# Cap States in Capped Carbon Nanotubes by Effective-Mass Theory

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**Abstract**

Localized cap states are studied by an effective-mass approximation in metallic armchair nanotubes closed by a cap consisting of $q$ graphene sheets of regular triangles ($q=6,5$).

*Key words:* cap, graphite, carbon nanotube, finite length, five- and seven-membered ring, energy level, effective-mass theory

## 1. Introduction

Localized cap states were obtained in some caps theoretically by the study of local density of states in a tight-binding (TB) model [1]. The presence of localized states was suggested also by a scanning tunneling microscopy [2,3]. In s previous study, resonance states in several less symmetric caps were obtained by a scattering of an electron wave by the caps [4]. Energy levels of these cap states were calculated in carbon nanotubes (CNs) with different diameters in a TB model [5]. The purpose of this work is to study such localized cap states by an effective-mass (EM) theory.

## 2. Effective-mass description

In the vicinity of K and K' points of the Brillouin zone of 2D graphite, the electronic states are well described by the EM equation $H\boldsymbol{F}(\boldsymbol{r})=\varepsilon\boldsymbol{F}(\boldsymbol{r})$ and an envelope function $\boldsymbol{F}(\boldsymbol{r})$ which has four components and

$$H=\gamma\begin{pmatrix}\hat{k}_x\sigma_x+\hat{k}_y\sigma_y & 0\\ 0 & \hat{k}_x\sigma_x-\hat{k}_y\sigma_y\end{pmatrix}, \tag{1}$$

where $\gamma$ is the band parameter, $\boldsymbol{\sigma}$ is the Pauli matrix, $\hat{\boldsymbol{k}}=-i\nabla$, and the $x$ and $y$ are chosen in the circumference and axis of CN, respectively.

We consider armchair CNs and caps consisting of $q$ graphene sheets of regular triangles. A cap with $q=6$ and 5 has been called a pencil and bowl cap, respectively. Figure 1 shows the structure of a pencil cap. The origin is chosen at the cap center and the polar coordinates $(r,\theta)$ are introduced also. The capped CN has $q$-fold rotation symmetry around the axis and states are specified by discrete "angular momentum" $\sigma$ given by an integer satisfying $-(q/2)<\sigma\leq(q/2)$. In the CN and cap regions, boundary conditions are given by

$$\boldsymbol{F}(x+r_0,y)=\mathrm{e}^{2\pi i\sigma/q}\,\boldsymbol{F}(x,y), \tag{2}$$

$$\boldsymbol{F}(R\boldsymbol{r})=\mathrm{e}^{2\pi i\sigma/q}\,T_{\pi/3}\boldsymbol{F}(\boldsymbol{r}), \tag{3}$$

respectively, where $r_0$ is the side of the equilateral triangle, $R$ denotes the $\pi/3$ rotation around the origin, and

$$T_{\pi/3}=\begin{pmatrix}0&0&0&1\\0&0&-\omega^{-1}&0\\0&-1&0&0\\\omega&0&0&0\end{pmatrix}, \tag{4}$$

which has been obtained for a junction system [6].

Under the boundary conditions (3), we obtain the wave functions in the cap region,

$$\boldsymbol{F}_{\mu_+}(r,\theta)=\begin{pmatrix}J_{\mu_+}(|\varepsilon|r/\gamma)\\(\varepsilon/|\varepsilon|)iJ_{\mu_++1}(|\varepsilon|r/\gamma)\,\mathrm{e}^{i\theta}\\s_m(\varepsilon/|\varepsilon|)iJ_{\mu_++1}(|\varepsilon|r/\gamma)\,\mathrm{e}^{i\theta}\\s_mJ_{\mu_+}(|\varepsilon|r/\gamma)\end{pmatrix}\frac{\mathrm{e}^{i\mu_+\theta}}{\sqrt{D_{\mu_+}}} \tag{5}$$

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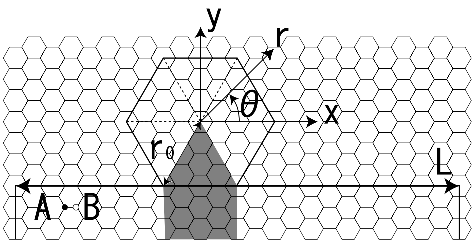


Fig. 1. The projection mapping of a pencil cap.

$$\boldsymbol{F}_{\mu_-}(r,\theta)=\begin{pmatrix}(\varepsilon/|\varepsilon|)J_{\mu_-+1}(|\varepsilon|r/\gamma)\\ -iJ_{\mu_-}(|\varepsilon|r/\gamma)\,\mathrm{e}^{i\theta}\\ -s_{m+1}iJ_{\mu_-}(|\varepsilon|r/\gamma)\,\mathrm{e}^{i\theta}\\ s_{m+1}(\varepsilon/|\varepsilon|)J_{\mu_-+1}(|\varepsilon|r/\gamma)\end{pmatrix}\frac{\mathrm{e}^{-i(\mu_-+1)\theta}}{\sqrt{D_{\mu_-}}} \quad (6)$$

where $J_\mu$ is the Bessel function, $\mu_+ = 3m+1+6\sigma/q$ and $\mu_- = 3m+1-6\sigma/q$ with integer $m$. The condition that the wave function is normalizable and the Hamiltonian be Hermitian gives $\mu_\pm > 1$ and $\mu_+ + \mu_- + 1 > 1$. The presence of localized cap states is determined by the condition that Fourier components of the wave functions in the tube and cap region are matched with each other. Energy levels of states with $\sigma$ are same as those with $-\sigma$ due to the mirror symmetry.

## 3. Results

Figure 2 shows some examples energy levels of the localized cap states for a pencil and a bowl cap. In EM method, these levels are at $\varepsilon(2\pi\gamma/L)^{-1}=0$, $\sim\pm1.75$, and $\sim\pm2.81$ for a pencil cap and at $\varepsilon(2\pi\gamma/L)^{-1}=0$ and $\sim\pm2.20$ for a bowl cap, where $L$ is circumference. They are all doubly degenerate and symmetric about $\varepsilon=0$.

Figure 2 contains also results of a TB method for a pencil cap with $L/\sqrt{3}a=30$ and a bowl cap with $L/\sqrt{3}a=25$, respectively. In actual capped CNs, the presence of five-membered rings destroys the symmetry between the positive and negative energies, giving rise to the slight asymmetry around $\varepsilon=0$. This asymmetry decreases with the increase of the CN thickness. In the EM scheme, this symmetry is not destroyed.

One important result is that the wave function at $\varepsilon=0$ for a pencil cap ($q=6$) is independent of $r$, while that for a bowl cap ($q=5$) is singular at $r=0$ like $r^{-1/5}$. This behavior corresponds to the main contribution of the wave function $\boldsymbol{F}_{\mu_-}$ with $\mu_-=1-6/q$.

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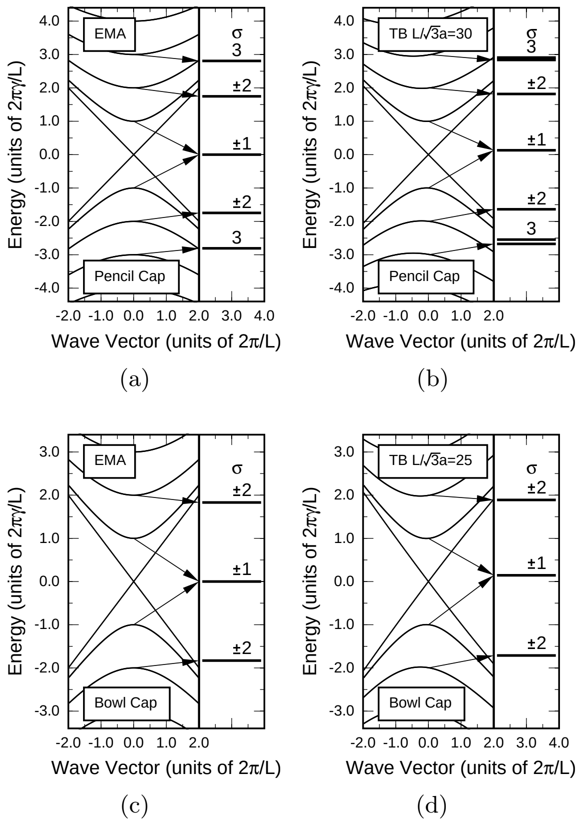


Fig. 2. Energy bands of armchair nanotubes and corresponding cap states. The results obtained by EM and TB method are shown in (a) and (b), respectively for a pencil cap. Those in a bowl cap are shown in (c) and (d). The left panel shows the energy bands and the right panel cap states. The correspondence between the band edges and the cap states is identified by the arrow.

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