Study of Cap States in Carbon Nanotubes

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Energy levels of states localized in a cap are calculated in a tight-binding model for pencil caps closing armchair nanotubes. They are at about 0, ±2, and ±3 in units of $2\pi\gamma/L$ in nanotubes with sufficiently large circumference $L$, where $\gamma$ is the band parameter.

1. Introduction

Some carbon nanotubes have caps at the end [1]. According to Euler’s theorem a cap contains six five-membered rings in a graphene sheet if it is constructed of only six- and five-membered rings. The presence of states localized in caps was indicated by the study of the local density of states in a tight-binding model [2] and by STM measurements [3]. The occurrence of resonance s-scattering was demonstrated by the study of a phase shift of scattering of an electron wave for several caps [4]. Further, patterns of six five-membered rings were observed by field emission microscopy [5], which may be related to the presence of cap states. In this paper, we study such localized cap states in a tight-binding model and elucidate their dependence on the circumference.

2. Cap States

In this paper we consider metallic armchair nanotubes closed by a pencil cap having highest rotation symmetry. A pencil cap consists of six five-membered rings located with equal distance along the boundary between a nanotube and a cap as shown in Fig. 1. Because of the six-fold rotation symmetry around the tube axis, we divide the states into six kinds of states by an angular momentum $\sigma=0, 1, \ldots, 5$.

Figure 2 shows energy bands of a tube with $L=18\sqrt{3}a$ ($a$ is the lattice constant) by solid ($\sigma=0$), dotted ($\sigma=1$ and 5), dashed ($\sigma=2$ and 4), and dot-dashed ($\sigma=3$) lines classified by the symmetry. Each band is doubly degenerate except those given by solid lines crossing the Fermi level and except the highest and lowest bands. The smallest gaps of bands with $\sigma=1$ and 5, $\sigma=2$ and 4, and $\sigma=3$ are approximately given by 1, 2, and 3 in units of $2\pi\gamma/L$, respectively, with $\gamma=\sqrt{3}\gamma_0a/2$ where $\gamma_0$ is the transfer integral between nearest-neighbor sites.

The calculation of cap states is straightforward in principle. For each symmetry $\sigma$ and at a given energy, the wave function in the cap region is matched with evanescent modes in the tube region which decay away from the cap. Such matching is possible only at a certain energy and when the connection is established, we have a cap state.

3. Numerical Results

Results are shown in Fig. 3. States with $\sigma=1$ and 5 are degenerate in energy and same is true of states with $\sigma=2$ and 4, while those with $\sigma=3$ have small splitting. In nanotubes with sufficiently large $L$, the energy of the states with $\sigma=1$ and 5 is about $\varepsilon=0$, that with $\sigma=2$ and 4 are near the band edges of the states with $\sigma=2$ and 4. For the states with $\sigma=3$, their splitting decreases and the energy is near the band edges of the states with $\sigma=3$.

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References


Figure Captions

Fig. 1. A cap structure of a pencil cap is shown by a projection mapping.

Fig. 2. Energy bands of an armchair CN with circumference $L=18\sqrt{3}a$ are described by solid, dotted, dash, dot-dash lines, being classified by the rotation symmetry $\sigma$ around the tube axis.

Fig. 3. Energy levels of localized states of the pencil caps as a function of the circumference.
Fig. 1

Fig. 2

Fig. 3