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VIEWPOINT

Filtering out the transmission of π electron Fermi states with odd symmetry through a carbon nanotube junction

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Some applications in nanoelectronics may require current transport through a nanowire with electrons that are in a coherent quantum state possessing full symmetry about the wire axis. Carbon nanotube multiple junctions may have this property. Carbon nanotubes are a cylindrical variety of graphite having the form of long, hollow molecules [1]. Single-wall nanotubes have just one atomic cylindrical layer. They behave like a metal or a semiconductor, depending on the way the graphene sheet is rolled up with respect to the axis [2]. Among them, armchair nanotubes have CC bonds perpendicular to the molecule axis; they are always metallic. Armchair nanotubes are periodic one-dimensional crystals. In their one-dimensional first Brillouin zone, two electronic bands with linear dispersion cross each other at the Fermi level for a positive wavenumber k [3] and two other bands do the same for negative k due to the $k \leftrightarrow -k$ inversion symmetry (see figure 1). The corresponding Fermi states mix the carbon 2p orbitals oriented normal to the graphene sheet, the so-called π orbitals.

Under a small voltage bias, two bands from the four metallic bands crossing the Fermi level transport electrons from the negative to the positive electrode. For that reason, it is said that a metallic nanotube has two conductive channels, each of them contributing one quantum of conductance to the electric conductance of the system when there is no defect. The two metallic states carrying the electric current in an armchair nanotube have different symmetries: one state is totally symmetric (a_1) with respect to the reflection through any mirror plane containing the axis of the nanotube and the other is antisymmetric (a_2) with respect to the same reflection.

In the presence of a defect that preserves at least an axial mirror plane (a vacancy, an impurity, some Stone–Wales defects, . . .), the transmission of electrons through one conduction channel may be strongly affected for some electron energies where the defect has a strong coupling with one metallic band of the nanotube, whereas the other channel is much less perturbed [4]. In the paper of Kim *et al* [5], an armchair nanotube with a 'needle-eye' defect is considered from a theoretical point of view. At a given location, the armchair nanotube separates into two armchair branches with smaller diameter, like the two legs of a pair of trousers, a structure that has indeed been observed experimentally in a TEM microscope [6]. Further away, the two branches fuse together to rebuild the original nanotube, while closing the eye of the needle. The structure is constructed such as to preserve a mirror plane containing the nanotube axis. Tight-binding calculations reveal that the transmission of electrons can be strongly reduced for those metallic states having the odd mirror symmetry (a_2) and is much less

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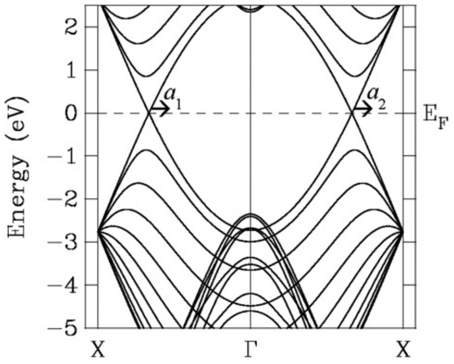

Figure 1. Tight-binding electron band structure of the (10, 10) armchair nanotube. The border points X of the first Brillouin zone correspond to $k = \pm\pi/a$, with a the lattice parameter of the nanotube. Two pairs of branches, with odd (a_2) and even (a_1) mirror symmetries, cross the Fermi level (taken as the zero of energy) for positive and negative wavevectors. Under a small potential bias, electrons are transported by these two branches on both sides of the Γ point that have, say, a positive slope (arrows).

so for the even symmetry (a_1), like for any one of the localized defects mentioned here above. However, there are now *continuous intervals* of energy where the 'needle-eye' junction filters out the a_2 symmetry instead of doing so only for a few *discrete* energies as before. The junction works like a valve that transmits electron states that have mirror symmetry around the armchair nanotube, whereas the second conduction channel is virtually closed over a continuous and sizable window of the applied voltage bias.

Interestingly, if such a system were used as a STM tip and provided there were no ending cap at the apex but a sharp armchair termination instead, it could be used to image the wavefunction character of a sample without distortion. Indeed, the wavefunction of the scanned sample has to couple to those electron states that the 'needle-eye' junction can transmit. These states are totally symmetric around an armchair end of the nanotube, preserving thereby the intrinsic character of the sample wavefunction that they couple to. For instance, it would then become possible to distinguish between d orbitals of the sample having $x^2 - y^2$ character and those with $3z^2 - r^2$ character.

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