Theoretical Studies of the Non-Linear Transport Properties of Molecular Wires

Massimiliano Di Ventra, Virginia Tech, DMR-0133075

Electronic circuits made up of nanoscale components (like, e.g., nanotubes, single molecules, atomic wires - see Fig 1a) may find an application beyond conventional silicon technology. Quantum effects are, however, responsible for a host of different phenomena not generally present in conventional electronics.

We predict that, under certain conditions, chaotic transport in arrays of quantum wires should be observed in the presence of an ac field (Fig.1b). Chaos is due to the formation of electric domains and domain walls in the wire when sequential resonant tunneling occurs between adjacent units (Fig. 1c).

Chaotic transport is an interesting effect but may be detrimental for actual electronic applications of quantum wires. This study shows under which conditions such an effect can be observed and technologically avoided.

This work has been done in collaboration with two undergraduate students:

Mike Zwolak (undergraduate)
David Ferguson (undergraduate)

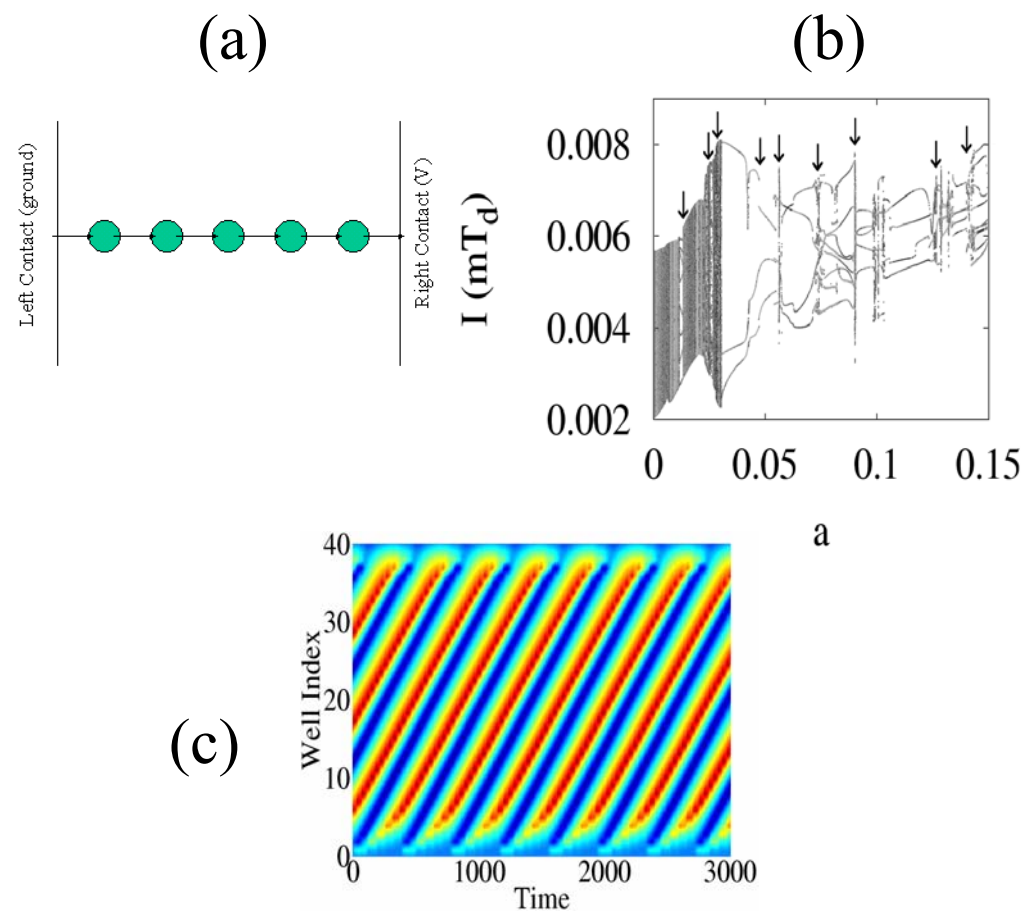

Figure 1. (a) Scheme of the quantum wire investigated. (b) Poincaré map of the current as a function of the strength *a* of the external ac field. The arrows indicate the onset of chaotic regions. (c) Charge density in a wire of 40 units as a function of time (internal units). Domain walls form at regular intervals.

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Educational:
2 undergraduates,
4 grad students,
2 post-docs.

The two undergraduate students are involved in several projects related to transport in quantum wires including the one highlighted here, and have learned several theoretical techniques and computational methods.

Book project:
The PI is co-editing a comprehensive textbook that would support courses on nanotechnology aimed at the senior undergraduate and masters level students (Fig. 2). The book will be published by Kluwer Academic. The text will consist of 25 chapters arranged in seven sections (Fig. 2). It will cover the techniques for fabricating and characterizing nanostructures, the various building-block materials for nanotechnology, and the applications of these novel technologies in electronic, magnetic, integrative, optoelectronic, and biological systems and devices. The book will also include a CD-ROM that will contain color versions of the figures appearing in each chapter, as well as supplemental set of slides that we have designed to support a class offered at Virginia Tech and the University of Pennsylvania.

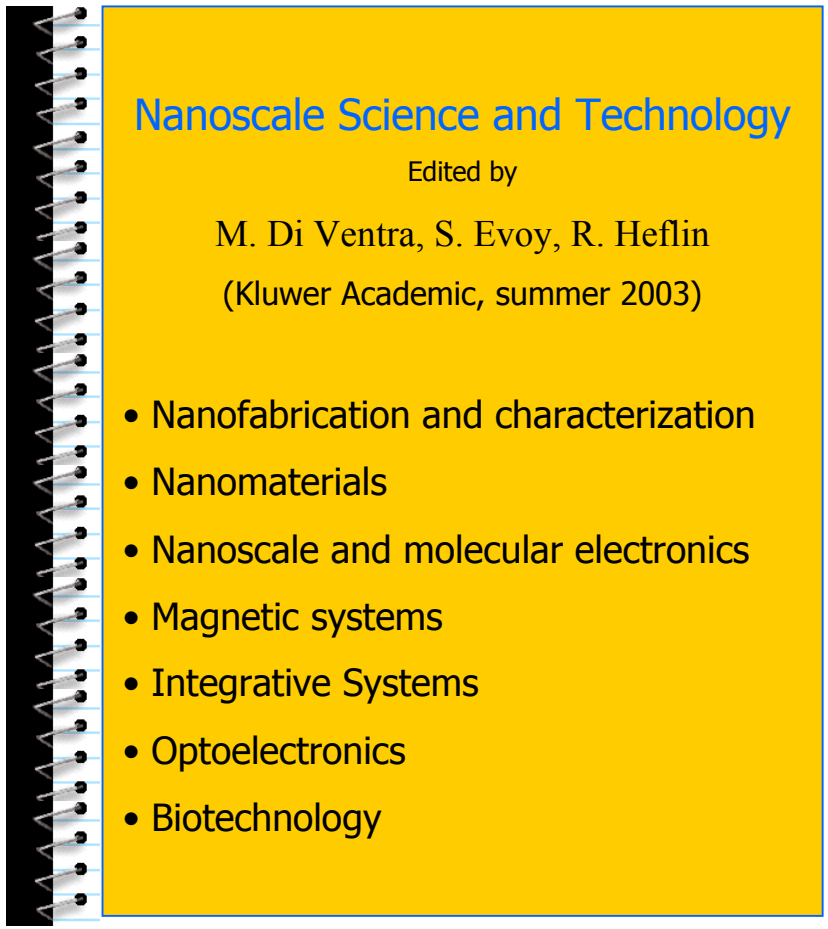

Figure 2. Outline of the textbook "Nanoscale Science and Technology" for senior undergraduate/junior graduate students.