

Conductance quantization in surface disordered nanoscale systems

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During the last decades the quantization of the conductance in nanoscale metallic contacts has been the subject of intense research. Before the contact breaks the conductance presents a stepwise behavior. The individual conductance traces are irreproducible, but, nevertheless, share some characteristics. The plateaus observed in the conductance traces are placed very close to integer multiples of the conductance quantum $G_0 = 2e^2/h$, suggesting the quantization of the conductance in nanocontacts. The irreproducibility of the traces is a consequence of mechanical instabilities occurring during the elongation process. Transitions from one stable atomic configuration to another take place at the same time as the conductance jumps.

The common features of the conductance of atomic-scale metallic contacts the study are revealed in a statistical way: the conductance of hundreds or even thousands of conductance traces are recorded and presented in the form of a histogram. These histograms present very well defined peaks at integer multiples of the conductance quantum. This has been taken by some groups as a proof of “true” conductance quantization, but the existence of some metals not displaying histograms with such a behavior cast doubts on this fact.

Here we present a theoretical analysis of the conductance in nanoscale systems with one restriction the contact cross-section does not vary when during the elongation process. The system consists in a two-dimensional wire whose central part presents a small amount of disorder in one of its surfaces (see inset of Fig. 1). This is to mimic the fact that, due to the atomic dimensions of the wire, there is no room for defects in the interior and the only source of scattering are the irregularities of the surface. The wire width (W_0) is such that the wire accomodates five propagating channels ($W_0/\lambda_F = 2.6$), in the central part, due to the

disorder, the width ranges from $W_0 - \delta$ to $W_0 + \delta$. Under these conditions the two electrodes (the two semi-infinite clean parts) are separated, leading to an increase of the disordered region that in its term leads to a decrease of the conductance. The individual traces, as well as the average, do not resemble to those obtained in nanocontact experiments. But, however, after performing thousands of individual traces, the histograms reveal clear peaks at integer multiples of G_0 (see Fig. 1).

From this result we can conclude that the conductance quantization phenomenon is a natural consequence of the nanoscale dimensions of the contacts, since there are no mechanical effects involved in the simulations.

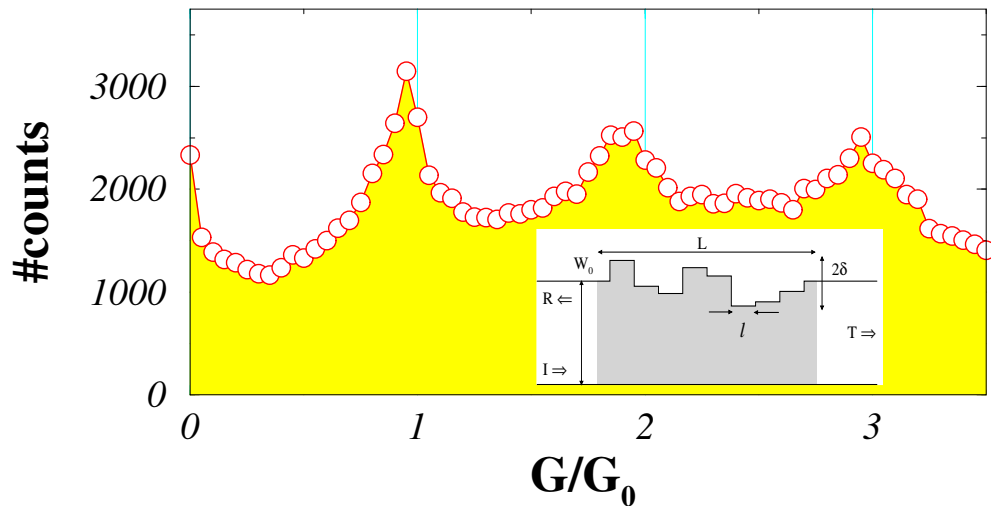


FIG. 1. Calculated histogram for a wire with the following parameters: $W_0/\delta = 7$ and $l/\delta = 3/2$ (i.e. $2\delta/W_0 = 0.286$ and $l/W_0 = 0.214$) where clear peaks close to integer multiples of G_0 are observed. The experimental displacement to slightly lower values is also reproduced. Inset: Schematic view of the geometry under consideration.