

Tayloring energy levels with curvature ? An illustration of Da Costa formalism

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Abstract. Nanotubes are generally not perfectly straight cylinders and the local curvature can influence transport properties. As shown by da Costa [1], charged particles moving on a curved surface experience an effective potential which modifies their dynamics. In this paper, we solve a one-electron Schrödinger equation in a distorted nanotube with open boundary conditions. We find that the deformations may open bandgaps suggesting their use in the design of nanotube-based electronic devices.

Keywords: Nanotubes, Ballistic transport, Geometric effects

1. Introduction

Single-walled nanotubes (SWNT) are made by rolling up a sheet of graphene into a cylinder. Graphene consists in a 2D honeycomb lattice of carbon atoms and because of its symmetries, one must view it as a hexagonal Bravais lattice with a two-atom basis. The distance between two nearest neighbours carbon atoms is about 0.142 nm. As there is one π -electron per carbon atom that is not involved in a covalent σ bond, there are as many valence electrons than carbon atoms and these electrons can propagate along the nanotube with peculiar properties [2].

This paper is concerned with ballistic electron transport, which is known to be drastically affected by variations of the tube geometry [3, 4] and therefore, of the local curvature. To simplify the study, we will restrict to physical situations where short-range electron-electron interactions have only weak effects: in practice, deviations from the behaviour of non-interacting electrons occur at low temperature and for nanotubes of small transverse size [5].

Our aim 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, understand the kind of impact that curvature may have on electronic band structure. To do so, we will consider deformed nanotubes in the following situations: shrunk nanotube, nanotube with a bump and a wavy peapod. The Schrödinger equation will be solved numerically for a single particle moving in the deformed cylinder, taking into account the modification of the kinetic energy caused by the non-Euclidean geometry and the effective potential induced by curvature. Then we will determine and discuss the transmittances as a function of the injection energy for all cases.



2. Differential geometry of SWNT

In their natural state, nanotubes are not perfectly straight cylinders and a practical way to model 2D carbon lattices is to work in the vanishing lattice spacing approximation: all characteristic lengths (such as de Broglie wavelength of electrons) are considered as large with respect to primitive lattice vectors (typically $a \approx 2.46 \text{ \AA}$). Hence, the discrete lattice appears as a smooth curved surface that is locally homeomorphic to \mathbb{R}^3 .

For a curved surface parametrized according to $\mathbf{r}(x^1, x^2) = (x(x^1, x^2), y(x^1, x^2), z(x^1, x^2))$, the induced metric tensor on the surface (or first fundamental form) is defined as

$$g_{ij} = \partial_i \mathbf{r} \cdot \partial_j \mathbf{r} = \begin{pmatrix} \mathbf{e}_1 \cdot \mathbf{e}_1 & \mathbf{e}_1 \cdot \mathbf{e}_2 \\ \mathbf{e}_2 \cdot \mathbf{e}_1 & \mathbf{e}_2 \cdot \mathbf{e}_2 \end{pmatrix} \quad (1)$$

In this expression, Einstein's summation convention on repeated indices was used, as will also be done in the remainder of this paper. The second quantity of interest is the shape tensor (or second fundamental form) defined as

$$h_{ij} = \begin{pmatrix} \mathbf{N} \cdot \partial_{11} \mathbf{r} & \mathbf{N} \cdot \partial_{12} \mathbf{r} \\ \mathbf{N} \cdot \partial_{21} \mathbf{r} & \mathbf{N} \cdot \partial_{22} \mathbf{r} \end{pmatrix} \quad (2)$$

These two objects are needed for computing the mean and Gaussian curvature scalars M and K , as prescribed by:

$$M = \frac{1}{2} \left(\frac{1}{R_1} + \frac{1}{R_2} \right) = \frac{\det h_{ij}}{\det g_{ij}}, \quad K = \frac{1}{R_1 R_2} = \frac{1}{2} \text{trace}(h_{ij} g^{ij}) \quad (3)$$

where R_1, R_2 are the local principal curvature radii and g^{ij} denotes the inverse metric of g_{ij} .

For a graphene sheet presenting one smooth ripple a relevant set of parametric equations is simply found to be $x = \rho(q) \cos \phi$, $y = q$, $z = \rho(q) \sin \phi$, where $q \in \mathbb{R}^1$ and $\phi \in \mathbb{S}^1$ (here the axis of the nanotube is chosen to be the y -axis). With such parametrization, the first and second fundamental forms are respectively:

$$g_{ij} = \begin{pmatrix} \rho(q)^2 & 0 \\ 0 & 1 + \rho'(q)^2 \end{pmatrix}, \quad h_{ij} = \frac{1}{\sqrt{1 + \rho'(q)^2}} \begin{pmatrix} \rho(q) & 0 \\ 0 & -\rho''(q) \end{pmatrix} \quad (4)$$

3. Quantizing constrained particles on a curved surface

The problem of a free quantum particle moving in a curved surface was solved by R. C. T. da Costa [1] in a seminal paper published in 1981. da Costa approach has ever since been successfully applied to a wide range of two-dimensional systems ([6],[7],[8]) and experimental verification was done in [9] by measuring the high-resolution ultraviolet photoemission spectra of a C₆₀ peanut-shaped polymer.

Introducing a confining potential given by an infinite square well in the normal direction, da Costa found that in-plane and out-of-the-plane dynamics decouple (adiabatic approximation) in such a way that the Schrödinger operator describing the particle reduces to [1]

$$H = -\frac{\hbar^2}{2m} \sum_{i,j} \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \left(\sqrt{g} g^{ij} \frac{\partial}{\partial x^j} \right) + V_{\text{geo}}, \quad (5)$$

where $g = \det g_{ij}$ and the geometric potential is given by

$$V_{\text{geo}} = -\frac{\hbar^2}{2m} (M^2 - K). \quad (6)$$

For the parametrization of the SWNT seen before, this potential can be found analytically as:

$$V_{\text{geo}} = -\frac{\hbar^2}{8m} \frac{[1 + \rho'(q)^2 + \rho(q)\rho''(q)]^2}{\rho(q)^2[1 + \rho'(q)^2]^3}. \quad (7)$$

Therefore, to obtain the stationary states of the Hamiltonian, one must solve:

$$\Psi'' + \frac{\rho'}{\rho} \left[1 - \frac{\rho\rho''}{1 + (\rho')^2} \right], \Psi' + (1 + (\rho')^2) \left[\frac{2m}{\hbar^2} (E - V_{\text{geo}}) \right] - \frac{\ell^2}{\rho^2} \Psi = 0. \quad (8)$$

E is the total energy, Ψ are the longitudinal eigenfunctions and $\ell\hbar$ the angular momentum. Taking Robin boundary conditions, solutions are used to compute the probability currents density $j = \frac{\hbar}{2mi} (\Psi^* \Psi' - \Psi \Psi'^*)$ and the transmittance $T = \frac{j_{\text{trans}}}{j_{\text{inc}}}$. From these expressions, we implemented a MAPLE code, with electron effective mass $m_e = 5.68 \times 10^{-27} \text{meV.s}^2/\text{nm}^2$.

4. Results

As shown in Figs. 1a, 2a and 3a, we considered a SWNT with a single bump, a single pinch and a wavy structure. Taking R as the radius of the straight nanotube, the corrugation was introduced by using

$$\rho(y) = R \pm \frac{\epsilon}{2} \left[1 - \cos \left(2 \frac{n\pi y}{L} \right) \right] \quad (9)$$

to generate the surface of revolution. ϵ is the strength of the deformation, the $+$ sign was used for the single bump and wavy structures, the $-$ sign for the pinched tube. We used $n = 1$ for the pinched/bumped nanotubes, and $n = 2, 3, 4, 5, 6$ for the wavy structures.

da Costa potential for a pinch and a bump is depicted in Figs. 1b and 2b, respectively. As the bump has only positive Gaussian curvature, the pinched case, due to its deeper potential well, lowers the quasibound energy levels thus lowering the resonance peak positions as compared to the bumped case. Fig. 3 shows the geometric potential and transmittance for wavy structures with varying number of bumps. As the number of bumps increases, the geometric potential starts to look like the Dirac comb. As in the Kronig-Penney problem, periodicity of the potential opens a gap in the energy spectrum which enlarges with the increasing number of oscillations. The effect on the transmittance is seen in Fig. 3. As expected, the energy gap sensibly reduces the transmittance and the effect becomes sharper with the number of bumps.

5. Conclusions

da Costa potential has to be used anytime a particle is constrained onto a surface (graphene sheets and alike) or a curve (rings). It shows that mean and Gaussian curvatures strongly impact ballistic transport of electrons and in particular, transmittance profiles show that periodic corrugation could lead to bandgaps opening [10]. Conversely, it could be a convenient tool to tune outer geometric properties of SWNT in order to obtain a prescribed band structure.

However, for that purpose, several refinements should be added to the present model. Among them, the influence of electron spin and its couplings to the chirality of nanotubes is of prime importance. Torsion is not accounted for in da Costa approach and a proper way to implement it is to derive the effective potential starting from Dirac equation on curved spacetime.

References

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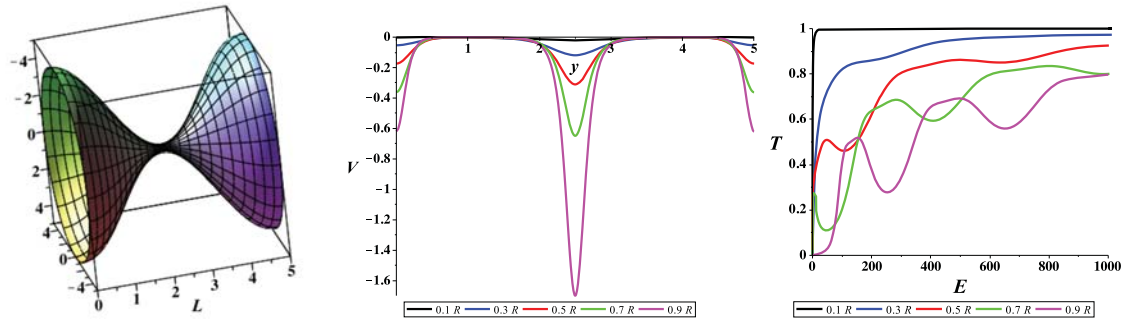


Figure 1: (a) Pinched nanotube. (b) Geometric potential due to the deformation shown in (a) and (c) transmittance as function of incident energy (in meV) for different waist sizes (ϵR).

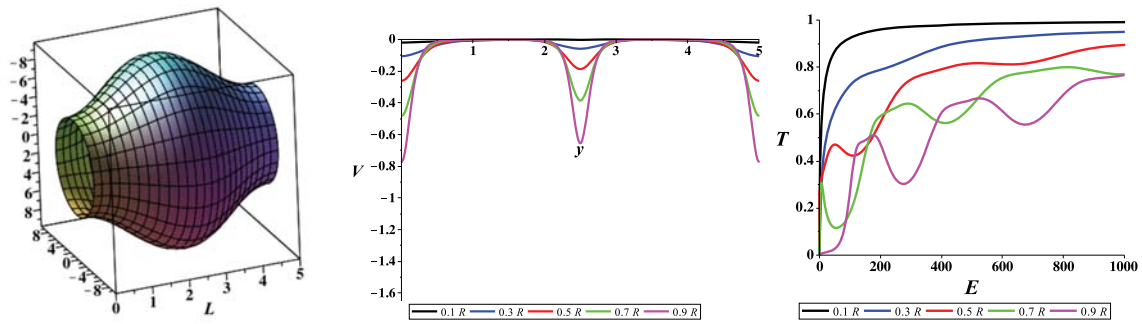


Figure 2: (a) Nanotube with a single bump. (b) Geometric potential due to the deformation shown in (a) and (c) transmittance as function of incident energy (in meV) for different bump sizes (ϵR).

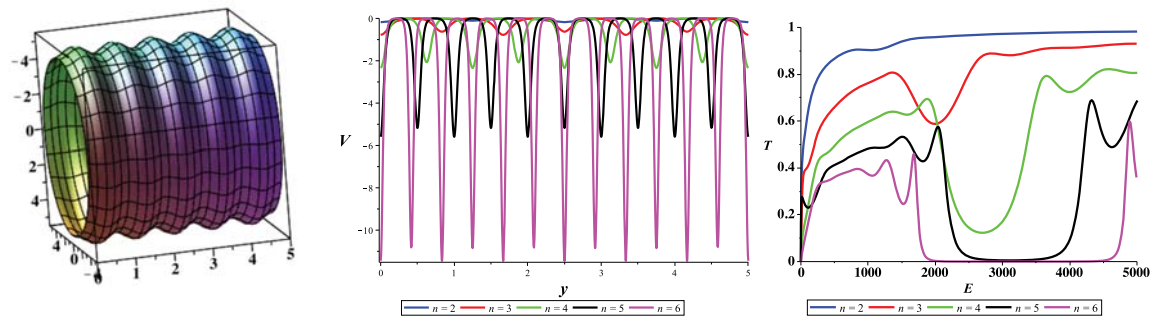


Figure 3: (a) Wavy nanotube. (b) Geometric potential due to the deformation shown in (a) for different numbers of bumps. (c) Transmittance as function of incident energy (in meV).

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