Electronic Transport in Nanotubes with Resonant Cavities.

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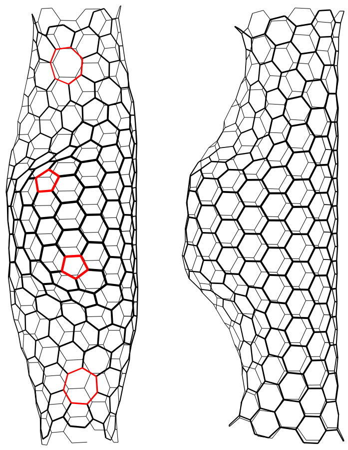
We investigate the properties of nanotubes sandwiched between other nanotubes with different geometry. This structure is shown in the Figure below. We use structures $(n, n)/N(m, m)/(n, n)$. Nanotubes with this kind of geometry are armchair. In the case $m > n$ this structure has, in its central part, a number of channels for transmission larger or equal to the number of channels in the leads. Henceforth, we refer to the central part of this structure as the cavity. This cavity behaves as a resonant box with quasi-bound states producing resonances and anti-resonances in transmission. This behavior is a consequence of the different band structures for nanotubes forming the cavity. Other authors have made similar studies but with another kind of structures: Sim *et al.* [1] worked with flattened-deformed nanotubes. Chico and Jaskolski [2] estudied a similar structure but with a conductance gap. In our study we employ metallic nanotubes with no gap in transmission in the whole range of energies, although dips in transmission arose due to the existence of quasi-bound states in the cavity.



In our calculations we employ a tight-binding model which only takes into account one π-orbital per atom. The overlap energy between nearest neighbors is taken as $t = -2.66$ eV where second-neighbor interactions are neglected. Curvature effects are not considered, as they are only significant when the diameter of the tube is small.

We calculate properties of our nanotube structures, as density of states and transmission function using the Green's function method [3], using the standard expression $\hat{G}(E) = \left(E\hat{I} - \hat{H}_n - \hat{\Sigma}_L - \hat{\Sigma}_R\right)^{-1}$, and the formalism developed by López Sancho *et al.* [4]. The latter has the advantage that converges very fast. We also calculate the eigen-energies E_n and eigen-functions Ψ_n, in order to obtain the participation number P_n: $P_n^{-1} = \sum_m |\Psi_n(m)|^4$, which gives a measure of the wavefunction extension and help to find out the localized or extended nature of an electronic state.

With the formalism developed above we show that transmission functions of nanotubes with cavities $(m > n)$ show resonances and anti-resonances. Differences between the band structures of the nanotubes forming the whole structure are responsible for this behavior. Anti-resonances in transmission are related to quasi-bound states formed inside the cavity, as it is shown by the peaks of the LDOS that coincide with dips in Transmission. These anti-resonances are produced by interferences between bound states of the central part of the nanotube and extended states along the leads. Resonances are produced by superposition of channels weakly scattered at the boundaries of the cavity, which modulate the transmission function even in the absence of quasi-bound states. We show that in the other hand, when the cavity has less transmitting channels than the leads $(m < n)$, there are not anti-resonances in transmission because of the lack of quasi-bound states inside the cavity, but transmission is slightly larger due to tunneling between leads.

We make also a deep extensive study of the behavior of the cavity as we modify its geometry. In this sense we show that 1) The larger N the less pronounced resonances in transmission while the number of peaks and valleys increases with the *length* of the cavity. 2) Increasing the *width* of the cavity makes transmission present more resonances and antiresonances. This effects are due to the interferences produced between waves weakly reflected at the boundaries of the cavity, as the number of possible energies that gives rise to interferences increases with the size of the system. Finally, properties of nanotubes with several cavities have been also studied.

References

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