

Spin transport in disordered single-wall carbon nanotubes contacted to ferromagnetic leads

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(Dated: April 17, 2007)

Abstract

Recent conductance measurements on multi-wall carbon nanotubes (CNTs) reveal an effective behavior similar to disordered single-wall CNTs. This is due to the fact that electric current flows essentially through the outermost shell and is strongly influenced by inhomogeneous electrostatic potential coming from the inner tubes. Here, we present theoretical studies of spin-dependent transport through disorder-free double-wall CNTs as well as single-wall CNTs with Anderson-type disorder. The CNTs are end-contacted to ferromagnetic electrodes modelled as fcc (111) surfaces. Our results shed additional light on the giant magnetoresistance effect in CNTs. Some reported results concern realistically long CNTs, up to several hundred nanometers.

PACS numbers: 85.35.Kt, 85.75.-d, 81.07.De, 73.63.-b, 79.60.Ht

INTRODUCTION

Over the last two decades, the magneto-electronics, based on all-metal multilayers, has proven to be very successful indeed [1]. The most important effect which should be invoked in this context is giant magnetoresistance (GMR) discovered in 1988 [2]. This effect makes it possible to control electric current flowing through magnetic materials by means of a magnetic field. In other words, the essence of the GMR effect lies in taking advantage of not just the electronic charge alone but also of its spin counterpart. Quite naturally researchers involved so far in physics of semiconductors, as well as those studying molecular systems have intensified their efforts in search for possible analogous effects in all-semiconducting [3] and/or hybrid systems (combinations among metals, semiconductors and molecules) [4, 5]. Consequently, a new field of science and technology has been triggered, under the name of spintronics [6, 7]. Here we report our results on the GMR effect in perfect and disordered carbon nanotubes sandwiched between ferromagnetic electrodes. There is no doubt nowadays that miniaturization requirements imposed on the emerging spintronics will be met by applying the so-called bottom-up approach as far as designing of new electronic devices is concerned. From this point of view carbon nanotubes are surely excellent candidates.

DOUBLE-WALL CNTS

We start our studies with carbon nanotubes (CNTs) end-contacted to metal electrodes. Our present approach is essentially that described in detail in [8] with an improved simulation method of CNT/metal-electrode interface developed in [9]. Spin-polarization of the ferromagnetic leads is defined as $P = 100(n_{\uparrow} - n_{\downarrow})/(n_{\uparrow} + n_{\downarrow})$, where n_{σ} stands for a number of σ -spin electrons per lattice site. It is noteworthy that the structures in question are relaxed under the Lennard-Jones potential in order to find energetically favorable relative positions of CNTs' and electrodes' interface atoms. During the relaxation process the external electrodes are allowed to rotate and shift independently of each other, similarly the inner tube is also free to rotate. As regards the inter-tube hopping integrals, they are taken in the form as proposed in [10], i.e. set to $t_{int} = -(t/8)\cos\theta_{ij}\exp[(d_{ij} - b)/\delta]$, where θ is the angle between the π orbitals, d is a relative distance, t stands for the nearest neighbor hopping integral (chosen as energy unit), $\delta = 0.45 \text{ \AA}$ and $b = 3.34 \text{ \AA}$. The GMR coefficient

is defined in terms of the conductances, G , as $\text{GMR}=1 - G_{\uparrow\downarrow}/G_{\uparrow\uparrow}$, with $\uparrow\uparrow$ ($\uparrow\downarrow$) denoting aligned (antialigned) magnetization orientation of the electrodes.

Most of the hitherto existing experiments on electronic transport suggest that current flowing through MWCNTs goes mostly through the outermost shell (see e.g. [11]). A precise role of the inner shells is still hardly known. Here we show the results on the GMR effect in two double-wall (DW) CNTs which have the same outer shell but different - though non-conductive in each case - inner shells. Specifically the DWCNTs in question are: (i) the zigzag at armchair (45-(5,0)@39-(8,8)) and (ii) the armchair at armchair (38-(3,3)@ 39-(8,8)), using a short-hand notation L-(n,m), for the length (in carbon rings) and the chiral vector, respectively. In the former case the corresponding lengths are roughly the same (ca. 5 nm each) so both the inner tube and the outer one are well contacted to the magnetic electrodes. In the latter case, in turn, the inner shell is artificially shortened and forced thereby to be out of contact to the drain electrode. Fig.1 presents giant magnetoresistance for the two DWCNTs. Despite the fact that both the systems are formally similar (at least in the presented "energy window" ($|E/t| < 0.2$), which falls into the zigzag-tube gap), the GMR curves are clearly different. We attribute these differences to intertube-quantum interferences which are present owing to the non-vanishing t_{int} . To mimic a possible effect of some additional disorder we present also GMR curves (thin lines) calculated from the energy-averaged conductances, where the averaging has been made over the most obvious energy scale in this context, namely over an energy bin equal to the inter-level spacing of the outer shell $\Delta E = \pi\sqrt{3}/L$ (in the present units). In the following subsection we present a more direct approach to the disorder issue.

SINGLE-WALL CNTS WITH ANDERSON DISORDER

The simplest way to include the effect of disorder in a system described in terms of the tight-binding model is to allow all on-site (atomic) potentials to take random values within a given energy interval. Such an approach has been already applied to CNTs [12], but to our knowledge, only for tubes with non-magnetic leads. In the case of disordered systems, it is necessary to perform statistical (ensemble) averaging of the results corresponding to particular sets of on-site potential distributions (to be referred to as samples hereafter). This is a purely technical problem easy to overcome at the expense of the computation

time. Another more serious problem is to develop a recursive procedure, which would make it possible to deal with big systems approaching macroscopic sizes of the order of several hundred nanometers. Recursive algorithms based on Dyson-type equations for the Green's function are well-known [13, 14]. Here however we modify those methods in order to make them work in the case of highly non-homogenous systems composed of disordered carbon nanotubes and two adjacent atomic layers from each electrode (to be referred to as the extended molecule). While conductance computations are usually rather fast, the computations of electronic charge at all atoms of a big system are extremely computer time consuming and expensive. In order to surmount this difficulty we impose a global charge neutrality condition only on a disorder-free "parent" system and self-consistently determine detailed values of all its on-site potentials (ca. 4000 and 40000 atoms for the SWCNT(8,8), 30 and 300 nm long). On introducing disorder, these on-site potentials are modified by random corrections fluctuating around zero within an interval $[-W/2, W/2]$. So, on the average the global charge of the Anderson-disordered extended molecule might be regarded as roughly close to that of the neutral parent system. Our computations proceed according to the following protocol: First the surface Green functions are found (see [9] for details). Second, the set of on-site potentials which ensure the charge neutrality of the parent system is found. Third, conductance calculations along with the corresponding GMR coefficients are performed for 100 different samples with random on-site corrections. Finally the results are ensemble-averaged. The main results of this study is presented in Fig.2, for the SWCNT (8,8) consisting of 240 carbon rings (120 unit cells \sim 30 nm). It is seen that although disorder suppresses the GMR, it happens to be of about the right value as compared to recent experiments on MWCNTs with transparent ferromagnetic contacts made from $Pd_{0.3}Ni_{0.7}$ (device resistances are then as low as $5.6 k\Omega$ at 300K) [15]. Other noteworthy points are: (i) on the average the GMR remains positive, and (ii) there exist some extra features in the GMR spectrum at energies close to ± 0.4 and ± 0.7 corresponding to higher sub-band onsets in the pristine (ideal) SWCNT.

For smaller W , GMR increases and eventually oscillates with the amplitude of roughly ± 0.2 in the disorder-free (parent) case, as shown in Fig.3 (l.h.s). Additionally the right-hand side of this figure highlights the length-effect on the period of oscillations. For the sake of simplicity this is shown for the paramagnetic leads. It is clearly seen that in the absence of disorder the observed periodicity reflects length-dependent interferences, as expected for

a (quasi) ballistic transport. In the magnetic case the peaks are split due to the lifting of spin-degeneracy. The quasi-periodic behavior does always occur when there is no disorder, regardless of whether the electrodes are ferromagnetic or not (c.f. the inset in Fig.3 with the thick solid curve on the r.h.s). From the present results one sees that the process of averaging of conductance and GMR spectra leads to a subtle interplay between the length and the amount of disorder in the CNTs.

SUMMARY

In this work it has been shown theoretically that the GMR effect in ferromagnetically contacted carbon nanotubes is quite considerable and may reach a few tens percent. Ideally, the GMR coefficient oscillates as a function of energy (gate-voltage) with a quasi-period close to the inter-level spacing of the CNT, which scales inversely proportional to the nanotube length. Yet, such a picture is to some extent too detailed if the system at hand is imperfect, e.g. due to some impurities, dopants or a presence of incommensurate inner shells in a MWCNT. The disorder-averaged GMR ranges from 6% down to 2% in the vicinity of the charge neutrality point, in conformity with recent experiments on MWCNTs with transparent ferromagnetic contacts. Furthermore, the aforementioned periodicity gets nearly completely suppressed, and there is no more tendency for the GMR to become negative.

S. K. thanks the KBN project (PBZ-KBN-044/P03-2001), the Centre of Excellence (contract No. G5MA-CT-2002-04049) and the Poznan Supercomputing and Networking Center for the computing time. This work was partially funded by the Volkswagen Foundation and the Vielberth Foundation.

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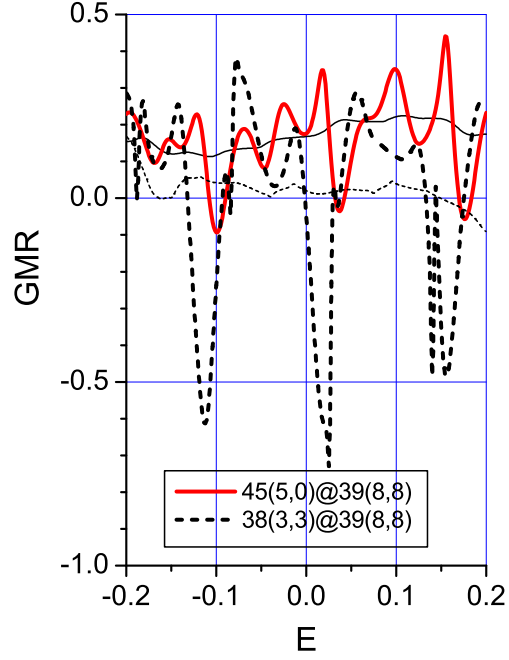


FIG. 1: GMR for the double-wall carbon nanotubes 45-(5,0)@39-(8,8) (solid thick line) and 38-(3,3)@39-(8,8) (thick dashed line) attached to ferromagnetic leads with 50% spin-polarization. To mimic a possible effect of disorder, there are also shown the GMR curves computed from ΔE -averaged conductances (thin curves of the same style), where ΔE is the inter-level spacing of the outer shell.

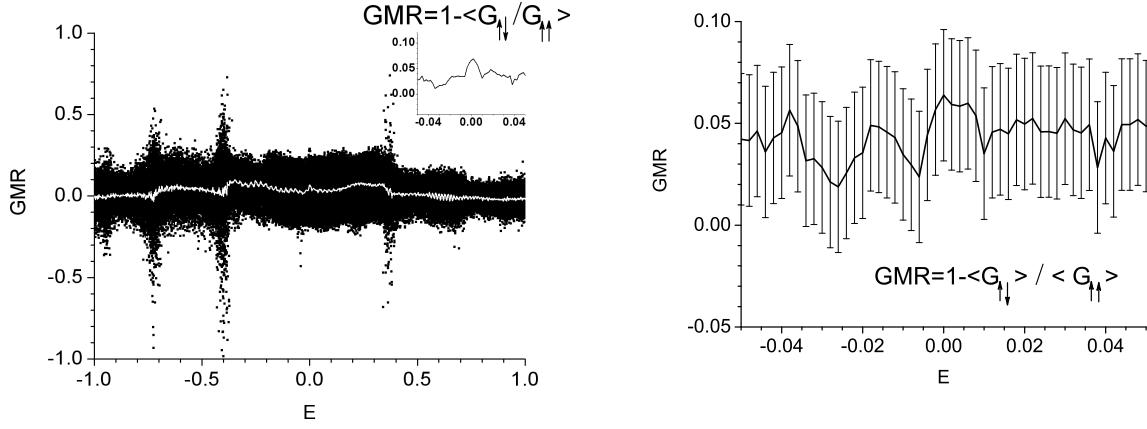


FIG. 2: Left hand side: GMR for individual SWCNTs (8,8), ca. 30 nm in length (points), along with the GMR (white curve) averaged over 100 samples with disorder-induced corrections to the on-site potentials (within $[-W/2, W/2]$ for $W=0.2$). On the right hand side the GMR computed from the disorder-averaged conductances together with the standard-deviation error bars are shown in the vicinity of the charge neutrality point.

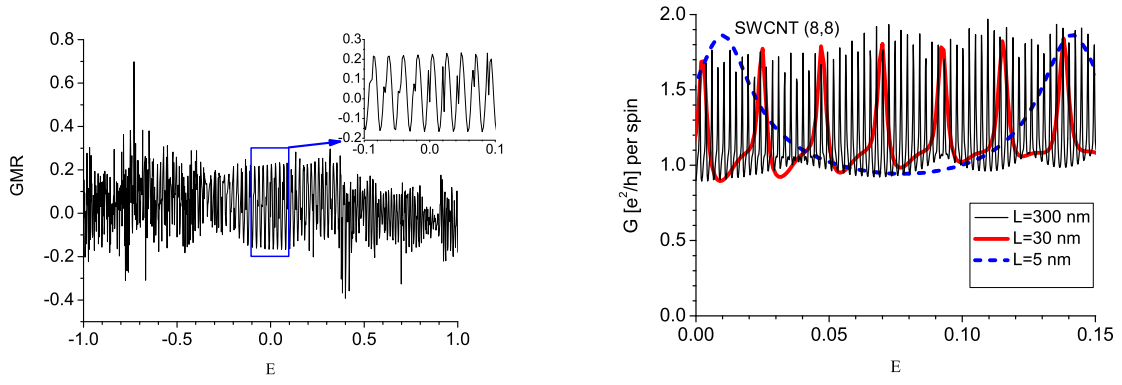


FIG. 3: Left hand side: GMR for disorder-free SWCNT (8,8), $P=50\%$, $W=0$, $L=240$ carbon rings (~ 30 nm). Right hand side: visualization of the length-dependent periodicity of the conductance for the case of paramagnetic leads, $P=0$, and $L=5$, 30 and 300 nm. Compare the inset with the thick solid curve to see that the quasi-period of oscillations is roughly maintained, but in the magnetic case the peaks are spin-split.