Conductance fluctuations in metallic nanocontacts

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It has been reported that conductance fluctuations in noble and monovalent metals nanocontacts oscillate with conductance, showing minima near integer multiples of the conductance quantum. Most observed features were reproduced by means of a model based on the Landauer-Büttiker approach, but the enhancement of the peak at conductances smaller than one quantum. Numerical simulations on metallic constrictions suggest that this enhancement could be a consequence of the large changes that disorder introduces at the conductance onset. Besides, our analysis shows that while the mentioned model does not apply to the case of wide contacts (large conductance) with relatively strong disorder, it satisfactorily works when disorder is weak, indicating that quantum suppression of fluctuations is also possible in this case.

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I. INTRODUCTION

The so-called break junction is one of the most common techniques actually used to investigate transport through metallic nanocontacts.[1] The method consists of breaking a metallic wire and, by means of a piezoelectric element, making a contact with the desired conductance. The piezoelectric element then allows one to smoothly vary the size of the contact and measure how the conductance falls down as the wire is pulled apart. Despite the great variability inherent to this technique, conductance histograms of noble metals show peaks at $G=mG_0$, where $G_0=2e^2/h$ is the conductance quantum and $m=1,2,\ldots$, [2] suggesting that channels contributing to the current are almost fully opened.[3,4]

More recently,[5] the combined statistical analysis of the conductance and its derivative with respect to the bias voltage $\partial G/\partial V$, measured over hundreds (or even thousands) of experiments, provided a tool to investigate the degree of opening of transmission channels contributing to the current. The results indicate that $\partial G/\partial V$ varied randomly (both in sign and magnitude) obeying a bell-shaped distribution with a standard deviation,

$$\sigma_{GV}=\sqrt{\langle(\partial G/\partial V)^2\rangle-\langle\partial G/\partial V\rangle^2} \tag{1}$$

that, for noble metals, shows minima near integer values of the conductance.[5,6]

The authors of Ref. 5 developed a model based upon the Landauer-Büttiker formalism[7] that led to the following result for the standard deviation:

$$\sigma_{GV}=A\sqrt{\sum_{n=1,\ldots,N}T_n^2(1-T_n)}, \tag{2}$$

where T_n is the transmission probability of channel n and N is the total number of conducting channels. On the other hand, A is a constant that depends on the bias voltage, several metal parameters (Fermi velocity, elastic scattering time, etc.) and the geometry of the constriction. Actually, A was adjusted in Refs. 5 and 6 to fit the experimental data. If, at any value of G, all channels but one have transmissions whose values are either 0 or 1, this equation is a periodic function of the conductance which vanishes whenever the conductance is an integer multiple of the conductance quantum ($G=mG_0$) and shows maxima at $G=(m+2/3)G_0$. Equation (2) was used to successfully interpret the oscillating standard deviations observed in noble and monovalent metals, although failed in describing an enhancement of the maximum that shows up at $G<G_0$.[5,6] This enhancement, albeit weak, was clearly observed in gold[5,6] (at several bias voltages, see Ref. 6), silver and less sharply in copper.[6] On the other hand, interpreting the standard deviation for trivalent metals, which steadily increases with G, by means of Eq. (2) requires assuming that several channels with randomly chosen weights contribute to the current.[6] Since the experimental and theoretical work of Ref. 5, the technique has became standard in identifying the number of open channels in a variety of systems.[8,9]

In this work we present extensive numerical calculations of conductance fluctuations in constrictions with a small amount of disorder. The use of a single orbital per lattice site makes our model closer to monovalent metals than to any else. The results for disordered nanoconstrictions are consistent with experimental data, and allow us to interpret the above-mentioned enhancement in terms of the rather large changes that disorder may introduce near and below the band bottom (or the conductance onset). This is a rather general result that should be valid in a wide variety of cases. Besides, our results for conductance fluctuations in stripes show that, when disorder is sufficiently weak, fluctuations do also show minima near integer values of the conductance.

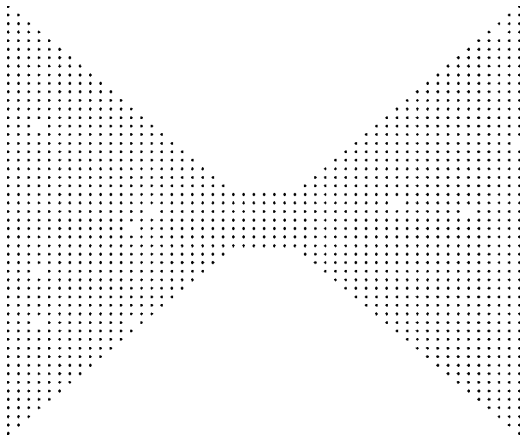

FIG. 1. Atomic arrangement in one of the nanocontacts used to investigate conductance fluctuations. In this particular case the constriction is a 7×7 square. The cluster is connected to semi-infinite stripes of width 51 (the maximum width of the cluster shown in the figure) on the left and right sides. The ten vacancies in a particular realization of disorder are clearly visible.

II. MODEL AND METHODS

A. General considerations

When a wire is pulled apart very complex atomic rearrangements occur that are surely largely different from one experiment to another. This is the source of the observed fluctuations. A detailed microscopic description of a single breaking process will require expensive molecular dynamics calculations. Besides, hundreds of them would be needed to attain a minimally trustable statistics. Here we adopt a much simpler approach. We fix the overall geometry of the system, and introduce disorder by randomly distributing a number of vacancies[11] in either the constriction (see Fig. 1) or in a $L\times L$ region in the case of the stripe. Averages over a sufficiently large number of realizations of disorder can then be easily carried out.

An additional approximation used in this work is to replace the bias voltage derivative of the conductance [see Eq. (1)] by its derivative with respect to the energy. In the present case (a tight-binding calculation) both coincide. But, even in the hypothetical case that an *ab initio* calculation would be feasible, the results of Ref. 4 support this approximation. Specifically, it was shown in Ref. 4 that the $I(V)$ numerical results for Au and Al nanocontacts derived from a full nonequilibrium treatment of the problem and those obtained by integrating the result for $V=0$ over the energy range $[-V/2, V/2]$, almost coincided for low bias voltages (in the case examined in Ref. 4 for V lower than 3 V). Finally the most crude aspect of our simulations is the way we vary the system conductance. In the experiments G changes as the wire is pulled apart. Here, instead, we vary the energy from the conductance onset up to a given energy which depends on the maximum conductance to be explored.

B. Hamiltonian and conductance calculations

The model we use is described by means of a tight-binding Hamiltonian with a single atomic level at sites of the square lattice,

$$\hat{H} = \sum_i \epsilon_i - t\sum_{\langle ij\rangle} \hat{c}_i^{\dagger}\hat{c}_j, \tag{3}$$

where the operator $\hat{c}_i$ destroys an electron on site i with energy ϵ_i. All hopping integrals t are taken equal to 1 (hereafter taken as the unit of energy) and restricted to nearest neighboring sites (indicated by the symbols $\langle\rangle$).

The Kubo formalism [10,11] was used to calculate the conductance and the conductance eigenchannels. [12] For a current propagating in the x-direction, the static electrical conductivity is given by

$$G = -2\left(\frac{e^2}{h}\right)\mathrm{Tr}[(\hbar\hat{v}_x)\mathrm{Im}\hat{\mathcal{G}}(E)(\hbar\hat{v}_x)\mathrm{Im}\hat{\mathcal{G}}(E)], \tag{4}$$

where the velocity (current) operator $\hat{v}_x$ is related to the position operator $\hat{x}$ through the equation of motion $\hbar\hat{v}_x = [\hat{H},\hat{x}]$, $\hat{H}$ being the Hamiltonian. Due to the simple form of $\hbar\hat{v}_x$ [10] only the matrix elements of the Green's function between the left- and right-end slabs of the cavity have to be calculated. This procedure saves a great amount of computing time. $\mathrm{Im}\hat{\mathcal{G}}(E)$ is obtained from the advanced and retarded Green's functions

$$\mathrm{Im}\,\hat{\mathcal{G}}(E) = \frac{1}{2\mathrm{i}}[\hat{\mathcal{G}}^R(E) - \hat{\mathcal{G}}^A(E)]. \tag{5}$$

The matrix elements of the retarded Green's function are given by

$$[E^+\mathbf{I} - \mathbf{H} - \Sigma_{\mathrm{l}}(E^+) - \Sigma_{\mathrm{r}}(E^+)]\mathcal{G}^R(E) = \mathbf{I}, \tag{6}$$

where $E^+ = \lim_{\delta\to 0^+}(E+\mathrm{i}\delta)$ and $\Sigma_{\mathbf{l},\mathbf{r}}(E^+)$ are the retarded self-energies matrices introduced by the left and right semi-infinite leads.

Simulations were carried out on constrictions such as that of Fig. 1 with N_v vacancies randomly distributed over the whole region. Vacancies were introduced by taking $\epsilon_i=\infty$ for $i=1,\ldots,N_v$. Constrictions of width L (all lengths are given in units of the lattice constant) with N_v vacancies distributed over a $L\times L$ region were also investigated. Semi-infinite leads of width L were connected at left and right sides of those regions. In order to make feasible including a large number of realizations of disorder, L was fixed at 51 (some checks with larger systems were also carried out). The energy was varied in steps of 0.001 (of the order of the mean level spacing for $L=51$). The derivative with respect to the energy E was calculated by taking also $\Delta E=0.001$. The results were averaged over at least 1000 realizations of disorder. This allowed us to build up histograms with more than one million points and conductances in the range $G=0-6G_0$ (wider ranges were also occasionally explored).

III. RESULTS

A. Nanoconstrictions

Figure 2 shows the results obtained on a constriction such as that of Fig. 1 with ten vacancies randomly distributed over the whole system. The conductance histogram shows peaks near integer values of the conductance in agreement with the

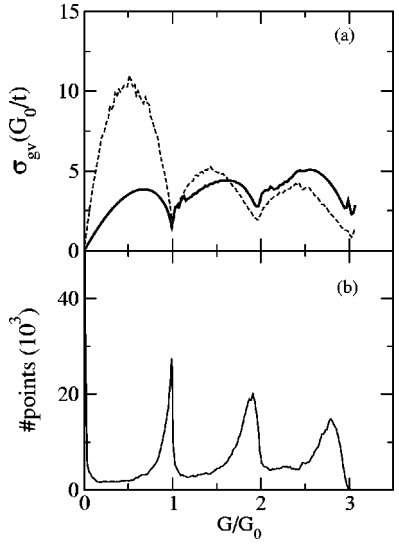

FIG. 2. Conductance fluctuations (a) and conductance histogram (b) in a nanocontact such as that of Fig. 1 with ten vacancies randomly distributed in the region depicted in the figure. Averages were taken over the energy range $[-4,-1]$ and 1000 realizations of disorder. The thick line in (a) corresponds to the numerical results derived from Eq. (2) with $A=10$.

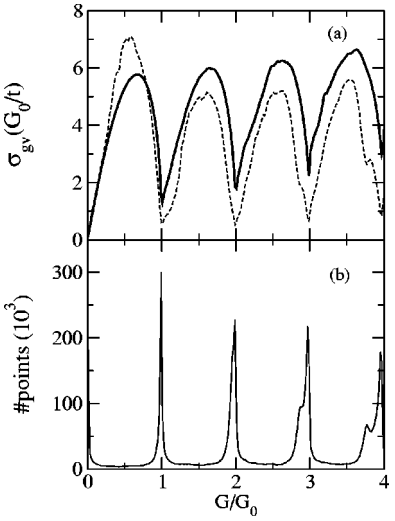

FIG. 3. As Fig. 2 with two vacancies in the region depicted in Fig. 1. In this case the thick line in (a) corresponds to the numerical results derived from Eq. (2) with $A=15$.

experimental data for nanocontacts.[6] There are, however, important differences (relative peak height and peak positions) that are likely due to actual atomic arrangements (the possibility of chain formation, see Ref. 13) and band structure effects not taken into account by our simple model. Fluctuations are also in line with data for noble metals, including the enhancement of the first conductance peak, although in the results shown in Fig. 2, this is more pronounced.[5] In order to check whether this difference is related to the amount of disorder introduced in the calculation, we have carried out a similar calculation with two instead of ten vacancies. The results shown in Fig. 3 clearly indicate that this may in fact be the case. Now the first peak is only 20% higher than the second peak.

In the upper panel of Figs. 2 and 3 we also plot the results obtained by inserting the computed eigenchannels (transmission probabilities T_n for each channel n) in each realization of disorder into Eq. (2) and averaging over realizations. It is clearly noted that Eq. (2) fails in reproducing the enhancement of the first peak in the conductance fluctuations, leading to fluctuations maxima that monotonically increase with conductance. Trying to identify the origin of this enhancement seems worthwhile. In Fig. 4 we show the conductance versus energy for two realizations of disorder in the nanoconstriction of Fig. 1 with ten vacancies. It can be clearly noted that just around the conductance onset there are large differences between the two realizations (indicated by an arrow in the figure) caused by the strong perturbations introduced by vacancies. This is surely the cause of the enhancement of the first peak in Figs. 2 and 3, and may help in attaining a full understanding of the experimental results.

B. Stripes

The results for a stripe of width 51 with ten vacancies distributed over a 51×51 region are shown in Fig. 5. The conductance histogram increases steadily with G and is quite different from those observed in the nanoconstrictions discussed above. Fluctuations show a peak at a conductance smaller than G_0 and then decreases steadily. This behavior is clearly not reproduced by Eq. (2). Although the agreement is, in general, rather poor, the most dramatic difference is the peak below one conductance quantum. As the conductance increases the difference between the two sets of data decreases, and both remain fairly constant (although one slightly increases with G while the other decreases). It is worth noting that increasing the number of vacancies (we have gone up to 200 vacancies in the same square region) does not change the qualitative features of Fig. 5. We have checked that the origin of the peak below one conductance

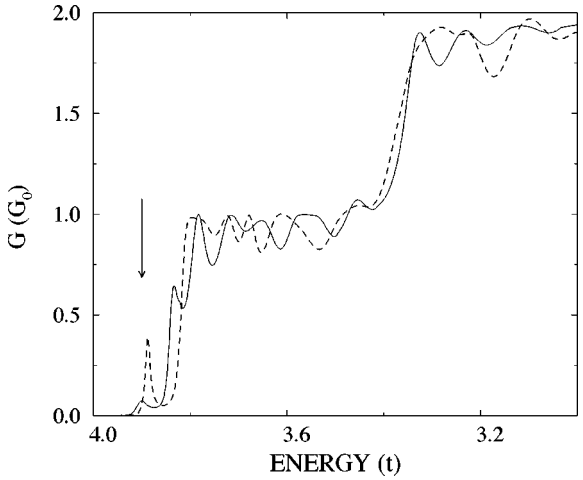

FIG. 4. Conductance versus energy in the nanocontact of Fig. 1 for two realizations of disorder (ten randomly distributed vacancies were included in the region depicted in Fig. 1). The large changes in the conductance just at onset (marked with an arrow) have to be noted. These are likely the origin of the enhancement of the peak in fluctuations that show up for conductances smaller than a conductance quantum (see Figs. 2 and 3 and text).

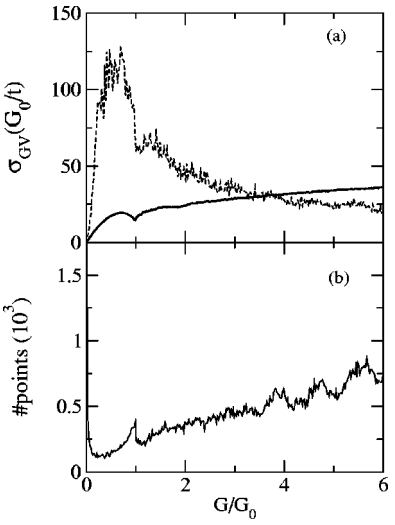

FIG. 5. Conductance fluctuations (a) and conductance histogram (b) in a stripe of width 51 with ten vacancies randomly distributed in a 51×51 region. Averages were taken over the energy range $[-4,-3.3]$ and 1000 realizations of disorder. The thick line in (a) correspond to the numerical results derived from Eq. (2) with $A=50$.

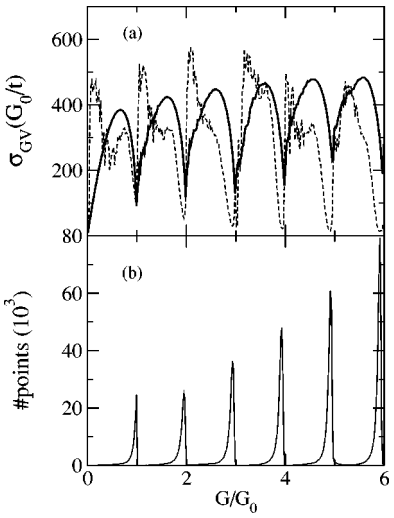

FIG. 6. Conductance fluctuations (a) and conductance histogram (b) in a stripe of width 51 with the energies of the atomic orbitals in a 51×51 region randomly distributed over the range $[-0.05,0.05]$. Averages were taken over the energy range $[-4,-3.8]$ and 4000 realizations of disorder. The thick line in (a) corresponds to the numerical results derived from Eq. (2) with $A=1000$. The unit of energy is the hopping integral t.

quantum is, again, the strong conductance variability around the conductance onset, as illustrated in Fig. 4.

Apparently, the results of Fig. 5 would suggest that there is no quantum suppression of fluctuations in wide nanocontacts where a large number of channels may be opened, in agreement with the results of Ref. 15. In order to further investigate this question we have carried out simulations for a stripe with a very weak Anderson disorder. In particular we chose the energies of atomic orbitals at all sites ϵ_i within a 51×51 region, randomly over the range $[-0.05,0.05]$. The results are reported in Fig. 6. Quantum suppression of fluctuations at integer values of the conductance is now clearly observed. Fluctuations oscillate in a manner similar to the results derived from Eq. (2) also shown in the upper panel of the figure. The rather noisy numerical results are probably related with a characteristic of the histogram shown in the lower panel of Fig. 6: The number of points in the histogram when G varies over the ranges $mG_0-(m+1/2)G_0$ is exceedingly low. In any case, the suppression of conductance fluctuations near integer values of the conductance in systems with a large number of conducting channels is clearly illustrated by these results.

IV. CONCLUSIONS

Conductance fluctuations in metallic nanocontacts and stripes with some degree of disorder have been investigated by means of a simple one-orbital tight binding model. Our results for nanoconstrictions indicate that fluctuations oscillate with conductance showing minima near integer multiples of the conductance quantum in a manner similar to experimental observations and to the results derived from a model based upon the Landauer-Büttiker approach.[5] Besides, our results show an enhancement of the first fluctuation peak that, being in qualitative agreement with experimental results for gold and silver, is not accounted for by the model of Ref. 5. Our analysis indicates that the origin of this enhancement may likely be due to the large effects that disorder introduces at the conductance onset. On the other hand the results for weakly disordered stripes do also show quantum suppression of fluctuations at integer values of the conductance. Instead, in stripes with relatively strong disorder, fluctuations show a maximum at a conductance smaller than one quantum, decreasing almost monotonically thereafter. The latter behavior is not reproduced by the simple expression of Ref. 5.

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