Comment on "Quantized Conductance in an Atom-Sized Point Contact"

In a recent Letter [1], Olesen *et al.* claim that they have clear evidence for conductance quantization in contacts between a W scanning tunneling microscopy (STM) tip and a metal surface at room temperature. We disagree both with their model calculations and with their experimental interpretation.

In irregular or atomically disordered systems, where there are no well-defined transverse modes, one loses the notion of conductance channels. Conductance jumps may still occur, as a result, say, of abrupt atomic rearrangements, but these jumps can be of arbitrary size and are not a sign of conductance quantization. Experimental evidence for this interpretation is given in [2] based on analysis of fluctuations at the jumps.

In their calculations, Olesen *et al.* find quantized conductance steps. This is an inevitable consequence of the assumption that the contact is a jellium constriction with smooth boundaries and an adiabatically varying cross section. By making this assumption, the authors exclude the very factors which could destroy the quantization effect, namely, the discrete atomic structure of the contact and irregularities in this structure. These features have the same length scale as the Fermi wavelength and cannot be ignored.

The stretch per conductance step is set by the mechanical instabilities, whether or not the two coincide exactly. Provided the strain is localized in a constriction of atomic dimensions, the stretch between instabilities must be of the order of the bond length. Thus, the stretch per step is not unique to a given contact geometry.

The smoothly decreasing minimal cross section, used in [1], is obtained by averaging the geometry from the dynamic simulations over 2.7 ps, which amounts to several atomic vibration periods. But, Fermi electrons crossing the contact see frozen atomic positions. Therefore, Olesen *et al.* have calculated a conductance for an average atomic configuration, whereas in reality one measures averages of *instantaneous* conductances.

We agree with Olesen *et al.* that provided well-defined transverse modes exist, and provided the minimal cross section of the contact decreases smoothly during stretching, the jumps in the conductance do not result from mechanical rearrangements. But these provisos are assumed and not proven in [1]. By contrast, in [3], *nonquantized* conductance jumps, which coincide unambiguously with mechanical instabilities, are found in a calculation which uses the exact atomic geometry at every stage of a dynamic simulation.

Our principal objection to the experimental results presented in Figs. 1 and 2 of [1] is that it is far from obvious whether or not the conductance curves show quantization. For comparison we show in Fig. 1 results which were obtained for a Au contact under ultrahigh vacuum at 4.2 K

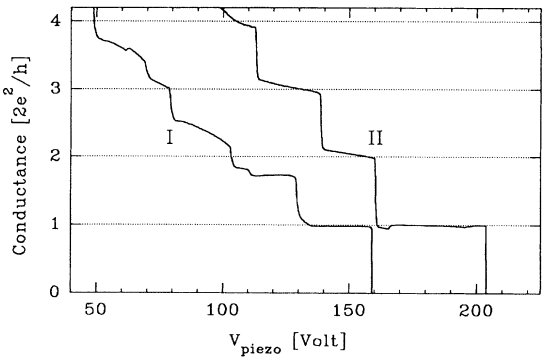

FIG. 1. Two examples of the conductance of an atom-sized Au junction as a function of the piezovoltage.

by the controllable break junction technique [4]. The great majority of our recordings is represented by curves similar to curve I in Fig. 1, which as a result of the much higher resolution compared to [1], clearly shows steps very different from quantum units. Some of the (less well-resolved) conductance plateaus presented in [1] also belong to this class and cannot be explained by the simplified model in [1]. In contrast, curve II of Fig. 1 is an example of a truly exceptional recording which also shows jumps in the conductance (due to the atomic rearrangements), but in this case with plateaus at multiples of the quantum unit. A possible explanation of these integer values in terms of conductance quantization is still under investigation.

In conclusion, we do not agree that the experimental results of [1] provide conclusive evidence for conductance quantization in metallic contacts. The calculations of [1] do not resolve this question because of the assumptions they are based on.

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