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Electronic properties of perturbed cylinder

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Abstract. The electronic structure of nanocylinder without and with a small perturbation is investigated with the help of calculation of the local density of states. A continuum gauge field-theory model is used for this purpose. In this model, Dirac equation is solved on a curved surface. The local density of states is calculated from its solution. The case of 2 heptagonal defects is considered. This paper is an extension of our previous work [1] where one heptagonal and one pentagonal defects in hexagonal graphene network were compared. The metallization for the perturbed cylinder structure is found.

1. Introduction

The carbon nanostructures play a key role in constructing nanoscale devices like quantum wires, nonlinear electronic elements, transistors, molecular memory devices or electron field emitters. Their molecules are variously-shaped geometrical forms its surface is composed of disclinated hexagonal carbon lattice. The main structure of this kind is graphene - the carbon lattice plane from which all other kinds are derived. Most often, the heptagons appear in pairs with pentagons in the connecting parts of the folded forms [2].

Because of the applications, the research of the electronic properties of the carbon nanostructures is important. One of the main characteristics is the local density of states (*LDoS*). In the presented model coming from the effective-mass theory, knowledge of the solution of the corresponding Dirac equation is necessary for the calculation [3]. This solution is represented by the wave-function and to find it, we have to know the geometry of the molecular surface. As discovered in [4] for the case of nanocones, the most suitable geometry for the description of the close vicinity of the defects is the hyperboloidal geometry. Very often, for a given geometry, the number of possible defects is limited.

The solutions for spherical, conical and 2-fold-hyperboloidal cases were found in [4, 5, 6]. In [1], we used the presented model for calculation of the electronic properties of the structures with the geometry of the 1-fold hyperboloid. The aim was to describe the electronic properties in the vicinity of the locally negative curvature of an arbitrary nanoparticle. This restriction did not enable us to do the calculations for the case of more than 1 defect. In this paper, we present a model describing the electronic properties of a simple nanocylinder and a curved nanocylinder including 2 heptagons at the opposite sides of the surface. The hyperboloidal geometry is used again. Because a nanocylinder is an opened nanotube, comparison with the case of the capped nanotube could be performed (see e.g. [7] for this purpose).

2. Computational formalism

To research the electronic properties, we have to solve the Dirac equation in (2+1) dimensions. It has the form

$$i\sigma^\alpha e_\alpha^\mu [\partial_\mu + \Omega_\mu - ia_\mu - ia_\mu^W] \psi = E\psi, \quad (1)$$

where ∂_μ means the partial derivation according to the μ parameter, i.e. $\partial_\mu = \frac{\partial}{\partial x^\mu}$.

In this equation, besides the energy E , the particular constituents have the following sense: $\sigma^\alpha, \alpha = 1, 2$, denote the Pauli matrices. The wave function ψ , the so-called bispinor, is composed of two parts:

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}, \quad (2)$$

each corresponding to different sublattices of the curved graphene sheet. The gauge field a_μ arises from spin rotation invariance for atoms of different sublattices A and B in the Brillouin zone and the gauge field a_μ^W is connected with the chiral vector (n, m) :

$$a_\varphi = N/4, \quad a_\varphi^W = -\frac{1}{3}(2m + n). \quad (3)$$

If we write the wave function in the form

$$\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \frac{1}{\sqrt{4g_{\varphi\varphi}}} \begin{pmatrix} u(z)e^{i\varphi j} \\ v(z)e^{i\varphi(j+1)} \end{pmatrix}, \quad j = 0, \pm 1, \dots \quad (4)$$

and substituting (4) into (1) we obtain

$$\frac{\partial_z u}{\sqrt{g_{zz}}} - \frac{\tilde{j}}{\sqrt{g_{\varphi\varphi}}} u = Ev, \quad -\frac{\partial_z v}{\sqrt{g_{zz}}} - \frac{\tilde{j}}{\sqrt{g_{\varphi\varphi}}} v = Eu, \quad (5)$$

where

$$\tilde{j} = j + 1/2 - a_\varphi - a_\varphi^W. \quad (6)$$

Each of the solutions u, v consists of two linearly independent components such that

$$u(E, z) = C_1(E)u_1(E, z) + C_2(E)u_2(E, z), \quad (7)$$

$$v(E, z) = \frac{C_1}{E} \left(\frac{\partial_z u_1}{\sqrt{g_{zz}}} - \frac{\tilde{j}u_1}{\sqrt{g_{\varphi\varphi}}} \right) + \frac{C_2}{E} \left(\frac{\partial_z u_2}{\sqrt{g_{zz}}} - \frac{\tilde{j}u_2}{\sqrt{g_{\varphi\varphi}}} \right), \quad (8)$$

where for a concrete value of E , the functions $C_1(E), C_2(E)$ stand for satisfying the normalization condition

$$2\pi \int_{-z_{max}}^{z_{max}} (|u(E, z)|^2 + |v(E, z)|^2) dz = 1. \quad (9)$$

For a given z_0 , the *LDoS* is defined as

$$LDoS(E) = |u(E, z_0)|^2 + |v(E, z_0)|^2. \quad (10)$$

2.1. Perturbed cylinder

In the case of a small perturbation, we have

$$\vec{R}(z, \varphi) = \left(a\sqrt{1 + \Delta z^2} \cos \varphi, a\sqrt{1 + \Delta z^2} \sin \varphi, z \right), \quad (11)$$

where Δ is a positive real parameter, $\Delta \ll 1$. For $\Delta = 0$, we get the defect-free cylinder discussed in previous chapter.

Then

$$g_{zz} = 1 + \frac{a^2 \Delta^2 z^2}{1 + \Delta z^2} \sim 1 + a^2 \Delta^2 z^2, \quad g_{\varphi\varphi} = a^2(1 + \Delta z^2) \quad (12)$$

and

$$g = g_{\varphi\varphi} = a^2(1 + \Delta z^2). \quad (13)$$

b For small Δ and neglecting the second order of Δ , it can be simplified as

$$\partial_z u - \frac{\tilde{j}}{a} \left(1 - \frac{1}{2} \Delta z^2 \right) u = E v, \quad -\partial_z v - \frac{\tilde{j}}{a} \left(1 - \frac{1}{2} \Delta z^2 \right) v = E u. \quad (14)$$

The solution is

$$u(z) = C_{\Delta 1} D_{\nu_1}(\xi(z)) + C_{\Delta 2} D_{\nu_2}(i\xi(z)), \quad (15)$$

$$v(z) = \frac{C_{\Delta 1}}{E} \left(\partial_z D_{\nu_1}(\xi(z)) - \frac{\tilde{j} D_{\nu_1}(\xi(z))}{a} \left(1 - \frac{1}{2} \Delta^2 z^2 \right) \right) + \frac{C_{\Delta 2}}{E} \left(\partial_z D_{\nu_2}(i\xi(z)) - \frac{\tilde{j} D_{\nu_2}(i\xi(z))}{a} \left(1 - \frac{1}{2} \Delta^2 z^2 \right) \right), \quad (16)$$

where

$$\nu_1 = i \frac{a^2 \Delta - 4a^2 E^2 + 4ia\sqrt{\Delta}\tilde{j} + 4\tilde{j}^2}{8a\sqrt{\Delta}\tilde{j}}, \quad \nu_2 = -i \frac{a^2 \Delta - 4a^2 E^2 - 4ia\sqrt{\Delta}\tilde{j} + 4\tilde{j}^2}{8a\sqrt{\Delta}\tilde{j}}, \quad (17)$$

$$\xi(z) = (-\Delta)^{1/4} \left(\sqrt{\frac{a}{2\tilde{j}}} + \sqrt{\frac{2\tilde{j}}{a}} z \right), \quad (18)$$

$D_\nu(\xi)$ being the parabolic cylinder function. The functions $C_{\Delta 1} = C_{\Delta 1}(E)$, $C_{\Delta 2} = C_{\Delta 2}(E)$ will be calculated in the same way as for the defect-free cylinder, i. e. from the normalization condition

$$\int_{-z_{max}}^{z_{max}} (|u(E, z)|^2 + |v(E, z)|^2) dz d\varphi = 4\pi \int_0^{z_{max}} (|u(E, z)|^2 + |v(E, z)|^2) dz = 1. \quad (19)$$

3. Conclusion

In Fig. 1, a comparison of the 2D plots of $LDoS$ is made for different values of Δ and similarly in Fig. 2, where the 3D plots are compared. The number of defects $N = 2$ and the other values are same as in the defect-free case. On the whole, we can conclude from the comparison that $LDoS$ is slightly increasing for higher Δ . Although this is only the first order approximation, we will see that the real solution of behaves in a similar manner. We found that for the defect-free case, the electronic properties can sometimes correspond to the case of infinitely long nanoribbons. For the case of perturbation, the metallic properties are more manifested.

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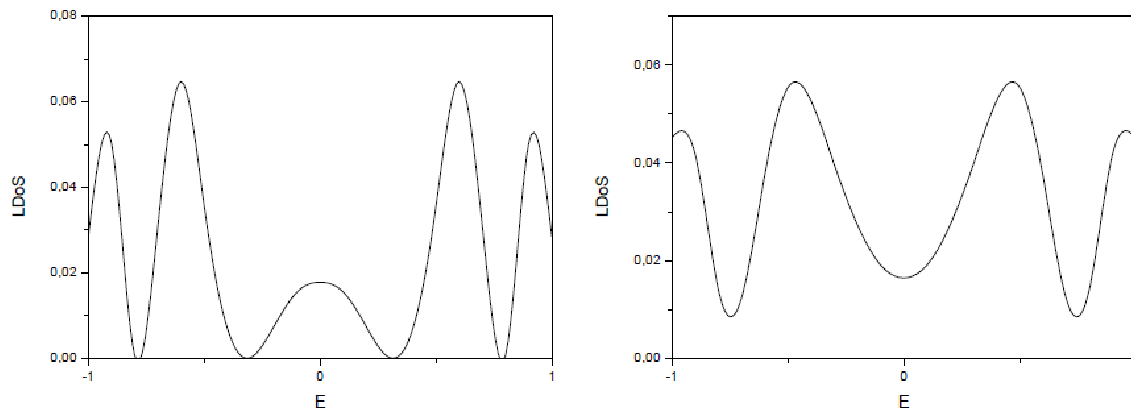


Figure 1. *LDoS* as a function of $E \in (-1, 1)$ and $z = 98$ for perturbed cylinder with $\Delta = 0.05$ (left) and $\Delta = 0.1$ (right)

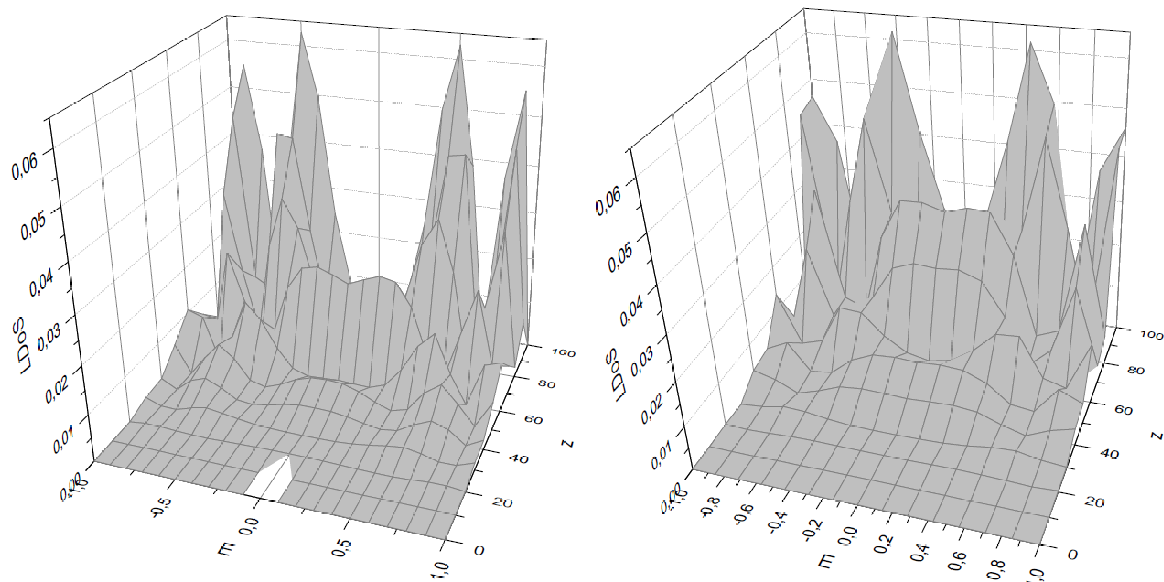


Figure 2. *LDoS* as a function of $E \in (-1, 1)$ and $z \in (0, 100)$ for perturbed cylinder with $\Delta = 0.05$ (left) and $\Delta = 0.1$ (right)

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