Effect of Contact Interfaces on Quantum Conductance of Armchair Nanotubes

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Abstract

Effect of contact interfaces, between metallic single-wall carbon nanotubes (SWCNT) and external electrodes made also of nanotubes, on the electrical conductance is studied. A tight-binding model with both diagonal and off-diagonal disorder, a recursive Green function technique as well as the Landauer formalism are used. The studies are carried out within the coherent transport regime and are focused on: (i) evolution from conductance quantization to resonant tunneling, (ii) SWCNT’s length effects and (iii) magnetoresistance. It is shown that the so-called on-resonance devices, i.e. nanotubes having a conductance peak at the Fermi energy, occur with a period of 3

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carbon inter-ring spacings. Additionally, the present approach provides an insight into magnetoresistance dependence of SWCNTs on conditions at the contact interface.

Since carbon nanotubes were discovered in 1991 [1], a great amount of research has been devoted to their mechanical, transport and electric properties [2]. Carbon nanotubes are already used as prototype devices such as field emitters, current rectifiers or single-electron transistors [3,4]. Also from the theoretical viewpoint the carbon nanotubes are a fascinating subject to study. Their electrical properties depend critically on the so-called chirality and range from metallic to semiconducting. The metallic properties are expected provided that the wrapping vector components \((n, m)\), defined on the graphene plane, satisfy the condition \(n - m = 3 \cdot \text{integer}\).

The system under consideration here is a purely molecular one, consisting of a central part made of a single-wall carbon nanotube (SWCNT) sandwiched between two semi-infinite defect-free lead wires made also of the SWCNTs. Such molecular systems can now be fabricated, with the central segment defined e.g. by creating either bent or twisted interfaces (see [5], [6] and the references therein). Hereafter the central part and the lead wires will be referred to as the sample and the electrodes, respectively. Although in practice molecular systems are coupled with the macroscopic world via extra metallic electrodes (usually Au), the latter have negligible effect on the total resistance which is nearly entirely due to the sample and the interfaces (contacts) between the sample and the electrodes. So formally the Au electrodes may be incorporated into the electron reservoirs and skipped.

The whole system is described by a single-band tight-binding Hamiltonian

\[
\hat{H} = \sum_{I,J} T_{I,J} |I><J| + \sum_I D_I |I><I|, \tag{1}
\]

where \(|I\rangle\) and \(|J\rangle\) stand for orbitals related to repeat units (principle layers) within both the electrodes and the sample. So the Hamiltonian has got a block-tridiagonal form, with off-diagonal matrices denoted by \(T\), and the on-diagonal ones \(D\). The theoretical approach applied here – based on the Landauer formula and the Green’s function method –
proceeds along the lines of Ref. [4]. In particular, the conductance is expressed in terms of the Green functions and the so-called broadening functions

\[ \Gamma^{L,R} = i[\Sigma^{L,R} - (\Sigma^{L,R})^\dagger], \] (2)

where \( \Sigma^L = T_{1,0}g^L(0,0)T_{0,1} \) and \( \Sigma^R = T_{N,N+1}g^R(N + 1, N + 1)T_{N+1,N} \) with the \( T \)s, \( g^L \), \( g^R \) standing for the coupling matrices, and the left- and right-electrode Green functions.

In this paper we want to achieve 3 objectives: (i) to explain the effect of conditions at sample-electrode interfaces and (ii) of the sample length on the electrical conductance, and (iii) to propose a simplistic approach to the spin-polarized transport (giant magnetoresistance, GMR) through the SWCNT. Letting the transport remain phase-coherent, it will be tested how the conductance evolves when the interface conditions change. The conditions are defined by means of just two parameters, namely the hopping across the interface, \( t_c \) and the on-site potential of the first carbon ring of the SWCNT sample and the last one. For armchair SWCNTs studied here (n=m) the repeat unit, \( a = 2.49 \text{Å} \), contains two carbon rings. The first carbon ring as well as the last one can have an arbitrary on-site potential, whereas the other on-site potentials are set to \( \epsilon = 0 \). Similarly, all the interatomic hopping integrals are \( t_{i,j} = -1 \) (\( |t_{i,j}| \) is the energy unit), except for those passing through the interfaces which are also arbitrary, \( t_c \). Figure 1 illustrates the effect of the interface hopping parameter on the conductance.
FIG. 1. Conductance (per spin) through the armchair SWCNT placed between electrodes made also of the SWCNTs (all with $n = m = 3$). The thick line corresponds to the pristine SWCNT ($t_c = -1$, $\epsilon = 0.0$), whereas the solid thin line and the dashed one correspond to the length $L = 7a$ and the interface parameters $t_c = -0.9$, $\epsilon = 0.0$, and $t_c = -0.5$, $\epsilon = 0.0$, respectively.

It is readily seen that the conductance evolves gradually from the continuous step-function quantized at integer multiples of $2e^2/h$ to the collection of narrow peaks – typical of the resonant tunneling. The overall picture does not depend on the tube diameter (determined by $m$) and varies in a quasi-periodic way with the sample length (apart from the trivial case of $t_c = -1$, $\epsilon = 0$ corresponding to the infinite perfect SWCNT). An interesting feature of Fig.1 is the existence of the central peak at energy corresponding to the Fermi energy $E=0$. The origin of this has been explained in terms of the so-called 3N+1 rule. If the sample length is equal to $L = (3N + 1)a$, with $N$ being an integer number, the allowed discrete values of the wave-vector include $k=2\pi/3a$ which zeros the electron dispersion relation. When the amount of disorder increases, the wave-vector is no longer a good quantum number, so there is no reason for the 3N+1 rule to be still valid. Fig. 2, plotted for $E=0$ ant $t_c = -0.5$, shows it very clearly since the ”on-resonance” peaks happen to depend strongly on the interface on-site parameters, and in fact they may also be described by the 3N rule (diamonds) or the 3N-1 rule (triangles).
FIG. 2. Length-dependent conductance (per spin) of the SWCNT for $E=0$ and various $\epsilon$ parameters. Depending on these parameters, the so-called on-resonance devices occur for the length $(3N+1)a$ ($\epsilon = 0$, circles), $3Na$ ($\epsilon = 1$, diamonds) and $(3N-1)a$ ($\epsilon = 0.5$, triangles), respectively with a period of $1.5a$.

Our calculation method makes it possible to sample the lengths with the resolution of the inter-ring length $a/2$ (half the unit cell). Owing to this we have found that the period of conduction oscillations is $3a/2$ rather than $3a$. Similarly as found for finite isolated (not coupled to any electrodes) SWCNTs[8] in the contest of their energy spectra. It is noteworthy that in the case of the on-resonance devices the conductance peak height does not vanish with decreasing $t_c$ (only its width does) and tends to the constant value.

Another point addressed in this paper is the giant magnetoresistance of a single-molecule system. It has been shown experimentally that carbon nanotubes electrically contacted by ferromagnetic cobalt show the GMR effect up to 9%[9]. The effect could be possibly even higher if there were single-domain electrodes and interfaces of better quality. To gain a closer insight into this we mimic spin-polarized electron injection to the SWCNT by applying fictitious magnetic electrodes which guarantee optimal matching of the interfaces, making it possible to single out the magnetic contribution. The fictitious electrodes have been constructed from the SWCNT electrodes by simply shifting, in a rigid way, the up- and down-spin bands with respect to each other. The GMR is defined as

$$GMR = (G_{\uparrow,\uparrow} - G_{\uparrow,\downarrow})/G_{\uparrow,\uparrow},$$

where $G_{\sigma,\sigma'}$ denotes the conductance for the parallel and antiparallel configurations. N.B.
the GMR problem in the SWCNTs has already been studied before by means of a similar approach in Ref. [10], where the electrodes have been treated as featureless leads which are taken into account indirectly by parametrizing spin-dependent self-energies in terms of corresponding line-width functions $\Gamma_{\uparrow, \downarrow}$ with a fixed ratio $\Gamma_{\uparrow}/\Gamma_{\downarrow} = 2$.

Fig. 3 represents the GMR dependence on the spin polarization of injected electrons for some typical interface parameters $\epsilon$ and $t_c$, and the sample lengths $N = 6a$ and $7a$. It is interesting to note that for the on-resonance device the inverse GMR may occur (thick solid curve), however it gives way to the positive GMR if some amount of diagonal disorder is present (thin solid line). As regards the off-resonance devices, their GMR is always positive (dashed curve). The reason for this peculiar behavior is that the density of states at the Fermi energy depends strongly both on the length and on conditions at the interfaces.

![FIG. 3. Giant magnetoresistance of the SWCNT coupled to fictitious electrodes, against their spin-polarization, P (lower x-axis) and the rigid band splitting, $\Delta$ (upper x-axis). The parameters are as follows: $L = 6a$, $t_c = -0.5$, $\epsilon = 0$ (dashed line); $L = 7a$, $t_c = -0.5$, $\epsilon = 0$ (thick line); $L = 7a$, $t_c = -0.5$, $\epsilon = 0.2$ (thin line). Note that the plot is restricted to the range where P scales roughly linearly with $\Delta$, in order to avoid electrode-specific features.](image)

In conclusion, quality of the sample-electrode interfaces is decisive for transport properties of single-wall carbon nanotubes. When the amount of disorder at the interfaces increases, the SWCNT conductance evolves from the continuous step function (discretized at integer multiples of $e^2/h$) to the set of peaks typical of the resonant tunneling. The conductance of armchair SWCNT oscillates with the period of $3a/2$ ($a$ is the repeat unit cell). The on-
resonance device is characterized by the existence of the conductance peak just at the Fermi energy. The on-resonance device length has been shown here to depend on the interface parameters, and not to satisfy the 3N+1-rule in general. The GMR effect in the SWCNT may be negative in the case of the on-resonance devices with no on-site interface disorder.

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