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Ballistic conductance in quantum devices: from organic polymers to nanotubes ☆

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Abstract

With the size of electronic devices approaching the nanometer scale, transition to self-assembly in molecular electronics systems appears to be technologically the next step to pursue. Quantum conductors with an especially high potential for applications are organic polymers and carbon nanotubes. The latter are being considered for use as both nonlinear electronic devices and as connectors between molecular electronics devices and the ''outside world''. Depending on their internal structure and the nature of the electric contact to leads, these systems may exhibit fractional conductance quantization. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

With the continually decreasing size of electronic and micromechanical devices, there is an increasing interest in the self-assembly of logic elements and nanoswitches [1]. Recent experiments suggest that specific polymers, such as oligo(phenylene ethynylene) [2], and functionalized carbon nanotubes are likely candidates for such logic gates and switches. It is conceivable that a complex logic device, containing many switching and memory elements that are connected by conducting carbon nanotubes, may form completely in a self-assembly process. Due to the nanoscale cross-section of conducting polymers and nanotubes, their conductance is quantized. In the following, I will discuss the unexpected conductance behavior that arises in nanotubes due to inhomogeneities, caused by changing number of walls along the tube axis.

Carbon nanotubes [3], consisting of graphite layers wrapped into seamless cylinders, are now being produced routinely using carbon arc, laser vaporization of graphite, catalytic decomposition of carbon monoxide at high pressures, and chemical vapor deposition techniques [4]. These methods yield single- and multi-wall nanotubes that are up to a fraction of a millimeter long, yet only nanometers in diameter. Virtual absence of defects suggests that these molecular conductors should be ideal candidates for use as nanowires that conduct electricity efficiently.

The present study has been motivated by recent observations of electron transport in nanotubes that is believed to be ballistic in nature, implying the absence of inelastic scattering. Recent conductance measurements of multi-wall carbon nanotubes [5] have raised a significant controversy due to the observation of unexpected conductance values in apparent disagreement with theoretical predictions.

2. Electrical conductance of carbon nanotubes

To address the conductance of multi-wall carbon nanotubes [6], we combined a linear combination of

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atomic orbitals (LCAO) Hamiltonian with a scattering technique developed recently for magnetic multi-layers [7,8]. The parameterization of the LCAO matrix elements is based on ab initio results for simpler structures [9]. Our calculations can build on a number of published theoretical studies of the electronic structure of single-wall [10–12] and multi-wall carbon nanotubes [13–15]. Calculations for single-wall nanotube ropes [16,17] have shown that interwall coupling may induce pseudo-gaps near the Fermi level in these systems, with serious consequences for their conductance behavior.

Our scattering technique approach to determine the conductance of inhomogeneous multi-wall nanotubes [6] is based on the quantum-mechanical scattering matrix S of a phase-coherent "defective" region that is connected to "ideal" external reservoirs [7]. At zero temperature, the energy-dependent electrical conductance is given by the Landauer–Büttiker formula [18]

$$G(E) = \frac{2e^2}{h} T(E), \tag{1}$$

where $T(E)$ is the total transmission coefficient, evaluated at the Fermi energy E_F.

For a homogeneous system, $T(E)$ assumes integer values corresponding to the total number of open conduction channels at the energy E. For individual (n, n) "armchair" tubes, this integer is further predicted [19] to be an even multiple of the conductance quantum $G_0 = 2e^2/h \approx (12.9\ \mathrm{k\Omega})^{-1}$, with a conductance $G = 2G_0$ near the Fermi level. In the (10,10)@(15,15) double-wall nanotube [15] and the (5,5)@(10,10)@(15,15) triple-wall nanotube, the interwall interaction significantly modifies the electronic states near the Fermi level and blocks some of the conduction channels close to E_F. This is shown in Fig. 1.

The experimental set-up of Ref. [5], shown schematically in Fig. 2(a), consists of a multi-wall nanotube that is attached to a gold tip of a scanning tunneling microscope (STM) and used as an electrode. The STM allows the tube to be immersed at calibrated depth intervals into liquid mercury, acting as a counter-electrode. This arrangement allows precise conduction measurements to be performed on an isolated tube. The experimental data of Ref. [5] for the conductance G as a function of the immersion depth z of the tube, reproduced in Fig. 2(e), suggest that in a finite-length multi-wall nanotube, the conductance may achieve values as small as $0.5G_0$ or $1G_0$.

As nothing is known about the internal structure of the multi-wall nanotubes used or the nature of the contact between the tube and the Au and Hg electrodes, we have considered several scenarios and concluded that the experimental data can only be explained by assuming that the current injection from the gold electrode occurs exclusively into the outermost tube wall, and that the chemical potential equals that of mercury, shifted by a contact potential, only within the submerged portion of the tube. In other words, the number of tube walls in contact with mercury depends on the immersion depth. The main origin of the anomalous conductance reduc-

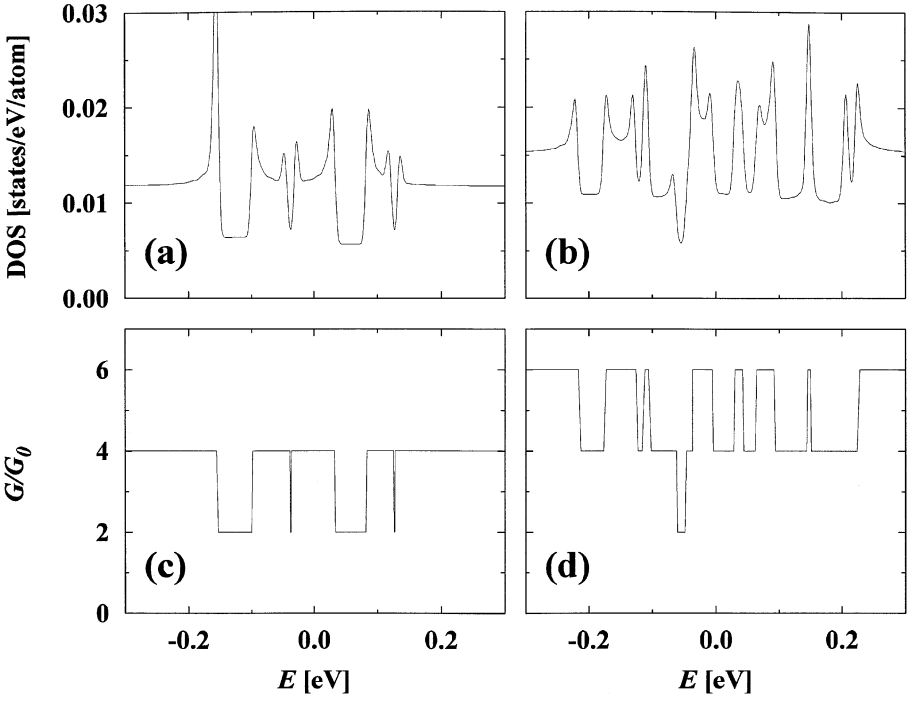

Fig. 1. Electronic density of states and conductance of a double-wall (10,10)@(15,15) nanotube ((a) and (c), respectively), and a triple-wall (5,5)@(10,10)@(15,15) nanotube ((b) and (d), respectively). From Ref. [6], © American Physical Society 2000.

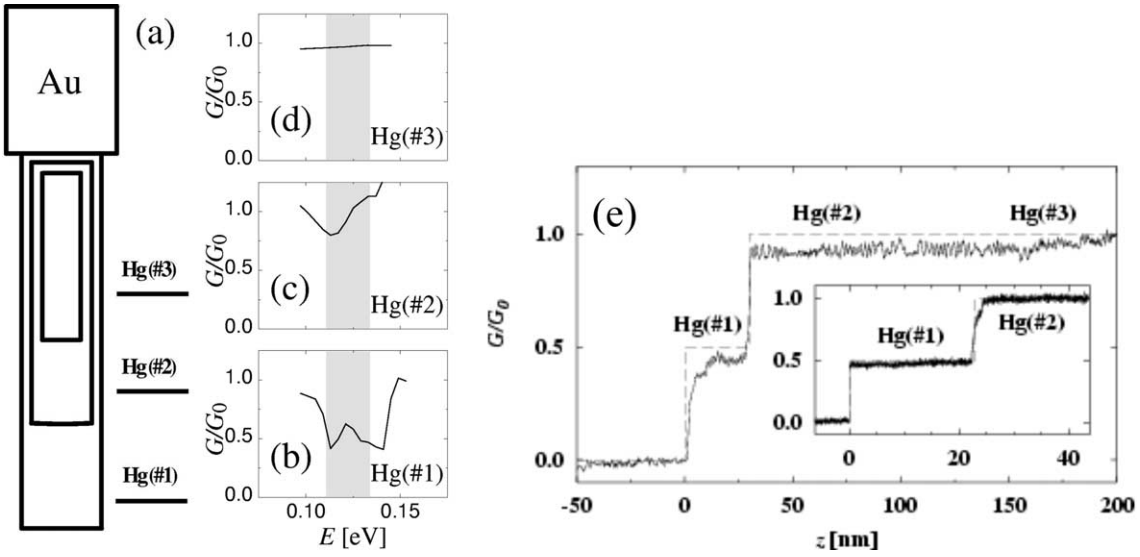

Fig. 2. (a) Schematic geometry of a multi-wall nanotube that is being immersed into mercury up to different depths labeled Hg(#1), Hg(#2), and Hg(#3). Only the outermost tube is considered to be in contact with the gold STM tip on which it is suspended. The conductance of this system is given in (b) for the immersion depth Hg(#1), in (c) for Hg(#2), and in (d) for Hg(#3) as a function of the position of E_F. The Fermi level may shift with changing immersion depth within a narrow range indicated by the shaded region. (e) Conductance G of a multi-wall nanotube as a function of immersion depth z in mercury, given in units of the conductance quantum $G_0 = 2e^2/h \approx (12.9\ \mathrm{k\Omega})^{-1}$. Results predicted for the multi-wall nanotube, given by the dashed line, are superimposed on the experimental data of Ref. [5]. The main figure and the inset show data for two nanotube samples, which in our interpretation only differ in the length of the terminating single-wall segment. From Ref. [6], © American Physical Society 2000.

tion from the theoretically expected integer multiple of $2G_0$ is the backscattering of carriers at the interface of two regions with different numbers of walls due to a discontinuous change of the conduction current distribution across the individual walls.

3. Summary and conclusions

The calculations discussed above indicate that carbon nanotubes show unusual electrical conductance behavior. Results for the electrical transport indicate that the interwall interaction in multi-wall nanotubes not only blocks certain conduction channels, but also re-distributes the current nonuniformly across the walls. The puzzling observation of fractional quantum conductance in multi-wall nanotubes can be explained by backscattering at the interfaces of regions with different numbers of walls. Sample-to-sample variations in the internal structure of the tubes offer a natural explanation for the observed variations of the conductance.

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