Quantum conductance of a helically coiled carbon nanotube

Wengang Lu*

State Key Laboratory for Surface Physics and International Center for Quantum Structures, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China

Received 15 March 2005; revised 9 June 2005; accepted 9 June 2005

Available online 29 September 2005

Abstract

Using a π-orbital tight-binding model, we investigate the transport properties of a coiled carbon nanotube (also called carbon nanotube spring), which we construct by connecting carbon nanotubes periodically in three-dimensional (3D) space. The conductance is quantized due to the translational symmetry in the coiled direction. However, the conductance behaviors differ greatly from those of pristine metallic carbon nanotubes but similar to those of carbon nanotube superlattices. We explain that conductance behaviors of the coiled carbon nanotube.

© 2005 Elsevier Ltd. All rights reserved.

Keywords: Coiled carbon nanotube; Quantum conductance; Tight-binding

1. Introduction

Carbon nanotubes have been extensively studied more than 10 years since their discovery in 1991[1]. Nowadays carbon nanotubes are still an active field for their unique properties and great potentials in future applications [2–4]. Because many physical properties are very sensitive to system geometries, we must handle the geometries of carbon nanotubes to obtain various properties in future actual applications. Many carbon nanotube based structures have been constructed [5–15]. Among them, carbon nanotube junctions, which are connected with different pristine single wall carbon nanotubes, are basic structures because they are bricks of more complex structures and have the virtue of manipulation and stabilization. Many experiments and theories have studied various carbon nanotube junctions [16–18].

There is a special family of carbon nanotube based structures, which are composed of carbon nanotube junctions periodically. Carbon nanotube sperlattice [19,20] is a linear structure composed of different carbon nanotubes periodically. The conductance of a carbon nanotube superlattice is found different greatly from those of pristine metallic carbon nanotubes. The conductance is quantized, but divided into segments by energy gaps, and each quantum step is one \( G_0(G_0 = 2e^2/h) \), for the lifting of energy band degeneracy. Coiled carbon nanotube (also called carbon nanotube spring), is another periodic carbon nanotube based structure. Akagi and coworkers [21,22] proposed a development map, which is a periodic plot on a two-dimensional (2D) graphite sheet, to describe the structures of coiled carbon nanotubes. And they studied the energy bands of coiled carbon nanotubes from the development maps and found the energy bands depend largely on the structures. As natural molecular solenoids, coiled carbon nanotubes must have vast electronic and magnetic applications. In this paper, we devote to study the electronic transport properties.

2. Methodology

In this section, we briefly introduce the tight-binding model and the Green’s function method used in this paper to calculate the conductance. The tight-binding Hamiltonian is

\[
H = - \sum_{\langle i,j \rangle} V_{pp} c_i^\dagger c_j + h.c.,
\]

where \( \langle i,j \rangle \) denotes that \( i \) and \( j \) are nearest neighbors, and \( V_{pp} = 2.7 \text{ eV} \) is the hopping parameter between \( p \)-orbitals. Even the parameter is not length dependent, this model gives good results because the strong C–C bonds do not vary
the bond length a lot in covalent systems. On-site energies are set to zero.

The conductance of a system can be obtained from Landauer formula, \[23–26\]

\[
C = \frac{2e^2}{h} T(E),
\]

(2)

where \(C\) is the conductance, \(T(E)\) is the transmission of channels between the two leads at energy \(E\) and it represents the probability of an electron tunnelling through the system.

Using the Green’s function approach, the transmission function \(T\) can be expressed as

\[
T = tr(\Gamma_L G^r \Gamma_R G^a),
\]

(3)

where \(\Gamma_L(R)\) is the coupling matrix between the left (right) lead and the system. It can be obtained from

\[
\Gamma_L(R) = i[\Sigma_L(R) - \Sigma_L(R)'],
\]

(4)

where \(\Sigma_L'(R) = (\Sigma_L(R))^\dagger\). \(\Sigma_L(R)\) is the self-energy due to the left (right) lead. \(G^{r(a)}\) in Eq. (3) is the retarded (advanced) Green’s function of the system. It can be written as

\[
G^r = (e - H_S - \Sigma_L^r - \Sigma_R^r)^{-1} = (G^a)^\dagger,
\]

(5)

where \(H_S\) is the Hamiltonian in the system. \(\Sigma_L\) and \(\Sigma_R\) are defined as

\[
\Sigma_L = h^g_{LS} g_L h_{LS}
\]

(6)

and

\[
\Sigma_R = h^g_{RS} g_R h_{RS},
\]

(7)

where \(h_{LS}(h_{RS})\) is the coupling matrix between the system and the left (right) lead, and \(g_{L(R)} = (e - H_{L(R)})^{-1}\) is the lead’s surface Green’s function and obtained through an iterative technique \[27\].

3. Results and discussion

Based on the fact that coiled carbon nanotubes are composites of single wall carbon nanotubes and because present softwares make the moving and connecting molecules fairly easy, we can easily use \((9, 0)\) and \((5, 5)\) tubes to construct coiled carbon nanotubes in three-dimensional (3D) space.

Fig. 1. Atomic structure of \((9, 0)/(5, 5)\) interface.

Fig. 2. Conductances of \((9, 0)/(5, 5)\) interface. The conductances of pristine tubes \((9, 0)\) and \((5, 5)\) tubes are plotted for comparison.

We construct firstly a \((9, 0)/(5, 5)\) interface by connecting pristine \((9, 0)\) and \((5, 5)\) tubes. The \((9, 0)/(5, 5)\) interface is shown in Fig. 1. We plot in Fig. 2 the conductance of the \((9, 0)/(5, 5)\) interface together with the conductances of pristine \((9, 0)\) and \((5, 5)\) tubes for comparison. The interface scatterings destroy the quantization of the conductance of pristine tubes and lower the conductance values. The two dents at the first conductance plateau at energies about 1.7 and \(-1.7\) eV are due to defect states.

Fig. 3. Atomic structures of \((9, 0)/(5, 5)/(9, 0)\) heterostructures. We denote the configuration using the angle between the two \((9, 0)\) branches after projecting them on a plane perpendicular to the middle \((5, 5)\) tube: (a) 0, (b) 72, and (c) 144°.
Next, we connect two (9, 0)/(5, 5) interfaces on the (5, 5) side to construct a (9, 0)/(5, 5)/(9, 0) sandwich heterostructure. Because of the $C_5$ rotational symmetry of the middle (5, 5) tube, there are totally three different configurations as shown in Fig. 3. We distinguish them with the angles between the two (9, 0) branches after projecting them on a plane perpendicular to the middle (5, 5) tube: (a) $0^\circ$, (b) $2\pi/5 = 72^\circ$, and (c) $2(2\pi/5) = 144^\circ$. Their conductances are shown in Fig. 4. The conductance curves are almost the same on the whole except for some small differences at high energies. That means that, at small energy regions, the angles of the two (9, 0) branches are not important for electrons transmitting through the (9, 0)/(5, 5)/(9, 0) heterostructure. In the (9, 0)/(5, 5)/(9, 0) heterostructure, the injected propagating electrons are multi-scattered between the two interfaces (9, 0)/(5, 5) and (5, 5)/(9, 0) before they passing through the middle (5, 5) part. Those electrons with their wave-lengths satisfying the resonance condition will tunnel through without decay. The conductance peaks in Fig. 4 with values of $2G_0$ at the vicinity of $E_F = 0$ are due to this resonance.

To construct a coiled carbon nanotube, we connect many identical (9, 0)/(5, 5)/(9, 0) heterostructures together under translational symmetry along the tube axis direction. The obtained structures of the coiled carbon nanotubes are plotted in Fig. 5(a) with longer composing tube lengths and (b) with shorter composing tube lengths. The angles between the neighboring (9, 0) tubes are taken to be 72° and the angles between neighboring (5, 5) tubes are taken to be $2\pi/9 = 40^\circ$. The definition of the angle between neighboring (5, 5) tubes is the same as the above definition for neighboring (9, 0) tubes in the (9, 0)/(5, 5)/(9, 0) sandwich structure. The conductances of the two coiled carbon nanotubes are plotted in Figs. 6 and 7, respectively. The main features of Figs. 6 and 7 are the same. Their conductances are both quantized but quite different from those of composing pristine carbon nanotubes. In the vicinity of $E_F = 0$, the conductances of pristine (9, 0) and (5, 5) nanotubes have a constant conductance of $2G_0$ because there are two double-degenerated bands available for transport. But the conductances of the coiled carbon nanotubes have been divided into several segments by energy gaps and they take values of $G_0$ and $2G_0$ in each segment.

In the following, we will explain the physics behind the features of the conductance curves shown in Figs. 6 and 7.

Because we construct the coiled carbon nanotubes under the translational symmetry, electrons travelling along the coiled carbon nanotubes undergo periodic potentials and scatterings just like they go through superlattices. Thus the discussions of carbon nanotube superlattices [19] apply to the coiled carbon nanotubes. The difference is that the wave vectors must change directions along the composing tube axes in a coiled carbon nanotube. As a consequence the period of a coiled carbon nanotube is difficult to be given an exact definition since the outer and inner spiral diameters of the coiled carbon nanotube can be largely different. Akagi et al. [21, 22] calculated the band structures of coiled carbon nanotubes based on their development maps. However, the lattice vector of the development map has not been proved suitable to be used as period of the coiled carbon nanotube. Even so, coiled carbon nanotubes are periodic structures and Bloch waves exist, and therefore the band structure exists.

Considering a pristine tube (5, 5) or (9, 0), the first band extends from $E_F = 0$ eV to several eVs till it reaches a boundary of the first Brillouin zone.
and (5, 5) tubes periodically, the period of the new structure becomes longer. The new first Brillouin boundary will be a fraction of that of a pristine tube and accordingly the first band can be looked as being folded some times in the new first Brillouin zone forming a series of mini-bands. Energy gaps are facile to open at high symmetric \( k \) points because of the broken of the original symmetries. Thus, gaps open between those mini-bands and the gap energies are only fractions of those of a pristine tube. That is the origin of the gaps appearing on the Conductance–Energy curves in Figs. 6 and 7.

The double degeneracy of a pristine carbon nanotube (9, 0) or (5, 5), is due to its rotational symmetry around its axis. In the coiled carbon nanotube, because the composing tubes (9, 0) and (5, 5) have different symmetries and also the interface defects have no rotational symmetry, the symmetries of pristine (9, 0) and (5, 5) tubes are destroyed and the band degeneracy is lifted. Since transmission in a non-interacting model is equal to the number of bands available for transport, with the increase of the energy, electrons are possible to probe one new band or leave one old band. Therefore, the conductance can take step value of \( G_0 \).

When we change the length of the composing tubes, we change the period and then the Brillouin zone boundaries. Then the position of the energy gaps are changed. And the degrees of destroying the symmetries are different for coiled carbon nanotubes with different periods, thus the degrees of lifting their band degeneracies are different. This render different shapes of the conductance segments between the gaps of coiled carbon nanotubes with different periods.

4. Summary

We have constructed a coiled carbon nanotube by connecting single wall carbon nanotubes (9, 0) and (5, 5), the conductance is quantized and divided into segments by energy gaps. The conductance steps are one \( G_0 \) because of the lifting of band degeneracy. The positions and widths of the gaps are adjustable by changing the lengths of composing tubes.

Acknowledgements

I thank Professors E.G. Wang and H. Guo for their helpful discussions. This work was supported by NSF, MOST and CAS of China.

References

[1] S. Iijima, Helical micro-tubules of graphitic carbon, Nature 345 (1991) 56–58 London.
[2] C. Dekker, Carbon nanotubes as molecular quantum wires, Phys. Today 52 (5) (1999) 22–28.
[3] R. Saito, G. Dresselhaus, M.S. Dresselhaus, Physical Properties of Carbon Nanotubes, Imperial College Press, London, 1998.
[4] S. Reich, C. Thomsen, J. Maultzsch, Carbon Nanotubes, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004.
[5] J.M. Ting, C.C. Chang, Multijunction carbon nanotube network, Appl. Phys. Lett. 80 (2002) 324–325.
[6] M. Terrones, F. Banhart, N. Grobert, J.C. charlier, H. Terrones, P.M. Ajayan, Molecular Junctions by Joining Single-Walled Carbon Nanotubes, Phys. Rev. Lett. 89 (2002) 075505–1–075505–4.
[7] J. Han, A. Globus, R. Jaffe, G. Deardorff, Molecular dynamics simulations of carbon nanotube-based gears, Nanotechnology 8 (1997) 95–102.
[8] Z. Yao, H.W.C. Postma, L. Balents, C. Dekker, Carbon nanotube intramolecular junctions, Nature 402 (1999) 273–276 London.
[9] A. Fonseca, K. hernadi, J.B. Nagy, Ph. Lambin, A.A. Lucasc, Model structure of perfectly graphitizable coiled carbon nanotubes, Carbon 33 (1995) 1750–1775.
[10] B.I. Dunlap, Constraints on small graphitic helices, Phys. Rev. B 50 (1994) 8134–8137.
[11] K. Tsukagoshi, B.W. Alpenaar, H. Ago, Coherent transport of electron spin in a ferromagnetically contacted carbon nanotube, Nature 401 (1999) 572–574 London.
[12] A.F. Morpurgo, J. Kong, C.M. Marcus, H. Dai, Gate controlled superconducting proximity effect in carbon nanotubes, Science 286 (1999) 263–265.
[13] R. Saito, G. Dresselhaus, M.S. Dresselhaus, Tunneling conductance of connected carbon nanotubes, Phys. Rev. B 53 (1996) 2044–2050.
[14] L. Chico, V.H. Crespi, L.X. Benedict, S.G. Louie, M.L. Cohen, Pure Carbon Nanoscale Devices: Nanotube Heterojunctions, Phys. Rev. Lett. 76 (1996) 971–974.
[15] M. Menon, D. Srivastava, Carbon nanotube ‘T junctions’: nanoscale metal-semiconductor-metal contact devices, Phys. Rev. Lett. 79 (1997) 4453–4457.
[16] H. Mehrez, J. Taylor, H. Guo, J. Wang, C. Roland, Carbon nanotube based magnetic tunnel junctions, Phys. Rev. Lett. 84 (2000) 2682–2685.
[17] Y. Wei, J. Wang, H. Guo, H. Mehrez, C. Roland, Resonant Andreev reflections in superconductor-carbon-nanotube devices, Phys. Rev. B 63 (2001) 1–5.
[18] Y. Zhang, T. Ichihashi, E. Landree, F. Nihey, S. Iijima, Heterostructures of single-walled carbon nanotubes and carbide nanorods, Science 285 (1999) 1719–1722.
[19] Wengang Lu, E.G. Wang, H. Guo, Quantum conductance of a carbon nanotube superlattice, Phys. Rev. B 68 (2003) 075407–1–075407–4.
[20] W. Jaskolski, L. Chico, Localized and conducting states in carbon nanotube superlattices, Phys. Rev. B 71 (2005) 155405–1–155405–5.
[21] Kazuto Akagi, Ryo Tamura, Masaru Tsukada, Satoshi Itoh, Sigeo Ihara, Electronic structure of helically coiled cage of graphitic carbon, Phys. Rev. Lett. 74 (1995) 2307–2310.
[22] Kazuto Akagi, Ryo Tamura, Masaru Tsukada, Satoshi Itoh, Sigeo Ihara, Electronic structure of helically coiled carbon nanotubes: Relation between the phason lines and energy band features, Phys. Rev. B 53 (1996) 2114–2120.
[23] R. Landauer, Electrical resistance of disordered one-dimensional lattices, Philos. Mag. 21 (1970) 863–867.
[24] M. Büttiker, Y. Imry, R. Landauer, S. Pinhas, Generalized many-channel conductance formula with application to small rings, Phys. Rev. B 31 (1985) 6207–6215.
[25] S. Datta, Electronic Transport in Mesoscopic System, Cambridge University Press, Cambridge, 1995.
[26] Marco Buongiorno Nardelli, Electronic transport in extended systems: Application to carbon nanotubes, Phys. Rev. B 60 (1999) 7828–7833.
[27] M.P. López Sancho, J.M. López Sancho, J. Rubio, Quick iterative scheme for the calculation of transfer matrices: application to Mo(100), J. Phys. F: Met. Phys 14 (1984) 1205–1215; Highly convergent schemes for the calculation of bulk and surface Green functions, 15 (1985) 851-858.