Electron confinement in Cavities of Carbon Nanotubes.

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We investigate the dynamical properties of electrons in cavities of nanotubes under the influence of an external electric field. The cavities of nanotubes are structures denoted as $(n_1, m_1)/N(n_2, m_2)/(n_3, m_3)$, where the diametre of the nanotubes used as contacts is smaller than the diametre of nanotubes used in the central part of the structure. There are many important properties associated to this kind of geometry as the generation of quasi-bound states inside the cavity for certain energies, or the behaviour as quantum-dot structures when the contacts are formed with semiconductor nanotubes [1, 2]. In this work we deal with cavities made of armchair nanotubes. We study the dynamical behaviour of waves when the structure is connected to two electrodes at different electric potential, that gives rise to a one-dimensional constant electric field along the structure.

According to the work of Bloch [3] and Zener [4], electrons in periodic linear chains of atoms under an electric field show Bloch oscillations. These oscillations take place due to Bragg reflections at the edges of the Brillouin regions. The behaviour of extended and localized waves under a constant electric field is quite different. The centre of the wavepacket oscillates in the case of extended waves but, on the other hand, for localized waves the electron changes its localization radius periodically with its center remaining at the same position In both cases, the period and the amplitude of these Bloch oscillations are given, respectively, by:

$$T_B = \frac{h}{eFd}, \qquad A_B = \frac{\Delta}{eF}, \tag{1}$$

where d is the period of the potential, Δ is the width of the energy band, and F is the electric field applied. We already checked that Bloch oscillations arise in carbon nanotubes [5].

In this work we study the behaviour of electrons under electric fields in cavities of carbon nanotubes. We obtain the Hamiltonian and solve the Schrödinger equation for CNT obtaining the wavefunction as a function of time. This allows us to calculate the occupation probability for any time. Furthermore, we obtain the averaged quadratic displacement and the inverse participation radius. Through the calculation of the Fourier transform of this function we obtain the frecuency of the oscillation, which we compare with the eq. 1, obtaining a good fit to the theoretical results.

The occupation probability along the nanotube axis can be represented versus time assigning a different colour for different values of probability. The figures obtained clearly show the behaviour of the wavefunction with time. The electric field can be placed in different regions of the structure, i. e. the central part of the cavity, one of the contacts, or the whole structure. We observe, for example, that if we place the electric field along the whole nanotube, the wave keeps confined at its initial region, instead of spread along the whole structure.

References

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