Geometric effects in the electronic transport of deformed nanotubes

Fernando Santos\textsuperscript{1,4}, Sébastien Fumeron\textsuperscript{2}, Bertrand Berche\textsuperscript{2} and Fernando Moraes\textsuperscript{3,5}

\textsuperscript{1} Wolfson Centre for Mathematical Biology, Mathematical Institute, University of Oxford, OX1 3LB Oxford, UK
\textsuperscript{2} Statistical Physics Group, IJL, UMR Université de Lorraine—CNRS 7198 BP 70239, 54506 Vandœuvre les Nancy, France
\textsuperscript{3} Departamento de Física and Departamento de Matemática, Universidade Federal da Paraíba, Caixa Postal 5008, 58051-900, João Pessoa, PB, Brazil

E-mail: moraes@fisica.ufpb.br

Received 2 December 2015
Accepted for publication 25 January 2016
Published 22 February 2016

Abstract
Quasi-two-dimensional systems may exhibit curvature, which adds three-dimensional influence to their internal properties. As shown by da Costa (1981 Phys. Rev. A 23 1982–7), charged particles moving on a curved surface experience a curvature-dependent potential which greatly influence their dynamics. In this paper, we study the electronic ballistic transport in deformed nanotubes. The one-electron Schrödinger equation with open boundary conditions is solved numerically with a flexible MAPLE code made available as supplementary data. We find that the curvature of the deformations indeed has strong effects on the electron dynamics, suggesting its use in the design of nanotube-based electronic devices.

Keywords: nanotubes, ballistic transport, geometric effects

1. Introduction

Graphene’s natural state is corrugated [2]. The curvature associated with it leads to interesting phenomena such as curvature induced p–n junctions, band-gap opening and decoherence [3]. Carbon nanotubes, on the other hand, are perfect cylindrical surfaces which can be deformed into wavy nanotubes from different techniques: axial compression [4], combination of defect formation and electromigration [5] or filling the nanotubes with fullerenes (‘peapods’ [6]). As curvature influences the dynamics of quantum particles, it can be used to manipulate the electronic properties of two-dimensional materials [3, 7] which can be measured. Experimental characterization of the electronic properties of imperfect nanotubes can be achieved via different techniques. The conventional approach requires making contacts and measuring transport properties of the device [5]. Microscopic probe based techniques, such as dielectric force microscopy [8] and scanning tunneling microscopy [9], offer the possibility to probe locally the electronic structure and properties without need of making contacts.

Ballistic electron transport in nanotubes is known to be drastically affected by variations of the tube geometry [10, 11] and therefore, of the local curvature. This effect is the main concern of the present article. Of course, carbon nanotubes are one-dimensional structures which can exhibit metallic, semimetallic, or insulating properties depending on their chirality, i.e. the way they are mapped from a graphene sheet [9, 12, 13]. Generically, the most conducting are the ‘armchair’ carbon nanotubes. Their behaviour is described by...
a Luttinger liquid rather than a Fermi liquid, the shorter the nanotube cylinder, the stronger the Luttinger behaviour. This has been shown experimentally, see, e.g. [14]. In spite of this, short-range electron–electron interactions have only weak effects and the deviations from the behaviour of non-interacting electrons occur only at a very low temperature and for nanotubes of very small transverse size [15].

Our aim in this paper is not to make a quantitatively realistic description of deformed nanotubes, but to use a simple independent electron approach in order to access qualitatively the ballistic transport regime, and possibly, arouse further studies on potential applications. With the examples reported here we intend to draw attention to the interest is to study corrugated nanotubes. A surface of revolution is obtained by rotation of a plane curve around an axis. The parametric equations for the surface of revolution can be written as \( x = \rho(q) \cos \phi \), \( y = q \), \( z = \rho(q) \sin \phi \), where \( q \in \mathbb{R}^3 \) and \( \phi \in \mathbb{S}^1 \). With such parametrization, the first and second fundamental forms are respectively:

\[
g_{ij} = \begin{pmatrix} \rho(q)^2 & 0 \\ 0 & 1 + \rho'(q)^2 \end{pmatrix}
\]

and

\[
h_{ij} = \frac{1}{\sqrt{1 + \rho'(q)^2}} \begin{pmatrix} \rho(q) & 0 \\ 0 & -\rho''(q) \end{pmatrix}.
\]

The mean and Gaussian curvatures are given respectively by

\[
M = \frac{1}{2g}(g_{11}h_{22} + g_{22}h_{11} - 2g_{12}h_{12})
\]

and

\[
K = \frac{1}{8g}(h_{11}h_{22} - h_{12}h_{21}),
\]

so that the geometric potential is analytically obtained in terms of the nanotube parametrization \( \rho(q) \):

\[
V_{geo} = \frac{h^2}{8m} \frac{[1 + \rho'(q)^2] + \rho(q)\rho''(q)]^2}{\rho(q)^2[1 + \rho'(q)^2]^3}.
\]

Therefore, from equations (1) and (2), the Hamiltonian follows

\[
H = -\frac{\hbar^2}{2m} \Delta_{LB} + V_{geo},
\]

where the Laplace–Beltrami operator is obtained from the curvilinear coordinates \( x^i \) intrinsic to the surface and the metric tensor \( g_{ij} \) (\( g \) its determinant)

\[
\Delta_{LB} = \sum_{i,j} \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \left( \sqrt{g} g^{ij} \frac{\partial}{\partial x^j} \right).
\]

and the geometric potential is given by

\[
V_{geo} = -\frac{h^2}{2m}(M^2 - K).
\]

Here, \( M \) and \( K \) refer to the mean and Gaussian curvatures, respectively. The geometric potential is a direct consequence of the quantization of the motion normal to the surface.

Let us now focus on surfaces of revolution since our interest is to study corrugated nanotubes. A surface of revolution is obtained by rotation of a plane curve around an axis. The parametric equations for the surface of revolution can be written as \( x = \rho(q) \cos \phi \), \( y = q \), \( z = \rho(q) \sin \phi \), where \( q \in \mathbb{R}^3 \) and \( \phi \in \mathbb{S}^1 \). With such parametrization, the first and second fundamental forms are respectively:

\[
g_{ij} = \begin{pmatrix} \rho(q)^2 & 0 \\ 0 & 1 + \rho'(q)^2 \end{pmatrix}
\]

and

\[
h_{ij} = \frac{1}{\sqrt{1 + \rho'(q)^2}} \begin{pmatrix} \rho(q) & 0 \\ 0 & -\rho''(q) \end{pmatrix}.
\]

The mean and Gaussian curvatures are given respectively by

\[
M = \frac{1}{2g}(g_{11}h_{22} + g_{22}h_{11} - 2g_{12}h_{12})
\]

and

\[
K = \frac{1}{8g}(h_{11}h_{22} - h_{12}h_{21}),
\]

so that the geometric potential is analytically obtained in terms of the nanotube parametrization \( \rho(q) \):

\[
V_{geo} = \frac{h^2}{8m} \frac{[1 + \rho'(q)^2] + \rho(q)\rho''(q)]^2}{\rho(q)^2[1 + \rho'(q)^2]^3}.
\]

Therefore, from equations (1) and (2), the Hamiltonian follows

\[
H = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sqrt{g}} \frac{\partial}{\partial q} \left( \sqrt{g} \frac{\partial}{\partial q} \right) \right) + V_{geo}.
\]

The potential \( V_{geo} \) depends only on the \( q \) coordinate, so we can separate the Schrödinger equation into two one-dimensional equations \( \Psi'' + \ell^2 \Psi = 0 \), with \( \ell \in \mathbb{Z} \) in order to satisfy angular periodicity and

\[
\Psi'' + F(q)\Psi' + G(q) \left( \frac{2m}{\hbar^2} (E - V_{geo}) \right) - \frac{\ell^2}{\rho^2} \Psi = 0.
\]

Here, \( E \) is the total energy, \( \Phi = A e^{i\ell \phi} \) are the eigenfunctions of the angular momentum \( \ell \) along the \( y \)-axis and \( \Psi(q) \), the longitudinal eigenfunction. The functions \( F \) and \( G \) in
equation (8) are
\[
F(q) = \frac{\rho^2}{\rho} \left[ 1 - \frac{\rho^2}{1 + (\rho^2)^2} \right], \quad G(q) = 1 + (\rho^2)^2. \tag{9}
\]

We model the corrugated nanotube as two semi-infinite cylinders of radius R, joined by a surface of revolution generated by a curve ρ(y) in the range 0 < y < L, such that ρ(0) = ρ(L) = R. In the region y < 0, total energy is the sum of the injection energy \( E_0 = \hbar^2 k_0^2 / (2 m^*L^2) \) and the angular part \( E_2 = \hbar^2 k_2^2 / (2 m^*) \). The mass \( m \) of the particle is replaced by its effective mass \( m^* = 0.173m_r \) in order to facilitate comparison with [10].

In the next section we solve equation (8) with open (Robin) boundary conditions using the quantum transmitting boundary method [21]. With these techniques we built a numerical code which we validated by reproducing the result for the electron transmittance in an axially symmetric cylindrical junction studied in [10].

### 3. Methodology

Recalling that \( \rho = \rho(y) \), we see that equation (8) is of the form

\[
\dot{\Psi}(y)^2 + V_1(y)\Psi(y)^2 + V_2(y)\Psi(y) = 0. \tag{10}
\]

By making \( \Psi(y) = \varphi(y)\lambda(y) \) we get

\[
\varphi'' + \left( 2\frac{\lambda'}{\lambda} + V_1 \right) \varphi' + \left( \frac{\lambda''}{\lambda} + V_1\frac{\lambda'}{\lambda} + V_2 \right) \varphi = 0. \tag{11}
\]

Now, for \( 2\frac{\lambda'}{\lambda} + V_1 = 0 \), one gets \( \lambda(y) = e^{-\int P(y)} \), where \( P(y) \) is the primitive for the function \( V_1(y) \). Therefore, (11) becomes

\[
\varphi''(y) + \left( -\frac{1}{4}V_1^2 - \frac{1}{2}V_1' + V_2 \right) \varphi = 0 \tag{12}
\]

and transforming back to \( \dot{\Psi} \): \( \dot{\Psi}(y) = e^{-\int P(y)}\varphi(y) \).

Since we are interested in the transmittance due to the deformation of the tube, we consider the injection and propagation of energy \( E_k \) from the negative part of the y-axis. Thus, we have

\[
\Psi(y) = a_0 e^{ik_0 y} + b_0 e^{-ik_0 y} \quad \text{for} \quad y \leq 0, \\
= a_L e^{-ik_L (y-L)} + b_L e^{ik_L (y-L)} \quad \text{for} \quad y \geq L, \tag{13}
\]

where
\[
k_0 = \sqrt{\frac{2 m^* (E_k - V(0))}{\hbar^2}} \tag{14}
\]
\[
k_L = \sqrt{\frac{2 m^* (E_k - V(L))}{\hbar^2}} \tag{15}
\]

are the incident and transmitted electron wave vectors, respectively. By doing this we are assuming that the field is perfectly matching contacts at both ends of the tube. Since our aim in this article is to present a way of designing specific electronic properties by manipulation of the nanotube shape we decided, following [10], to use this simpler approach. A complete treatment of the boundary conditions including the input and output leads can be found in [21].

Notice that \( V_1(y) = 0 \) for \( y \neq 0 \) in the range \( 0 < y < L \), which makes equations (10) and (12) identical. So, equation (13) is also valid for \( \varphi(y) \) and then \( \Psi(0) = \varphi(0) \) as well as \( \Psi(L) = \varphi(L) \). As we will see below, this implies that the reflectance and transmittance do not depend on \( \lambda(y) \) and can be obtained from \( \varphi(y) \) directly. We choose the normalization of the incident wavefunction such that \( a_0 = 1 \). Also, considering only outgoing waves, in the \( y \geq 0 \) region we have \( a_L = 0 \).

For the above normalization, the transmittance may be obtained from the probability current density

\[
J = \frac{\hbar}{2mi} (\dot{\Psi}^* \dot{\varphi} - \dot{\Psi}^* \dot{\varphi}^*), \tag{16}
\]

such that the incident current is \( J_{inc} = \frac{\hbar}{n_0} |b_0|^2 \), the reflected current is \( J_{ref} = \frac{\hbar}{n_0} |a_0|^2 \), and the transmitted current \( J_{trans} = \frac{\hbar}{n_0} |a_L|^2 \). Hence, the transmittance is

\[
T = \frac{J_{trans}}{J_{inc}} = \frac{2|b_0|^2}{|a_0|^2} \quad \text{and} \quad R = \frac{|a_0|^2 - 1}{|a_0|^2}. \tag{17, 18}
\]

Then, the problem reduces to finding \( \varphi(0) \) and \( \varphi(L) \) by solving the coupled differential and algebraic equations (equation (12) and boundary conditions) in the range \( 0 \leq y \leq L \). This is the essence of the open boundary condition method for solving ordinary differential equations with Robin boundary conditions. With the above expressions we implemented a MAPLE code to find, for each injection energy, \( \varphi(0) \) and \( \varphi(L) \) and, consequently, the transmittance and the reflectance as specified by equations (17) and (18), respectively. In order to input the energy in meV and distances in nm we use a mixed units system where the electron mass is \( m_e = 5.68 \times 10^{-27} \text{meV.s}^2/\text{nm}^2 \) and Planck’s constant is \( \hbar = 6.58 \times 10^{-16} \text{meV.s} \).

### 4. Results

Resonance peaks correspond to quasibound states. These are states associated with a quantum well where a particle is primarily confined but has a finite probability of tunnelling out and escaping. In the nanotube, the geometric potential, if deep enough, may have such states. Although most of the incident electrons are reflected back by the geometric potential, if the energy of the electron coincides with that of a quasibound state this makes it easier for it to tunnel to the inner region of the potential, and thus tunnel out of it on the opposite side. If the potential becomes deeper, the energy levels of the quasibound states shift downward implying a
shift of the resonant peaks to lower energies. This is in fact what is seen in the results described below.

Looking at equation (8) we see that for angular momentum \( \ell \neq 0 \) a repulsive term \( \ell^2 \) is added to the geometric potential (6). So, the effect of the centrifugal term is to make the potential well shallower and consequently reduce the number of quasibound states, therefore of the resonances in the transmittance. For this reason, in what follows we consider only the cases of zero angular momentum (\( \ell = 0 \)) which gives the general physical picture of the system.

We look at three generic situations: a nanotube with a single bump, one with a pinch and a wavy structure.

**Figure 1.** (a) Pinched nanotube. (b) Geometric potential due to the deformation shown in (a), and (c) transmittance as function of incident energy (in meV) for different waist sizes (\( \epsilon R \)).

**Figure 2.** (a) Nanotube with a single bump. (b) Geometric potential due to the deformation shown in (a), and (c) transmittance as a function of incident energy (in meV) for different bump sizes (\( \epsilon R \)).

**Figure 3.** (a) Wavy nanotube. (b) Geometric potential due to the deformation shown in (a) for different numbers of bumps. (c) Transmittance as a function of incident energy (in meV).
shown in figures 1(a), 2(a) and 3(a), respectively. We create the corrugations by using the curve
\[ \rho(y) = R \pm \frac{\epsilon}{2} \left[ 1 - \cos \left( 2 \frac{n \pi y}{L} \right) \right] \] (19)
to generate the surface of revolution. In equation (19) the parameter \( \epsilon \) regulates the strength of the deformation while \( R \) gives the radius of the undistorted nanotube. The + sign was used to generate the single bump and wavy structures and the − sign for the pinched tube. We used \( n = 1 \) for the pinched and bumped nanotubes and \( n = 2, 3, 4, 5, 6 \) for the wavy structures.

The geometric potential of a nanotube with a pinch and with a bump is seen in figures 1(b) and 2(b), respectively. Differently from the pinch, the bump has only positive Gaussian curvature. The result is a stronger geometric potential for the pinch which results in lower quasi bound states and therefore resonances in the transmittance shifted to lower energies. Figures 1(c) and 2(c) show the transmittance as function of the incident energy. The pinched case, due to its deeper potential well, lowers the quasi bound energy levels thus lowering the resonance peak positions as compared to the bumped case (see supplementary data for a direct comparison of the resonance peaks of the pinch and of the bump).

In figure 3 is shown the geometric potential and transmittance as a function of incident energy for wavy structures with a varying number of bumps. As the number of bumps increases, a one-dimensional lattice on the tube starts to take form and the geometric potential starts to look like the Dirac comb [22], as seen in the figure. The periodicity of the potential minima opens a gap in the energy spectrum which becomes better defined with the increasing number of oscillations. The effect on the transmittance is seen in figure 3. As expected, the energy gap sensibly reduces the transmittance and the effect becomes sharper with the number of bumps. For the curves displayed we fixed the tube length in 5 nm and changed the number of bumps. Therefore the wavelength of the wavy perturbation changes with the number of bumps. Thus the width of the gap changes accordingly. The reader might ask why with a few bumps the gap is already so well defined. In order to answer this we evaluate the geometric potential at the position of its minima. There are two kinds: the deeper minima correspond to the pinched regions while the other ones correspond to the bumped regions. The result for the deeper minima is
\[ V_{\text{gap}} = \frac{\hbar^2}{8L^2mR^2} \left( L^2 - 2 \pi^2 R \alpha^2 \right)^2 \] (20)
which means that the deepness of the minima grows with \( n^4 \). For the other minima, change \( R \rightarrow R - \epsilon \). The dependence on \( n \) is therefore the same. The half-width of the potential minima goes like \( 1/n \) since we are increasing the number of oscillations in a fixed nanotube and keeping its length \( L \) fixed. So, the potential quickly approaches a Dirac comb, giving the observed result. The periodic array of potential wells defines a Kronig–Penney look-alike resulting in the opening of bandgaps in the electronic structure. This is clearly seen in figure 3. As the number of wells increase the band gap becomes better defined.

5. Conclusions

The main object of this article is to illustrate how geometry can be used to manipulate electronic properties of nanostructures. This was used to study its effects on transport in three different examples involving nanotubes. The influence of perturbations of the cylindrical form of conducting nanotubes on their electronic transport properties was studied in this article with particular focus on the transmittivity. Curvature introduces a potential in the free particle Hamiltonian which is diagonalized numerically for chosen nanotube profiles. These include: a pinched nanotube, a tube with a bump and one with a sinusoidal deformation. In the first two cases we obtained results for different pinch/bump sizes. The results agree qualitatively with those of reference [11]. In the third case, for different numbers of oscillations of the tube, the energy gap becomes better defined with the increasing number of oscillations. This suggests the possibility of using corrugated nanotubes as electronic filters. In general, our results indicate the importance of curvature in the transport properties of ballistic electrons. The geometric approach used in this article can be easily generalized for different perturbations of the cylindrical geometry intrinsic to the nanotubes. Naturally, for a more realistic description of the transport properties, the geometric approach presented here must be extended to include interactions between the charge carriers. This is presently under investigation and will be the subject of a follow-up article.

Acknowledgments

FS and FM are thankful for the warm hospitality at the Institut Jean Lamour of Université de Lorraine where part of this work was done. FM is also grateful for financial support from the Institut Jean Lamour. This work has been partially supported by CNPq, CAPES and FACEPE (Brazilian agencies) and CNRS (France).

References

[1] da Costa R C T 1981 Phys. Rev. A 23 1982–7
[2] Meyer J C, Geim A K, Katsnelson M I, Novoselov K S, Booth T J and Roth S 2007 Nature 446 60–3
[3] Atanasov V and Saxena A 2010 Phys. Rev. B 81 205409
[4] Ozaki T, Iwasa Y and Mitani T 2000 Phys. Rev. Lett. 84 1712–5
[5] Yuzvinsky T D, Mickelson W, Aloni S, Begtrup G E, Kis A and Zettl A 2006 Nano Lett. 6 2718–22
[6] Smith B W, Monthioux M and Luzzi D E 1998 Nature 396 323–4
[7] Medina E, González-Arraga L A, Finkelstein-Shapiro D, Berche B and Mujica V 2015 *J. Chem. Phys.* **142** 194308
[8] Li Y, Ge J, Cai J, Zhang J, Lu W, Liu J and Chen L 2014 *Nano Res.* **7** 1623–30
[9] Ouyang M, Huang J L, Cheung C L and Lieber C M 2001 *Science* **292** 702–5
[10] Marchi A, Reggiani S, Rudan M and Bertoni A 2005 *Phys. Rev. B* **72** 035403
[11] Taira H and Shima H 2007 *Surf. Sci. Proc. 10th ISSP Int. Symp. on Nanoscience at Surfaces* **601** 5270–5
[12] Kane C L and Mele E J 1997 *Phys. Rev. Lett.* **78** 1932–5
[13] Egger R and Gogolin A O 1997 *Phys. Rev. Lett.* **79** 5082–5
[14] Bockrath M, Cobden D H, Lu J, Rinzler A G, Smalley R E, Balents L and McEuen P L 1999 *Nature* **397** 598–601
[15] Kane C, Balents L and Fisher M P A 1997 *Phys. Rev. Lett.* **79** 5086–9
[16] Chang C H, van den Brink J and Ortix C 2014 *Phys. Rev. Lett.* **113** 227205
[17] Gaididei Y, Kravchuk V P and Sheka D D 2014 *Phys. Rev. Lett.* **112** 257203
[18] Chen K C and Chang C R 2013 *SPIN* **03** 1340006
[19] Atanasov V and Saxena A 2011 *J. Phys.: Condens. Matter* **23** 175301
[20] Onoe J, Ito T, Shima H, Yoshioka H and ichi S 2012 *EPL* **98** 27001
[21] Lent C S and Kirkner D J 1990 *J. Appl. Phys.* **67** 6353–9
[22] Sakurai J J 1993 *Modern Quantum Mechanics (Revised Edition)* 1st ed (Reading, MA: Addison-Wesley)