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INFLUENCE OF DENSITY, OCCUPANCY AND LOCATION OF ELECTRON TRAPS ON SHOT NOISE IN NONDEGENERATE QUASIBALLISTIC TRANSPORT

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An ensemble Monte Carlo simulator self-consistently coupled with a Poisson solver is used to study the influence of the density, occupancy and location of electrons traps on the current fluctuations in nondegenerate quasiballistic structures. Transport and noise are found to depend significantly on the density and location of the traps. In particular, the presence of traps increases the noise level as compared with the purely ballistic case. The nonuniformity of the trap occupancy profiles along the active region of the structures affects markedly (specially for low trap densities) the dependence of shot noise on the applied voltage. The location of the traps with respect to the potential minimum appearing in the structures because of the presence of space charge determines their influence on the noise level, fact which can be of help to identify the trap position.

Keywords: Shot noise; suppression/enhancement; electron traps; MC simulation; ballistic transport.

1. Introduction

The analysis of shot noise in mesoscopic structures has become a subject of extensive research activity in recent years [1], mainly due to the possibility of obtaining relevant information about the carrier dynamics inside the structures from the knowledge of the shot-noise properties [2]. A wide variety of interactions and mechanisms, by introducing correlations between carriers, may have an influence on the shot-noise behavior [1]. Some of them are related to the quantum nature of transport in the conductors, and must be analyzed by using phase-coherent models [3]. In contrast, some others admit of a semiclassical description, like in the case of nondegenerate systems, both ballistic [4] and diffusive [5], where long-range Coulomb interaction between carriers has been found to play a very important role.

It is well known that the presence of electron traps can substantially modify the noise spectrum of semiconductor devices [6], specially at low frequency; their density and position being relevant parameters to determine their influence on the noise [7]. However, little attention has been paid to the effect that trapping-detrapping (TD) processes may have on the shot-noise behavior in mesoscopic structures. In a previous work [8] we showed that the presence of electron traps in nondegenerate structures, otherwise ballistic, may lead to a significant increase of the shot-noise level with respect to that found in the purely ballistic case. In the absence of electron traps, when transport is completely ballistic, these structures exhibit suppressed shot noise due to the action of long-range Coulomb interaction, which introduces negative correlations between carriers by means of the fluctuating potential barrier (related to the presence of space charge) that controls the current [4, 9, 10]. When TD processes are present, trapped carriers act as a negative and fluctuating fixed charge that, via Coulomb interaction, can modify the amplitude of the mentioned potential barrier, thus inducing positive correlations between carriers and increasing the level of noise [8]. To evidence clearly this effect, in [8] it was assumed that the concentration of electron traps N_t was uniform and much higher than the density of trapped electrons n_t, $N_t >> n_t$ (negligible trap occupancy). However, these conditions are far from those found in real structures, where typically only a few traps are present, and thus in low concentration and nonuniformly distributed.

The aim of this work is to analyze the influence of electron traps on shot noise in nondegenerate quasiballistic conductors when the trap occupancy is significant (n_t is of the order of N_t) and the trap density is position dependent [$N_t(x)$]. We will show how the noise increase induced by the presence of the electron traps depends on their density, occupancy and location. On the one hand, the noise enhancement is conditioned by the existence of free traps. On the other hand, it is found to be more pronounced if the potential barrier is close to a given trap or between the location of the trap and the cathode. We will illustrate how, because of these facts, the knowledge of the shot-noise behavior can help to identify in some cases the location of the electron traps. For the calculations we make use of an ensemble Monte Carlo (MC) simulator self-consistently coupled with a Poisson solver to account for Coulomb interaction.

2. Physical Model and Monte Carlo Simulation

We consider a lightly doped active region of length *L*, where electron traps are present, sandwiched between two heavily doped contacts that act as thermal reservoirs by injecting carriers into the active region [10]. The transversal size of the structure is sufficiently thick to allow a 1D electrostatic treatment. So, the simulation is 1D in real space and 3D in momentum space. Electrons are emitted from the contacts according to a thermal-equilibrium Maxwell-Boltzmann distribution at the lattice temperature *T* and following a Poissonian statistics [8]. The scattering mean free path ℓ is assumed to be much longer than the sample length, $\ell >> L$; consequently, electrons move ballistically inside the active region, only interrupted by trapping processes.

The following set of parameters is used in the simulations: $T = 300$ K, $L = 200$ nm, relative dielectric constant $\varepsilon_r = 11.7$, contact doping $n_c = 4\times10^{17}\,\mathrm{cm}^{-3}$, and effective mass $m = 0.25m_0$ (m_0 being the free-electron mass). The above set of values yields for the dimensionless parameter $\lambda = L/L_{Dc}$ (L_{Dc} is the Debye length corresponding to n_c) the value $\lambda = 30.9$, which implies the presence of significant space-charge effects inside the structures [4, 9, 10].

A single type of electron traps [11, 12], initially neutral and empty, at a depth E_n below the bottom of the conduction band is considered to be present in the active region. These traps only interact with electrons in the conduction band. The two time constants involved in the TD processes are the generation time τ_g (average *captured time* of an electron) and the recombination time τ_r (average *free time* of an electron). In the general case of having a position-dependent density of traps $N_t(x)$, the recombination time depends on the position, $\tau_r(x)$, and electrons disappear by trapping at the rate [11]:

$$1/\tau_r(x) = N_t(x) v_{th} s \left[(N_t(x) - n_t(x)) / N_t(x) \right], \tag{1}$$

where v_{th} is the thermal velocity and s is the capture cross section of the traps, which, as a first approximation, is assumed to be energy independent in our calculations. In order to implement in the MC simulation this position-dependent recombination probability, we proceed as follows. In those meshes where traps are present, a position-independent probability $1/\tau_r = N_t^{max} v_{th} s$ is considered to calculate the duration of free flights, N_t^{max} being the maximum value of $N_t(x)$ along the sample. Once the free flight finishes, we determine if a trapping process actually takes place by means of the rejection technique according to the probability $(N_t(x) - n_t(x))/N_t^{max}$, which accounts for the local density and instantaneous occupancy of traps. To this end, $n_t(x)$ is recalculated every time step.

The values of τ_r and τ_g considered in our calculations are $\tau_r = 1/(N_t^{max} v_{th} s) = 20$ ps, and $\tau_g = 5$ ps (independent of position), which, being still within the range of real values [11], are short enough to bring about affordable computation times. The average transit time τ_T of electrons through the active region (about 1.05 ps under equilibrium conditions) fulfills $\tau_r > \tau_T$, so that electrons cross the sample in a quasiballistic way, with a very low probability of suffering a trapping process. Anyway, due to the continuous flux of carriers, a significant density of (fluctuating) trapped charge is present in the active region, which affects the carrier transport and noise behavior [8].

In our analysis, a constant voltage U is applied to the contacts and current noise is analyzed. The temporal correlation between carriers is studied by means of the autocorrelation function of current fluctuations $C_I(t)$. The corresponding spectral density $S_I(f)$ is determined by Fourier transform, and then the Fano factor, the key parameter to characterize the shot-noise behavior, is evaluated as $\gamma = S_I(0)/2qI$.

More details about the physical model and MC simulation can be found in [8−10].

3. Results

In this section we will analyze the influence on the noise of: (i) the density and occupancy of electron traps when their distribution is uniform, and (ii) the location of the traps when they are present only at given positions inside the active region.

3.1. *Influence of density and occupancy of electron traps*

Here we will consider the case of a uniform distribution of electron traps with different values of density, $N_t = 2\times10^{16}$, 10^{16}, 4×10^{15} and 2×10^{15} cm^{-3}. The results corresponding to $N_t = 0$ (ballistic structure) [9] and $N_t >> n_t$ (very high density of electron traps) [8] will be used as reference of asymptotic behaviors. To allow the comparison with the case $N_t >> n_t$ reported in [8], we will consider that $\tau_r = 20$ ps independently of N_t [a], so that the recombination probability in each case differs only in the local occupancy factor $(N_t - n_t(x))/N_t$.

Figure 1 shows the *I-U* characteristics of the structures with the different values of N_t. The current I is normalized to the saturation value $I_S = q\Gamma$ (with Γ the injection rate), which is the maximum current that contacts can provide [10]. Starting from the case when $N_t >> n_t$, for a given value of U the current increases and approaches the ballistic limit as N_t decreases. It is also observed that a lower value of U is necessary to reach

[a] This is equivalent to consider that the capture cross section of the traps s is different for each value of N_t, so that the product sN_t remains constant.

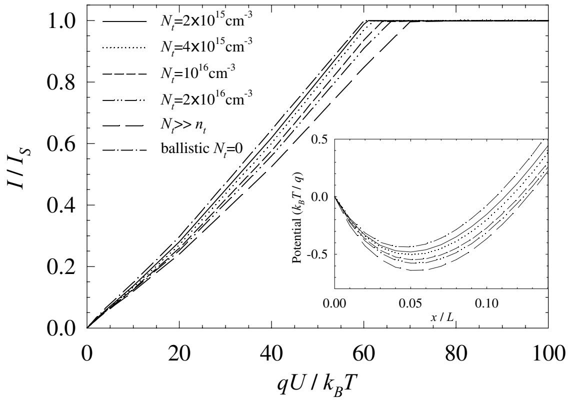

Fig. 1. Current flowing through the structure normalized to the saturation value I_S as a function of the applied voltage for different values of trap density. The ballistic ($N_t = 0$) and $N_t >> n_t$ cases are also plotted for comparison. The inset shows the normalized potential profile $q\varphi / k_BT$ near the cathode (for an applied voltage of $40k_BT / q$), where the potential barrier can be observed.

saturation (U_{sat}). The higher values of the current found for decreasing N_t are due to the lower density of negative fixed charge present in the active region, which leads to a smaller amplitude of the potential minimum controlling the current flowing through the structure (shown in the inset of Fig. 1 for $U = 40k_BT / q$) [8].

This can be observed in Fig. 2, which shows the profiles of the density of free and captured electrons (n and n_t , respectively), and the trap occupancy (n_t / N_t) along the active region for the different values of N_t and $U = 40k_BT / q$. The presence of space charge leads to the shape of free carrier density observed in the figure, higher near the contacts and lower around the center of the active region [10]. For higher N_t the concentration of free carriers decreases slightly (Fig. 2(a)) due to the lower amount of electrons injected with sufficient energy to surpass the increasing potential barrier (inset of Fig. 1). As expected, the density of trapped electrons n_t decreases when a lower density of traps N_t is present in the active region (Fig. 2(b)). This happens specially near the contacts, where there are more free electrons susceptible of being trapped and, as a consequence, the trap occupancy is higher (Fig. 2(c)). Thus, contrary to the case $N_t >> n_t$, for which the trap occupancy plays no role and the ratio n / n_t is constant along the active region, when n_t is of the order of N_t and the trap occupancy must be taken into account the ratio n / n_t becomes position dependent. As one could expect, the trap occupancy is higher the lower N_t is[b] and the closer the contacts are (Fig. 2(c)), thus preventing the occurrence of a significant number of TD processes and reducing the fluctuations of the negative fixed charge, fact that has important consequences on the shot-noise behavior of the structures.

Figure 3 illustrates the evolution of the Fano factor γ with the applied voltage for the same previous values of N_t. In the limits of thermal noise ($qU < k_BT$) and saturation ($U > U_{sat}$), where long-range Coulomb interaction plays no role, the different curves coincide. However, for intermediate voltages significant differences are observed: (i) as N_t increases, the shot-noise behavior goes from the pronounced suppression ($\gamma < 1$) found in the ballistic case ($N_t = 0$) [9] to the enhancement ($\gamma > 1$) observed when

[b] In the case that τ_r scales with N_t, the occupancy profiles become independent of N_t, and none of the related effects discussed in the following would take place.

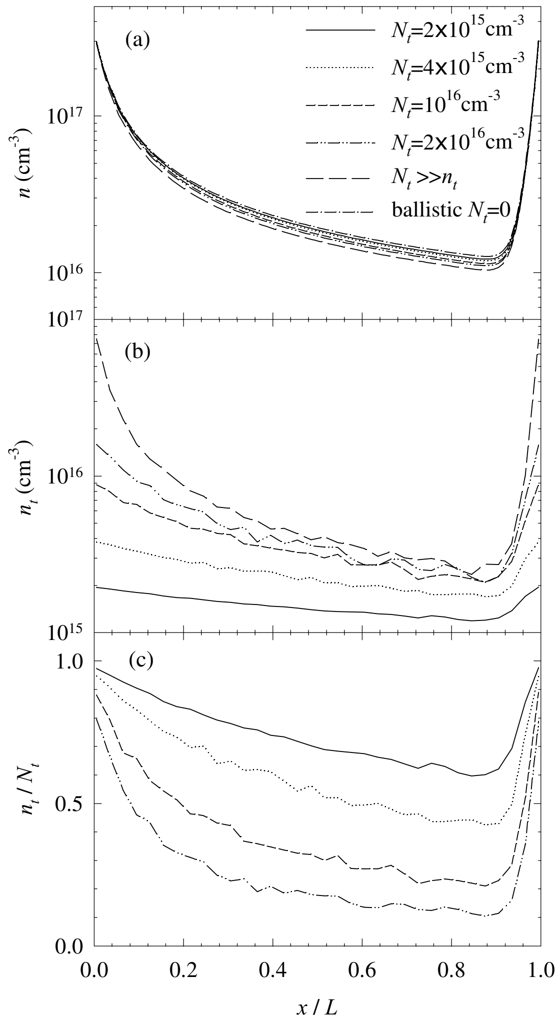

Fig. 2. Spatial profiles along the active region of density of (a) free and (b) trapped electrons, and (c) trap occupancy at an applied voltage of $40k_BT/q$ for different values of the trap density. The ballistic ($N_t = 0$) and $N_t >> n_t$ cases are also plotted for comparison.

$N_t >> n_t$ [8], and (ii) the dependence of γ on U changes notably with N_t due to the different trap occupancy. In the two limit cases ($N_t = 0$ and $N_t >> n_t$), the suppression/enhancement effects are more pronounced the closer the structure is to saturation, since it is under these conditions when long-range Coulomb interaction has a stronger effect on the current fluctuations.

For the lowest value of N_t under analysis ($2\times10^{15}\,\mathrm{cm}^{-3}$), even if an increase of the noise related to the presence of the traps is observed with respect to the ballistic case, shot-noise suppression is dominant and the dependence of γ on U is very similar to the ballistic one. This is due to the fact that, on the one hand, n_t is still low (see Fig. 2(b)) to have an important effect on the noise via Coulomb correlations and, on the other hand, the trap occupancy is very high (see Fig. 2(c)), thus preventing the fluctuations of n_t that

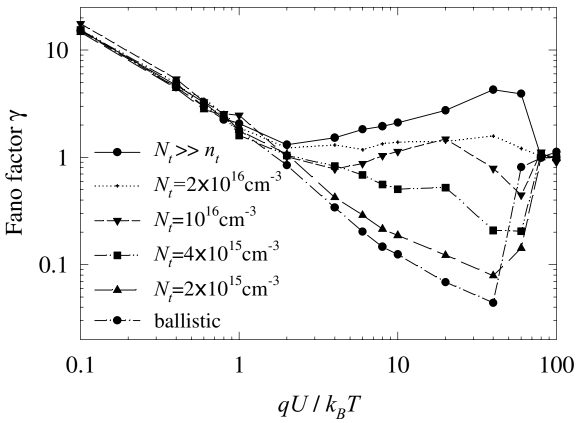

Fig. 3. Fano factor vs. bias voltage U for several densities of electron traps uniformly distributed along the active region. The ballistic ($N_t = 0$) and $N_t >> n_t$ cases are also plotted for comparison.

lead to the increase of shot noise. For higher N_t, the influence of TD processes on the noise is more pronounced due to both the increase of n_t and the decrease of n_t / N_t, and, as a consequence, higher values of the Fano factor are obtained, even corresponding to shot-noise enhancement ($\gamma > 1$) for $N_t = 10^{16}$ and 2×10^{16} cm^{-3}. In contrast with the limit case $N_t >> n_t$, the peak value of the Fano factor is not found just before saturation, where a decrease of γ is observed, but for a value of U significantly lower. This peculiar behavior of the γ-U curves and the associated peak can be explained in terms of the trap occupancy profiles as follows. Near saturation, when the potential minimum is close to the left contact and affects the highly occupied low-energy states of injected carriers, the maximum influence of the trapped electrons on the noise could be expected, like in the case $N_t >> n_t$. However, it is precisely near the left contact where the trap occupancy takes the highest values (Fig. 2(c)), thus reducing considerably the fluctuations of n_t at the origin of the noise enhancement so that the suppression effect related to the ballistic carriers passing over the barrier prevails, persisting for voltages higher than in the ballistic case (like $60k_BT / q$) due to the increase of U_{sat} with N_t observed in Fig. 1. For lower values of U not so close to saturation the potential minimum is located in a position more distant to the cathode where the trap occupancy is lower. Hence, relevant fluctuations of n_t may take place, the noise enhancement is more pronounced and γ takes its highest value. We conclude that the shot-noise behavior depends substantially on the trap density and occupancy profile in the active region.

3.2. *Influence of trap location*

In this section we will analyze how the location of the traps x_{trap} modifies the noise behavior. To this end, we will consider that traps are present only in some specific zones of the active region. For the simulation, the sample is divided into 100 meshes; we will take into account the existence of traps only in two consecutive meshes, and we will cover all possible locations in the left half of the structure ($0 < x_{trap} < 0.5L$, with x_{trap} the coordinate of the boundary separating the two meshes).

Firstly we study the case in which the density of traps present in these meshes satisfies that $N_t >> n_t$. This condition implies that TD processes are not limited by the trap occupancy. Fig. 4 shows the Fano factor as a function of the applied voltage for several values of x_{trap}. The cases $N_t = 0$ and uniform trap density $N_t >> n_t$ in the whole active

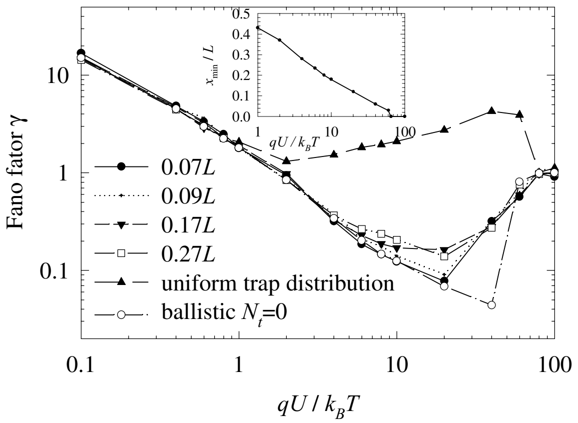

Fig. 4. Fano factor as a function of bias voltage U for several trap locations with $N_t >> n_t$. The ballistic case and that in which a uniform trap distribution is considered are plotted for comparison. Inset: location of the potential minimum, $x_{\min}/L$, vs. bias voltage.

region are plotted for comparison. The position of the potential minimum x_{min} is represented in the inset as a function of the applied voltage, being nearly the same for all the cases considered in the figure. It can be observed that the presence of the traps has practically no influence on the noise for applied voltages for which $x_{min} > x_{trap}$. In particular, $x_{min} \cong 0.27L$ for an applied voltage around $5k_BT/q$, $0.17L$ for $10k_BT/q$, $0.09L$ for $25k_BT/q$ and $0.07L$ for $35k_BT/q$. Thus, for $qU \le 4k_BT$ all the curves coincide with the ballistic case, while for higher voltages the Fano factor departs from the ballistic case when x_{min} approaches x_{trap}, showing an increase of the noise that persists until saturation is reached, this is, while $0 < x_{min} < x_{trap}$. Accordingly, the closer the traps are to the cathode, the higher the applied voltage necessary to have a significant noise increase is. This fact constitutes a valuable hint to determine the location of the traps. Of course, the noise increase found when the traps are present only in two meshes of the active region is much lower than when a uniform distribution is considered, but it is still quite significant. Near saturation, for voltages high enough ($qU \ge 40k_BT/q$) to detect the influence of the traps in all the cases under analysis, all the curves are similar, since the fluctuations of n_t have an analogous influence on the potential barrier once $x_{min} < x_{trap}$. The most significant difference with respect to the ballistic case occurs in all cases for $40k_BT/q$, when the potential barrier affects to the most populated sates [10].

Now we will consider the more realistic situation in which n_t is of the order of N_t, and therefore the trap density and occupancy must be taken into account. Again, the traps will be situated only in two meshes of the active region. The previous case, in which $N_t >> n_t$, will be also considered for the sake of comparison. Fig. 5 shows the Fano factor as a function of x_{trap} (for $0 < x_{trap} < 0.5L$) for an applied voltage of $40k_BT/q$ and $N_t >> n_t$, $N_t = 2\times10^{16}\text{cm}^{-3}$ and $N_t = 10^{16}\text{cm}^{-3}$. As expected, the Fano factor increases with N_t for every x_{trap}, since the density of fixed charge is higher and the trap occupancy is lower, thus permitting more important fluctuations of n_t. For $N_t >> n_t$, γ takes its maximum value close to the position of the potential minimum ($x_{min} \cong 0.07L$), while in the other two cases the maximum value appears for a trap position more distant from the cathode the lower N_t is. This behavior is associated to the different occupancy of the traps depending on their position. In a similar way to that observed in Fig. 2(c), n_t/N_t is higher when the traps are located near the contacts, what reduces their influence on the

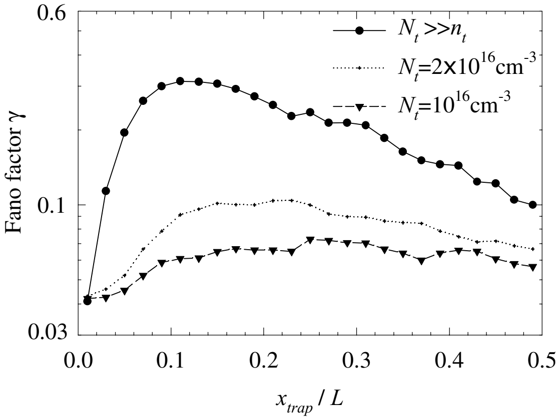

Fig. 5. Fano factor vs. trap location in the range 0-0.5L for several densities of electron traps and an applied voltage of $40k_BT/q$.

noise, so that the maximum effect is achieved in a position closer to the middle of the structure the lower N_t is, where, even if the traps are distant from x_{min}, the value of n_t/N_t is low enough to have relevant fluctuations of n_t. In the case of $0 < x_{trap} < x_{min}$, the values of γ decrease with x_{trap}, becoming very close to those obtained in the ballistic limit, indicating that the traps practically play no role, firstly because they are located at the left of the potential minimum, and secondly because at those positions the traps are near to be fully occupied.

To illustrate more clearly how the occupancy of traps (depending on their position) modifies their influence on the shot-noise behavior, Fig. 6 shows the ratio between the Fano factor obtained for different values of x_{trap} (with traps in two meshes, as in previous cases, and $N_t = 2\times10^{16}\,\mathrm{cm}^{-3}$) and the ballistic one as a function of the applied potential. Again, it can be observed that the noise departs from the ballistic behavior ($\gamma/\gamma_{bal} > 1$) for lower voltages (for which $x_{min} \le x_{trap}$) the higher x_{trap} is. For $U = 40k_BT/q$, when the traps have the maximum influence on the noise, γ/γ_{bal} takes the highest value for $x_{trap} = 0.17L$, and not for $x_{trap} = 0.09L$ or $0.11L$, as one could expect because of the closer position of the traps to $x_{min} \cong 0.07L$. Once more, it is the high trap occupancy at $x_{trap} = 0.09L$ or $0.11L$ as compared to that at $x_{trap} = 0.17L$ which leads to this result.

4. Conclusions

By using an ensemble MC simulation, we have investigated the influence of the density, occupancy and location of electron traps on the shot-noise behavior of quasiballistic nondegenerate structures. An increase of the noise level with respect to the purely ballistic case is detected in all the cases under analysis due to the presence of the traps. This enhancement is more pronounced the higher the trap density is. The high values taken by the trap occupancy near the contacts (specially for low trap densities), by reducing the fluctuations of the fixed charge, prevent the increase of shot noise for applied voltages near saturation. When the electrons traps are present only in some given positions of the active region, the shot noise is enhanced at applied voltages for which the potential barrier is between the cathode and the traps, fact which can be of help to determine the trap position. The most significant difference with respect to the ballistic case occurs in all cases near saturation, when the potential barrier affects to the most populated sates.

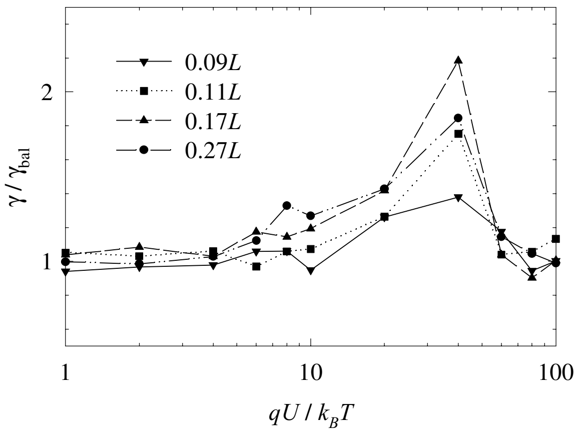

Fig. 6. Ratio between the Fano factor obtained for different trap locations and the ballistic one vs. bias voltage U, for a density of electron traps $N_t = 2\times10^{16}\,\mathrm{cm}^{-3}$.

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