

Geometrical Effects of Wave Functions of Carbon Nanosystems

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Abstract. Networks built from carbon nanostructures and in particular from nanotubes promise exciting nanoelectronic applications. It is thus important to fully understand the quantum mechanical rules of charge propagation through these nanostructures. Some features of the electronic properties of the nanosystems are of purely geometrical origin. These can be investigated in the framework of the jellium model [1]. Wave packet dynamical calculations showed that, when the current is tunneling in a transversal direction through a carbon nanotube "sandwiched" between two electrodes, the energy dependence of tunneling probability shows a plateau in a well defined range. In this work, by solving analytically the stationary Schrödinger equation of a model system, we demonstrate that this plateau is due to electrons being trapped in stationary states of the nanotube. Geometrical features, like diameter dependence of the wave functions and binding energies are studied. Comparison of the results of the widely used zone folding technique with exact jellium wave functions shows a discrepancy at small diameters and an excellent agreement for $d > 1$ nm.

INTRODUCTION

Electron transport through carbon nanosystems is a basic phenomenon for the understanding of the Scanning Tunneling Microscopy (STM) investigation of these structures and also provides the principal operational principles for carbon nanotube based nanoelectronics. Understanding the current flow through a carbon nanotube during the STM measurements is of great interest in the interpretation of experimental STM images, which contain always a mixture of geometrical features and the electronic structure of both the sample and the STM tip. In our former wave packet dynamical simulations [2] following the time evolution of the electron tunneling through the full three-dimensional system the tunneling problem was regarded as a problem in potential scattering theory with a jellium model potential and the time dependent Schrödinger equation was solved numerically. The study of energy dependent transmission of a wave packet showed [3] when the tunneling occurs in a transversal direction through a carbon nanotube "sandwiched" between the STM tip and the support surface, the energy dependence of the tunneling probability shows a constant plateau (instead of typical exponential behavior), in a well defined energy range (Fig.1a.). This means an increased transition probability from tip to support in that energy range compared to the case when the nanotube is not present between the electrodes. This is a signature of resonant tunneling, i.e. the existence of quasi-stationary states in the mentioned energy range.

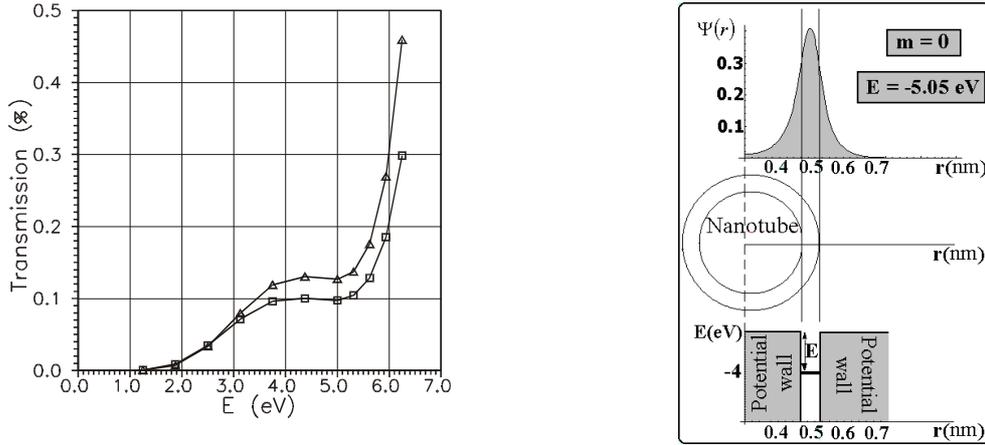


FIGURE 1. a) Energy dependent transmission of a wave packet tunneling through a nanotube in an STM model for tip positive (triangles) and negative (squares) 1 V bias potential (taken from ref.[3]). b) The potential model used in analytical calculations, and the stationary solution of the Schrödinger equation corresponding to the zero angular momentum state of a jellium tube.

CALCULATION METHOD AND RESULTS

The stationary states of the system can be found by solving the stationary Schrödinger equation for the given model. Due to the simplicity of the jellium model, this can be done analytically. The potential model is shown in figure 1b. The potential inside the walls of the tube is set to -9.81eV . Outside the walls of the tube the potential is zero. The diameter of the tube is taken 1 nm corresponding to a typical SWCNT value, while the width of the wall is chosen 0.14 nm. See ref. [3] for details. Because of the cylindrical symmetry it was feasible to solve the Schrödinger equation in cylindrical coordinates. The solutions can be written as a combination of first and second order, Bessel, and modified Bessel functions.

$$y_m(r) = A_m^i I(r, m) + B_m^i J(r, m) + C_m^i Y(r, m) + D_m^i K(r, m)$$

The coefficients of the Bessel functions were obtained from matching conditions at the boundaries of the three potential regions.

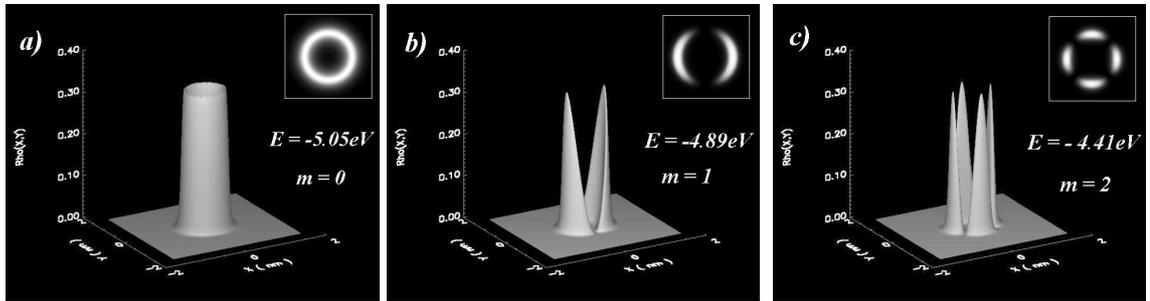


FIGURE 2. Analytical solutions of stationary Schrödinger equation for jellium tube. (x,y) are the cross sectional coordinates in nm while the vertical coordinate corresponds to the probability density. The insets show the $\rho(x,y)$ in nanotubes cross section in grayscale. E is the binding energy for the different angular momenta.

DISCUSSION AND CONCLUSIONS

As shown in figure 3a, for a jellium tube with 1 nm diameter there are six allowed energy states, corresponding to angular momentum quantum numbers $m = 0, 1, 2, 3, 4,$ and 5 . The energy distribution of the wave packet used in the time dependent simulations is also shown.

As can be seen in Fig. 3a, the incoming wave packet can excite with significant probability only three states of the jellium tube, for $m = 0, 1,$ and 2 . This means that the quantum mechanical state of the electrons at every moment can be obtained as the superposition of these three states with different, time dependent, coefficients.

During the time evolution of the system there can occur time intervals when only one of the coefficients of these three states is significant, then we can say that the system is in a quasi-stationary state.

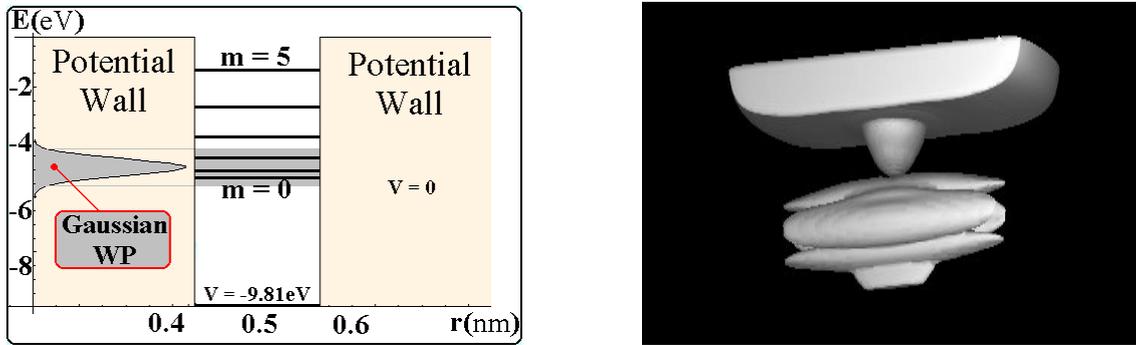


FIGURE 3. a) The stationary energies and the energy distribution of wave packet used in time dependent simulations. b) A snapshot taken from simulation at $t=5.4$ fs showing a quasi-stationary state.

Following the time evolution of our system (the tunneling process) in simulations, we have found states that shows evident similarity with our analytical results, in the Fig 3b it is shown the system in a quasi-stationary state that corresponds to our analytically calculated stationary state for $m = 2$. The metastability of these states can explain the increased dwell times of the electron (see Ref. [4]) in the tube region.

Knowing the analytical wave functions of the system, the jellium model enables us to investigate the geometrical effects such as diameter dependence of the stationary energies for different angular momentum quantum states. As expected, with increasing diameter, the binding energies for all m values tend to that calculated for the graphene layer using also the jellium potential model.

It is worth emphasizing that the zero angular quantum momentum state has inverse diameter dependence.

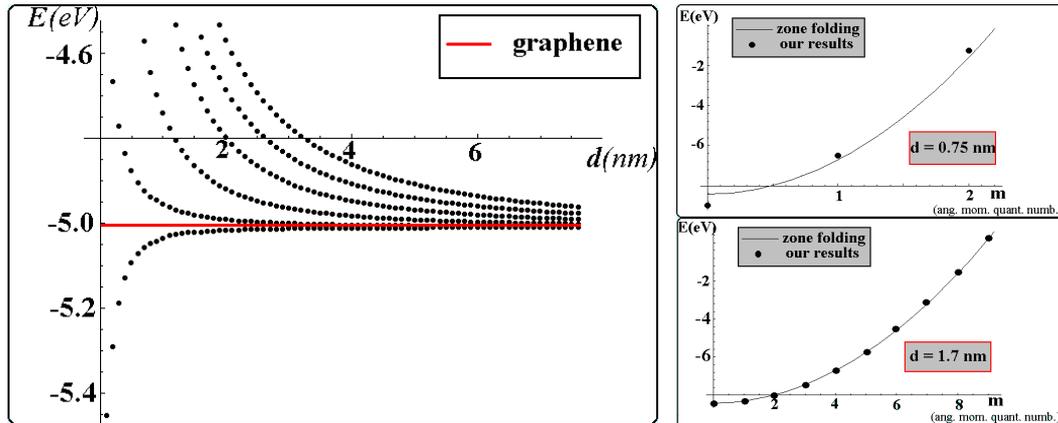


FIGURE 3. a) diameter dependence of binding energies for electrons with different angular momenta. b) comparison between the exact results and the results using zone folding approximation, for small and large tube diameters.

A widely used simple approximation is the so-called zone folding method. In tight binding approximation one calculates the wavefunctions and energies for the graphene sheet, then applies a periodic boundary condition in the rolling direction to find out the wavefunctions for the carbon nanotubes. However it is obvious from experimental findings that there are problems applying the zone folding approximation to tubes with small diameters [5]. This error was attributed to the hybridization of the s and p orbitals of the graphene, that are no more perpendicular to each other when the graphene sheet is rolled up to form a cylinder. As seen in fig 3.b. zone folding leads differences when applied to small diameter tubes even *from purely geometrical effects*.

In conclusion our analytical results are in excellent agreement with numerical simulation results, and can explain some interesting features of earlier simulations. Geometrical effects like diameter dependence of binding energies, and geometrical corrections to zone folding approximation were found.

ACKNOWLEDGMENTS

This work was supported by the EU5 contracts NANOCOMP, HRPN-CT-2000-00037 and EU5 Centre of Excellence ICAI-CT-2000 70029 and by OTKA grant T 043685 in Hungary, and the IUAP program P5/01 of the Belgian state OSTC office.

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