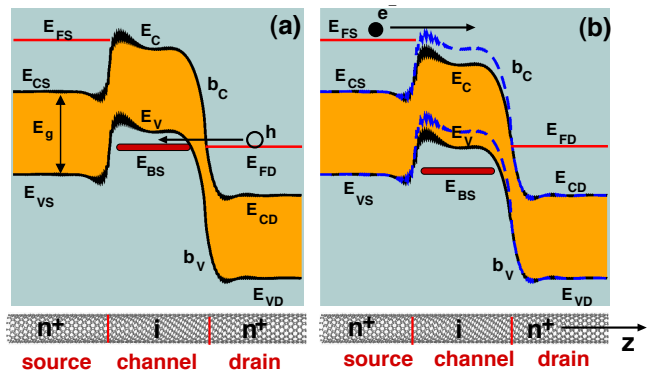

Fig. 3. Sketch explaining the physical process behind the shot noise enhancement in CNT devices.

enhancement can be then explained by the current modulation due to trapping/detrapping of holes in the bound state. Since (13,0) CNTs have a much wider gap E_{gap} =0.75 eV, E_V in the channel is always below E_{CD} in the drain, and hole injection is completely inhibited, as well as noise enhancement.

To justify our assertion, let us focus on the local density of states (LDOS) computed for the (25,0) CNT. In Figs. 4a-b the LDOS averaged on each carbon ring is shown as a function of the coordinate along the transport direction z for two gate voltages in correspondence of the peaks in Fig. 2a, i.e. $V_{GS} = 0$ V and 0.3 V, and a drain-to-source bias $V_{DS} = 0.5$ V: two localized states appear in the valence band, due to the local confinement. Since the energy of the highest quasi-bound state is close to the drain Fermi energy, hole tunneling in and out of the channel can occur, with a zero net current flow. As shown in Fig. 2a, shot noise enhancement ($F = 1.22$) is observed whenever the applied gate voltage roughly aligns E_{BS} with E_{FD}, i.e. in the range -0.4 V$< V_{GS} - V_{th} <$ 0.1 V.

In Figs. 5 and 6, we show the scatter plots obtained from Monte Carlo simulations. In particular, Figs. 5a-b show E_C as a function of the number of injected thermionic electrons for $V_{DS} = 0.5$ V and $V_{GS} = 0.7$ V for (13,0) CNTs ($F = 0.27$) and 0 V for (25,0) CNTs ($F = 1.15$). As can be noted in Fig. 5a, the net result of an electron entering the channel of the (25,0) CNT is a decrease of the conduction band in the channel, that is at first counterintuitive, and opposite to the trend observed in (13,0) CNTs [5], [9] (Fig. 5b). The different behavior is not due to a different screening of the gate field, since the quantum capacitance in the channel $q\partial Q/\partial E_C$ (Q is the net charge in the channel) is expected to be positive in both cases (Figs. 6a-b).

Actually, the apparently strange behavior of Fig. 5a is due to the positive correlation between holes in the quasi-bound state and thermionic electrons. This is further confirmed by Fig. 6c, which highlights a strong correlation between statistical fluctuations of holes and electrons in the channel, as proved by the almost unity correlation factor ($R = 0.96$). In addition the slope of the line is close to 0.5, which means that for every two holes that are injected in the channel, electron count in the channel roughly increases by one.

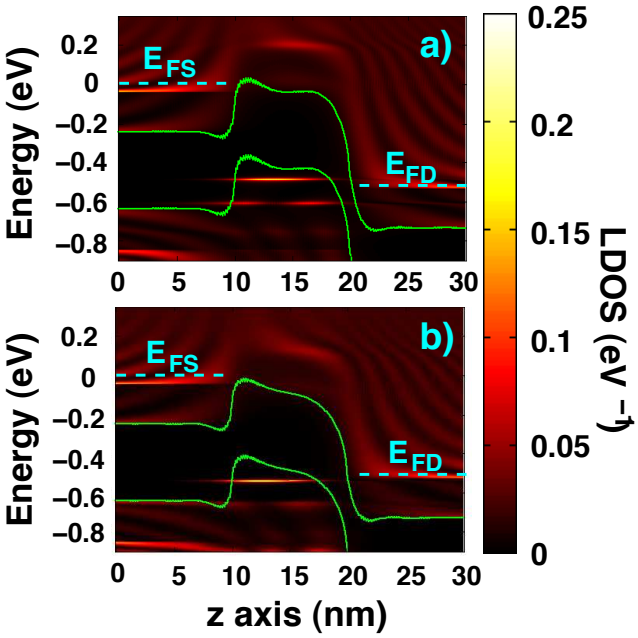

Fig. 4. Local density of states (LDOS (eV^{-1})) as a function of the longitudinal direction z for two different V_{GS}: 0 V (a) and 0.3 V (b). The bias V_{DS} is 0.5 V.

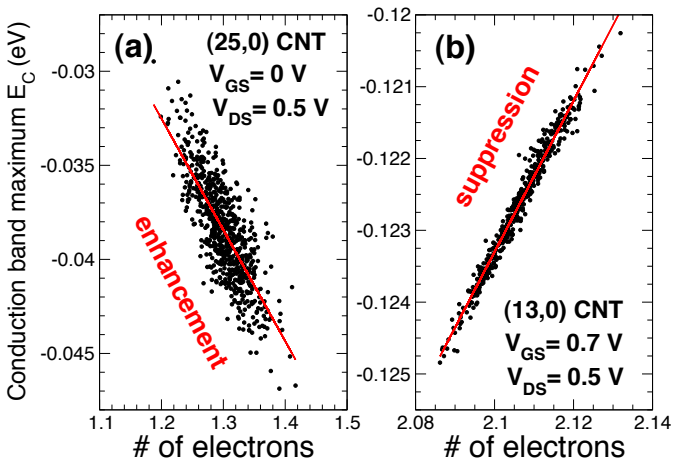

Fig. 5. Conduction band maximum E_C as a function of the number of electrons transmitted in the channel for (a) (25,0) and (b) (13,0) CNTs.

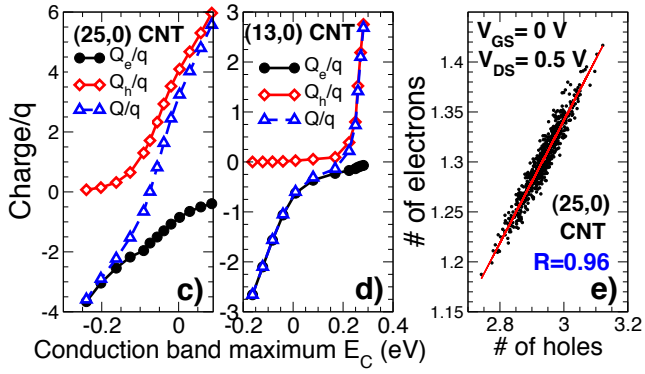

Fig. 6. Electron, hole and total charge as a function of E_C for (a) (25,0) and (b) (13,0) CNTs. (c) Number of electrons transmitted in the channel as a function of the number of holes tunneling from the drain.

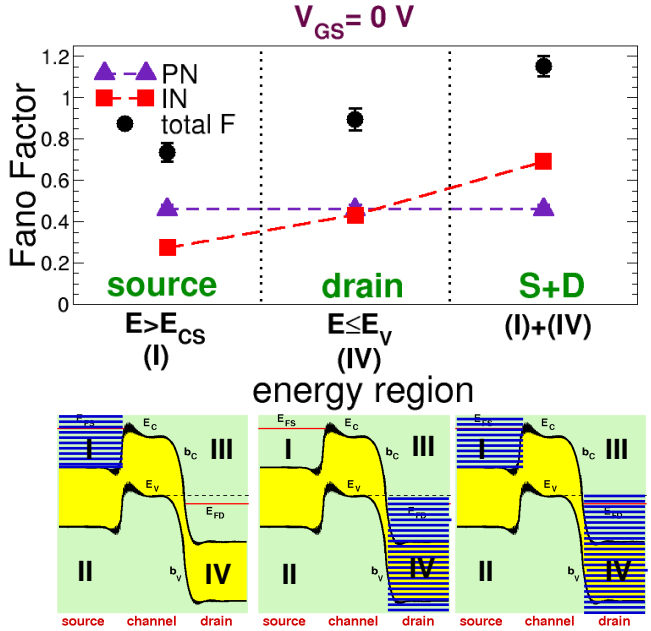

Fig. 7. F, F_{PN} and F_{IN} when randomizing the occupancy at different energy regions and at different reservoirs (source (S): I,II; drain (D): III, IV) for $V_{GS} = 0$ V. Blue shaded areas indicate energy regions where the occupancy is randomized.

To further highlight the correlation between electrons and holes, we can divide the states injected from the reservoirs in 4 regions: regions I ($E > E_{CS}$) and II ($E \leq E_{CS}$) refer to source injected states, whereas regions III ($E > E_V$) and IV ($E \leq E_V$) to drain injected states. Regions II and III of course do not contribute neither to transport, nor to charge fluctuations. Instead turning on random injection of states only for region I or IV, the enhancement disappears (Fig. 7a), confirming our interpretation. In addition, the total injection noise obtained by randomizing the statistics everywhere can be roughly expressed as the sum of the injection noise contributions obtained by separately randomizing the statistics in regions I and IV. Partition noise is instead not affected by the considered statistics (Fig. 7a), because it is fully taken into account by the shot noise formula [5], [9].

Now, we discuss the temperature dependence of shot noise. As can be observed in Fig. 8a and 8b, lowering the temperature suppresses shot noise enhancement by reducing the injection noise, due to the suppression of the hole trapping-detrapping process. We want now to evaluate the cutoff frequency of noise enhancement. In order to do that, we need to evaluate the total capacitance C of the channel from Fig. 6a, obtaining $C \approx 5.5$ aF. Then we need to compute the conductance G between the channel and the drain due to interband tunneling. Following Bardeen [10], tunneling can be treated as an electronic transition between energy levels in different regions. The matrix element for a transition at energy E from a state

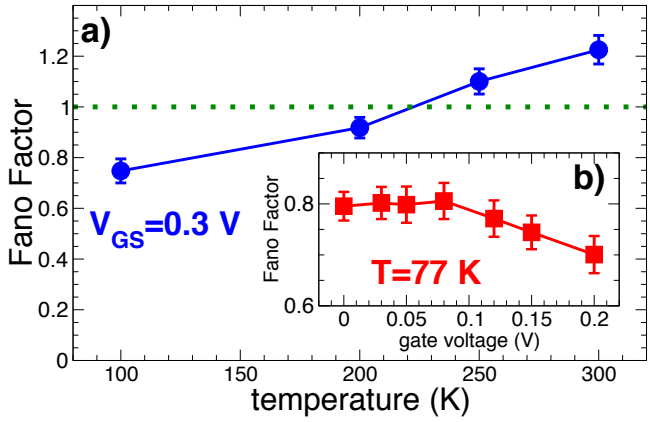

Fig. 8. (a) F at $V_{GS} = 0.3$ V as a function of temperature and (b) as a function of V_{GS} for T=77 K.

in b_C at the drain into a state in b_V in the channel can be expressed as [11]:

$$M(E) = \hbar^2 T(E) J_V(E) J_C(E) \tag{1}$$

where $J_V(E)$ ($J_C(E)$) is the current probability incident on the barrier from S (D), while $T(E)$ is the transmission probability for injected states from S. The transition probability per unit time is given by the Fermi's golden rule:

$$\nu(E) = \frac{2\pi}{\hbar} \left|M(E)\right|^2 \rho_V(E) \tag{2}$$

where $\rho_V(E)$ is the density of states in b_V in the channel. The tunneling frequency g can be obtained by summing on all empty states in b_C at the drain and on all occupied states in b_V in the channel:

$$g = 4\pi\hbar \int_{E_{VS}}^{E_V} dE\, T(E) J_V(E) J_C(E) \rho_V(E) \rho_C(E) \left(1 - f_D(E)\right) , \tag{3}$$

where $\rho_C(E)$ is the density of states in b_C at the drain and the occupancy in b_V in the channel has been approximated to $f_D(E)$. By exploiting $J_C(E)\rho_C(E) = 2\pi\hbar$ [11], [12], we finally obtain G as:

$$G = \left(\frac{q^2}{KT}\right) g \, . \tag{4}$$

From a numerical point of view, $T(E)$ has been evaluated by considering the band profile in correspondence of S constant and equal to the value assumed at source/channel interface. We finally obtain $G \approx 4.7 \times 10^{-5}$ S. Note that G and C are such that we are at the limit of the Coulomb blockade regime. The cutoff frequency of shot noise enhancement f_H can be simply evaluated as the cutoff frequency of an R-C circuit: $f_H = G/(2\pi C) \approx 1.36$ THz.

II. Conclusion

In conclusion, noise enhancement in CNT device can be explained by the correlation between trapping of holes from the drain into quasi-bound states in the channel and thermionic injection of electrons from the source. Such enhancement can lead to an appreciable Fano factor of 1.22 even at room temperature, it is observable down to a temperature of 200 K and up to frequencies of order 1 THz.

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