Numerical investigation of shot noise in nanostructures including chaotic cavities and potential barriers

M. Macucci and P. Marconcini
Dipartimento di Ingegneria dell’Informazione
Università degli Studi di Pisa
Via Diotsalvi 2, I-56122 Pisa, Italy

ABSTRACT

A numerical approach for the evaluation of conductance and shot noise suppression in mesoscopic structures is presented and applied to a few relevant cases. Details are provided both of the technique based on a recursive Green’s function procedure that is used for calculations in the absence of a magnetic field and of the recursive scattering matrix method that is applied to simulations with nonzero magnetic field.

Shot noise suppression in cascaded chaotic cavities is studied and discussed in comparison with the suppression obtained for cascaded potential barriers. It is observed that the Fano factor for multiple cascaded cavities is the same as that for a single cavity, as long as its apertures are small compared to its width.

Finally, a particular structure, consisting in a cavity with a central potential barrier, is studied and from its noise behavior conclusions are drawn about the very different role played by a constriction or by a potential barrier in the presence of edge states.

Keywords: Shot noise suppression, mesoscopic devices, Fano factor, chaotic cavity

1. INTRODUCTION

Recent experiments have raised the interest in shot noise suppression in mesoscopic systems, by confirming the predictions of several groundbreaking theoretical papers by Beenakker, Büttiker, Nagaev, Blanter and others.1-3

Most theoretical approaches have been based either on a quantum mechanical treatment, relying on Random Matrix Theory,4 or on semiclassical approaches,5 coupling the Boltzmann-Langevin equation with the Pauli exclusion principle. These are powerful methods that allow to obtain general results analytically or semi-analytically, but they may be difficult to apply to complicated structures, and in the presence of a magnetic field. We have developed a numerical approach to the evaluation of the low-frequency noise power spectral density in generic nanostructures, with which we have retrieved the results in the literature and made predictions for coupled cavities,4 partially diffusive structures,5 antidot lattices,6 the transition between ballistic and diffusive transport.7

Here we present the application of our technique to some further analysis of cascaded cavities (also in the light of some other theory that recently appeared in the literature8) and to the analysis of somewhat more complex structures, with the inclusion of a magnetic field orthogonal to the plane of the device. More specifically, we will present our results for shot noise suppression in cascaded cavities, pointing out that, based on our coherent model, the shot noise suppression factor for multiple cascaded cavities with input and output apertures that are symmetric and small with respect to the cavity width turns out to be the same as for a single cavity. This is in contrast with the results of Ref.8, according to which shot noise suppression in a series of cascaded cavities should tend to the 1/3 limit as in the case of a series of barriers.9 We have applied our method also to a structure with multiple cascaded barriers, showing that, under appropriate conditions, the 1/3 value is retrieved, and we discuss why a series of barriers is intrinsically different from a series of quantum point contacts.

Such a difference becomes much more pronounced in the case of the presence of a magnetic field, because of the formation of edge states and their quite different interaction with a barrier or a quantum point contact. We

Further author information: E-mail: macucci@mercurio.ieo.unipi.it, Telephone: +39 050 568537
present some results for shot noise suppression in the presence of magnetic field for a chaotic cavity, as well as the behavior, as a function of magnetic field, of a cavity with a potential barrier in the middle, whose investigation sheds more light on the differences between the properties of barriers and of quantum point contacts.

2. NUMERICAL MODEL

Both the conductance and the low-frequency shot noise power spectral density for the structures of interest are evaluated from the transmission matrix, with a few simple steps that will be described in the following. The transmission matrix, in turn, is computed using two different approaches, depending on whether a magnetic field is present. If there is no magnetic field, we use a recursive Green’s functions technique, based on subdividing the structure in a number of transverse slices (transverse with respect to the direction of electron propagation), which are thin enough that within them the transverse confinement potential can be assumed to be constant along the longitudinal direction. Each section is initially considered as separated from the others, so that its Green’s function can be computed analytically in the form of a diagonal matrix, with a dimension corresponding to the number of transverse modes that we consider. Then, starting from one end of the device, the Green’s function matrix of two coupled slices is computed with the procedure described in Refs., which is then applied recursively until the overall Green’s function matrix of the whole structure has been obtained. From such a matrix, the transmission matrix can be computed with a straightforward procedure. The recursive Green’s function technique is very efficient from a numerical point of view, and this is the reason why we use it for the simulations without magnetic field.

Inclusion of a magnetic field is simpler within an approach based on a recursive scattering matrix technique: we choose a gauge for the vector potential that has a single nonzero component along the direction of propagation for the electrons. With such a choice the wave function within each section can be written as the product of plane waves times transverse wave functions that, depending on the transverse width of the structure and on the magnetic field intensity, may be strongly distorted with respect to those in the absence of magnetic field.

In the literature, several methods can be found for the calculation of such transverse wave functions, but many of them become numerically unstable in the case of relatively wide structures and high magnetic fields. We have chosen the technique proposed by Tamura and Ando, which consists in expanding each transverse wave function over a basis of transverse wave functions for zero magnetic field and in solving an eigenvalue problem to determine the expansion coefficients. This method is very stable, but a very large basis may be required (with more than 600 elements for the calculations that we shall present in the following). The scattering matrix for each discontinuity between adjacent sections is computed with the mode-matching technique, and then the scattering matrices are combined recursively, obtaining the overall scattering matrix of the structure. From its submatrix $t_n$, representing the relationship between the complex amplitudes of the modes exiting from the output port of the device and those of the modes impinging into the input port, we derive the matrix $t_n'$ of the transmission coefficients normalized with respect to the probability current flux. The generic element of $t_n'$ reads

$$t_n' = t_{nm} \sqrt{\frac{v_n}{v_m}},$$

where $v_n$ is the group velocity of the $n$-th mode.

The conductance of the device is computed with the Landauer-Büttiker formula:

$$G = \frac{2e^2}{h} \sum_{n,m} |t_{nm}'|^2,$$

where $e$ is the electron charge and $h$ is Planck’s constant. The low-frequency noise current power spectral density is then computed following Büttiker:

$$S_I = 4 \frac{e^2}{h} |eV| \text{Tr} \left( t'^\dagger t'^\dagger t' t' \right),$$
where $V$ is voltage applied between the reservoirs to which the input and output leads are connected and $r'$ is the reflection matrix (notice that there is a factor 2 difference with respect to Ref.\textsuperscript{15}, because we include spin degeneracy). Due to the unitarity of the scattering matrix, we can write

$$S_I = 4\frac{e^2}{\hbar} |eV| \text{Tr}[t'_t t'_e (I - t'_e t'_t)] ,$$

(4)

which, considering the invariance properties of the trace of a matrix for rotations, can be written as

$$S_I = 4\frac{e^2}{\hbar} |eV| \sum_i w_i (1 - w_i) ,$$

(5)

where $w_i$ is the $i$-th eigenvalue of $t'_e t'_t$. Since the modulus of the average current reads

$$|I| = G |V| = 2\frac{e^2}{\hbar} |V| \sum_{nm} |t'_{nm}|^2 = 2\frac{e^2}{\hbar} |V| \sum_i w_i ,$$

(6)

the Fano factor $\gamma$ can be written

$$\gamma = \frac{\sum_i w_i (1 - w_i)}{\sum_i w_i} .$$

(7)

If the temperature is different from zero, averaging over a range of energies around the Fermi level (using the derivative of the Fermi function as a weighting factor) is needed. It is important to point out that, in order to reproduce the experimental results, the quantities appearing at the numerator and at the denominator must be separately averaged:

$$\gamma = \frac{\langle \sum_i w_i (1 - w_i) \rangle}{\langle \sum_i w_i \rangle} .$$

(8)

This is particularly important in the case of few propagating modes, and therefore of large relative amplitude of the fluctuations as a function of the value of the Fermi energy, due to quantum interference effects.

3. CASCADeD CHAOTIC CAVITIES AND CASCADeD BARRIERS

We have derived our model cavities from the layout of the device on which several recently published measurements have been performed.\textsuperscript{8,15,17} In order to limit the computational complexity, we have considered a hard-wall model with cavities that are 8 $\mu$m wide and 5 $\mu$m long, defined by constrictions that are 750 nm long and with a width $W$, variable, depending on the calculations, between 400 nm and 1.6 $\mu$m. A sketch of such a cavity is shown in Fig. 1.

For our initial calculations we have considered 300 energy values centered around a Fermi level of 7.9 meV, over a total range of 35 $\mu$eV. Conductance and noise results are obtained by averaging over such a set of values. With respect to previous calculations\textsuperscript{4} that focused on smaller structures and fewer propagating modes, the present simulations require a very large computational effort, because in the leads and in the cavities we are considering 400 transverse modes (the number of propagating modes in such regions is 323). Evaluation of the conductance and of the noise power spectral density for 300 energy values requires, for the simplest structure including a single cavity, over ten hours of CPU time on an Alpha XP1000 workstation. A large number of energy values is needed to obtain good statistics, because, as we shall show in detail, there are very ample fluctuations of the computed quantities versus the energy, as a consequence of the fully coherent nature of the problem and of the relatively large length of the cavity.

To limit the relative amplitude of the fluctuations we have considered a minimum width of the constrictions of 400 nm, which corresponds, at the mentioned value of the Fermi energy, to 15 modes propagating through them. This leads, consistently with the experimental results reported in Ref.\textsuperscript{17}, to a shot noise suppression for a single cavity slightly lower than the “universal” value of 0.25 expected for a symmetric cavity with apertures much smaller than its width. The actual value of the Fano factor that we obtain from our calculations for a single cavity with the previously mentioned dimensions and $W = 400$ nm is 0.226. In Fig. 2 we report the
Figure 1. Hard-wall model for a chaotic cavity used in the simulations.

Figure 2. Fano factor as a function of the Fermi energy for a single cavity with $W = 400$ nm.
Figure 3. Fano factor as a function of the Fermi energy for two (a), three (b), and four (c) cascaded cavities with $W = 400$ nm.

Fano factor as a function of energy, in order to show the ample fluctuations that, although we are considering a relatively large number of modes propagating through the constrictions, take place around the average value of 0.226, indicated with a dashed line.

If we consider two cascaded cavities, we get a very similar behavior for the Fano factor, with a slightly higher averaged value, of 0.234. For three cavities we get a Fano factor 0.237, and for four cavities 0.229. In Fig. 3 we report the Fano factor as a function of energy for the case with two (a), three (b) and four (c) cavities: we notice that fluctuations grow in amplitude as the number of cavities is increased. From the averaged values of the Fano factor we conclude that our coherent model does not exhibit any significant trend toward the 1/3 Fano factor predicted in Ref$^9$; it rather seems that we have just a fluctuation, due to the residual variance of the results after the averaging process, around a constant value of about 0.23.

Calculations on other cavities with comparable or smaller apertures have yielded analogous results, with a Fano factor that does not seem to have any significant dependence on the number of cascaded cavities.

In Fig. 4 we report the behavior of the conductance through one (a), two (b), three (c) and four (d) cavities. While the Fano factor is substantially invariant with respect to the number of cascaded cavities, the conductance appears to be decreasing as the number of cavities is increased.

The invariance of the Fano factor as a function of the number of cavities disappears if we consider cavities delimited by relatively large apertures, which are therefore far from the limiting condition leading to the Fano factor 1/4. We have considered apertures that are 1.6 $\mu$m wide, defining cavities with the same other geometrical dimensions as the ones previously described. For $W = 1.6$ $\mu$m, a single cavity is characterized by a Fano factor of 0.12, which raises to 0.15 in the case of a double cavity and to 0.198 for a quadruple cavity.

In Ref$^8$ an analogy is drawn between a structure with cascaded quantum point contacts and one with cascaded barriers, for which it has been shown in the literature$^9$ that, under some simplifying conditions, the Fano factor...
Figure 4. Conductance in units of $G_0 = 2e^2/h$ as a function of the Fermi energy for one (a), two (b), three (c), and four (d) cascaded cavities with $W = 400$ nm.

tends to $1/3$ as the number of barriers is increased. We have tested our code on a series of cascaded barriers, in order to verify whether our coherent model can reproduce the $1/3$ limit, obtained in Ref.9 with a semiclassical approach. If we choose barriers with relatively low transparency (with a height of 50 meV and a width of 2.5 nm) and we place them within a hard-wall quantum wire 8 $\mu$m wide, with an interbarrier separation of 5 $\mu$m, our model yields the Fano factor behavior reported in Fig. 5 as a function of the Fermi energy. The thick curve represents the result for 3 barriers, which has substantially converged to the $1/3$ limit value (indicated with a dashed line), while the Fano factor for 2 barriers is indicated with the thin curve, and is slightly below the theoretical value$^9$ of 0.5 (dotted line).

Our model is thus able to retrieve the expected results for cascaded barriers, but we must point out that these results are not general, and deviations are observed, depending on the height and thickness of the barriers. Such deviations are probably due to the fact that the results of Ref.$^9$ are obtained making a few strong assumptions that are not verified for generic barriers, i.e. that the transmission coefficient is independent of the impinging wave vector and of the energy.

There is thus a clear discrepancy between the results of Ref.$^8$ and ours, which we believe cannot be simply explained on the basis of the presence of phase coherence across the whole structure in one model and of the loss of coherence between adjacent cavities in the other model: in the recent literature many indications can be found that the noise behavior in mesoscopic systems is not sensitive to the loss of phase coherence. Therefore some further work is needed to understand the actual origin of the difference between the results of the two approaches and, in particular, additional experimental data are required (in Ref.$^9$ only a single relevant data point is available).
4. CHAOTIC CAVITIES IN THE PRESENCE OF A MAGNETIC FIELD

It has been experimentally shown\textsuperscript{17} that application of a magnetic field perpendicular to the plane of a symmetric chaotic cavity further decreases the Fano factor below the value 0.25. In particular, it has been shown that the Fano factor decreases linearly with increasing magnetic field. Our numerical approach correctly reproduces such an effect and provides clues for an intuitive explanation of the origin of this phenomenon.

For our simulations we have considered the same structure that has been previously described, with a few choices of the aperture width \( W \) that correspond to different numbers of propagating modes in the constrictions. In particular, we consider the values \( W = 200, 100, \) and 60, which correspond to 8, 4, 2 propagating modes, respectively. The Fano factor as a function of magnetic field is shown in Fig. 6, with solid dots for 8 propagating modes, empty circles for 4 propagating modes, and empty squares for 2 propagating modes.

All calculations are performed assuming a Fermi level of 9.14 meV, corresponding to that of the sample used in Ref.\textsuperscript{16,17} The dashed lines interpolate among the data points available for each value of \( W \): we observe a larger dispersion around the interpolating line for the smallest value of \( W \), this is due to the fact that the relative amplitude of the fluctuations due to quantum interference effects increases as the number of modes propagating through the constrictions decreases.

We propose a very simple and intuitive explanation for this further noise suppression effect, based on a classical description. As the magnetic field is increased, the cyclotron radius decreases: for a large enough value of the magnetic field the cyclotron radius becomes smaller than the width of the apertures defining the cavity. In such a case, the edge states that crawl along the walls of the structure can pass the entrance aperture, proceed along the internal walls of the cavity and exit through the exit aperture, without undergoing significant scattering. This unimpeded flow of charge corresponds to a noiseless current, therefore it is expected that the Fano factor will drop down. The expression for the cyclotron radius is

\[
R_c = \frac{\sqrt{2m^*E_f}}{eB},
\]

where \( m^* \) is the effective mass of the electron, \( E_f \) is the Fermi energy, and \( B \) is the value of the magnetic field. If we evaluate \( R_c \) for \( B = 1 \) T, we obtain 83.4 nm, which is definitely smaller than 200 nm, but just slightly

Figure 5. Fano factor as a function of the Fermi energy for a structure with two (thin curve) and five (thick curve) cascaded barriers. Each barrier has a height of 50 meV and a thickness of 2.5 nm.
Figure 6. Fano factor as a function of magnetic field for cavities with $W = 200$ nm (solid dots), $W = 100$ nm (empty circles), and $W = 60$ nm (empty squares).

smaller than 100 nm. The results of Fig. 6 are consistent with these results: for $W = 200$ nm at 1 T noise is completely suppressed, as expected, while for $W = 100$ nm noise is only partially suppressed (with a Fano factor around 0.1), because the cyclotron radius is just slightly smaller than $W$ and therefore some scattering still takes place at the apertures. Based on this interpretation, we can state that the inner dimensions of the cavity (width and length) have no effect on shot noise suppression, as long as they are large compared to the aperture widths. We have verified this by computing the Fano factor for cavities with varying width or length: as long as $W$ is kept constant, the Fano factor for a given value of the magnetic field is substantially constant, confirming our conjecture.

Another structure that we have studied consists in a cavity in the middle of which a potential barrier has been inserted, as shown in Fig. 7. The height of the barrier is $14$ meV and its width is $20$ nm, while the width $W$ of the apertures is $125$ nm. We have computed the Fano factor as a function of the Fermi energy, in an interval between $9.03$ meV and $9.06$ meV, for $B = 0$ and for $B = 1.25$ T.

Results are presented in Fig. 8 as a function of the Fermi energy. We immediately notice that, while in the case of $B = 0$ the Fano factor has a behavior that is substantially the same as the one in the absence of the barrier, with an average value of approximately $0.242$, for $B = 1.25$ T the Fano factor is rather close to 1 and exhibits a very regular behavior, compared to the complex fluctuations that can be observed for $B = 0$. There is a relatively simple explanation for this behavior, based on the essential difference existing, in the presence of edge states, between a constriction and a potential barrier.

Let us first analyze the behavior of the edge states in the case that no potential barrier is present: the edge state enters, with a relatively large transmission probability, through the input constriction, then travels along the wall of the cavity, until it reaches the output constriction, from which it exits with relatively high probability. Therefore multiple scattering inside the cavity is significantly suppressed and a Fano factor of $0.0176$ results from our calculations. In the presence of the relatively opaque barrier we are considering, the edge state that has entered from the input constriction has a good probability of bouncing back, in which case it crawls back to the input aperture moving along the opposite wall of the cavity and, with reasonably high likelihood, exits and is reflected. If, instead, the edge state impinging into the barrier goes through, it reaches the output constriction and is likely to exit, being transmitted. The situation is thus very close, apart from the moderate scattering occurring at the input and output apertures, to that of a simple barrier with low transmission, for which a Fano

138 Proc. of SPIE Vol. 5115
Figure 7. Layout of a chaotic cavity with a potential barrier in the middle that is 14 meV high and 20 nm thick.

Figure 8. Fano factor as a function of the Fermi energy for a cavity with a potential barrier in the middle, for $B = 0$ and $B = 1.25$ T.

factor around unity is expected, which is consistent with the numerical results. Due to the moderate scattering at the constrictions, multiple reflections within the cavity are negligible, and this explains why the Fano factor as a function of energy does not exhibit any complex structure associated with quantum interference.

Thus the difference in behavior between a constriction and a potential barrier can be simply explained: a constriction with a width larger than the cyclotron radius does not represent an obstacle for edge states, while
a potential barrier has the same behavior both for edge states and for plane waves.

5. CONCLUSION

We have presented numerical simulations of conductance and noise in mesoscopic structures defined by quantum point contacts and potential barriers, including the effects of a magnetic field perpendicular to the plane of the device. Our results show that the Fano factor of cascaded cavities does not exhibit a significant dependence on the number of cavities if each of them is in the limit of suppression down to 1/4 of the full shot value (i.e., it has symmetric apertures that are much narrower than the cavity width), while it exhibits a clear dependence for cavities with large apertures. This result is compared with that for the Fano factor for cascaded potential barriers and with the recent literature. Further work, both theoretical and experimental, is needed to provide a final answer on this point.

We then provide results for the dependence of the Fano factor in a chaotic cavity on the applied perpendicular magnetic field: our results are in good agreement with published experimental data, and we present a simple, intuitive explanation for the behavior of the Fano factor, based on the ratio of the cyclotron radius to the width of the apertures defining the cavity.

Finally we discuss the effect of a potential barrier located in the middle of a cavity: there is a striking difference between its action in the absence of a magnetic field and in the presence of a magnetic field large enough to make the cyclotron radius smaller than the input and output apertures of the cavity. In the former case the presence of the barrier does not produce any significant variation in the noise behavior, while in the latter case a large increase in the noise is observed, with a Fano factor close to unity if the barrier is opaque enough. This interesting behavior of the Fano factor is explained as the consequence of the different interaction of edge states with constrictions and with potential barriers.

ACKNOWLEDGMENTS

This work has been supported by the Italian CNR (National Research Council) through the “5% Nanotecnologia” project and by the University of Pisa.

REFERENCES