

Electronic structure of negatively curved graphene

D. V. Kolesnikov¹⁾, V. A. Osipov¹⁾

*Joint Institute for Nuclear Research, Bogoliubov Laboratory of Theoretical Physics,
141980 Dubna, Moscow region, Russia*

Submitted 4 March 2008

We study the electronic structure of graphene in the presence of either sevenfolds or eightfolds by using a gauge field-theory model. The graphene sheet with topological defects is considered as a negative cone surface with infinite Gaussian curvature at the center. The density of electronic states is calculated for a single seven- and eightfold as well as for a pair of sevenfolds with different morphology. The density of states at the Fermi energy is found to be zero in all cases except two sevenfolds with translational factor $M \neq 0$.

PACS: 73.22.-f, 73.22.-Dj

Nowadays graphene and related graphene-based nanostructures are the subject of great interest. It is well known that some number of fivefolds must be included in the honeycomb graphene lattice to produce various nanostructures with positive Gaussian curvature of the surface: nanocones, nanohorns, closed nanotubes, fullerenes, etc. There is another type of possible defects, sevenfolds and eightfolds, which results in a surface with negative Gaussian curvature. Experimentally the presence of sevenfolds in various nanostructures was observed by Iijima [1]. The structures with sevenfolds only are rather exotic [2], however, the presence of fivefold-sevenfold pairs is expected in some cases and, what is important, leads to new features of the graphene-based materials. For example, in the carbon nanotube this pair changes chirality, which allows one to connect metallic and semiconducting nanotubes without breaking of π -bonds (see, e.g., [3]). Therefore the question of the electronic structure of carbon nanostructures containing sevenfolds has the definite theoretical and practical interest.

Earlier computations on the carbon lattice [4] shows the general decrease of the density of states (DoS) near the sevenfolds in the sixfold plane. Notice that the influence of the curvature was not taken into account in [4]. Effects of both topological defects and local curvature on the electronic properties of planar graphene has been recently studied in [5, 6] within the effective low-energy field-theory model proposed to study the electronic structure of slightly curved graphene sheets with an arbitrary number of pentagon-heptagon pairs.

In the present paper, we investigate the electronic structure of the graphene plane with either a single sevenfold or two sevenfolds/one eightfold inserted (which

corresponds to the negative 60° and 120° disclination, respectively). The surface of the plane is assumed to be free to bend but impossible to stretch. This results in appearance of the “surplus-angle cone” surface with infinite (negative) Gaussian curvature in the center, but with absence of the rotational symmetry. We use a field-theory model suggested in [7–9] and, in final form, in [10], which includes two gauge fields to take into account both the presence of sevenfolds and the influence of surface curvature.

Let us consider the planar honeycomb lattice, which can be bent but can not be stretched. A single sevenfold can be inserted in this lattice by using the standard “cut-and-paste” procedure. The surface of the lattice due to the presence of negative disclination will appear to be curved (see Fig.1). Let us assume the curved surface in

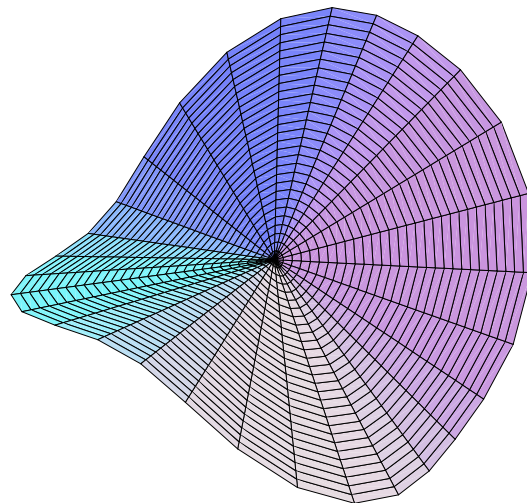


Fig.1. The curved surface of the honeycomb lattice with a single sevenfold inserted at the center (a “surplus-angle cone”).

¹⁾e-mail: kolesnik@theor.jinr.ru, osipov@theor.jinr.ru

the form

$$\mathbf{r} = (r \cos \varphi \sin \theta(\varphi), r \sin \varphi \sin \theta(\varphi), r \cos \theta(\varphi)), \quad (1)$$

where

$$\theta(\varphi) = \frac{\alpha}{2} \cos(2\varphi) + \frac{\pi}{2}.$$

After the cut-and-paste procedure, the length of the line of a constant distance R from the sevenfold (which is also the line of intersection of the 3d-sphere and the surface) is larger than for the same line in the planar case. Since the sevenfold leads to an additional 60° sector, the length should have the value $(7/6)2\pi R$. One can define it from the condition

$$R \int_0^{2\pi} \sqrt{\sin^2 \theta(\varphi) + (\theta'(\varphi))^2} d\varphi = 2\pi R \frac{7}{6}, \quad (2)$$

which allows us to fix the only parameter α . The metrical tensor for the described surface is written as

$$g_{rr} = 1, g_{\varphi\varphi} = r^2 [\sin^2 \theta(\varphi) + \alpha^2 \sin^2(2\varphi)], g_{r\varphi} = 0, \quad (3)$$

and the non-zero metrical connection coefficients read

$$\begin{aligned} \Gamma_{\varphi\varphi}^r &= -g_{\varphi\varphi}/r, \\ \Gamma_{\varphi r}^\varphi &= \Gamma_{r\varphi}^\varphi = 1/r, \\ \Gamma_{\varphi\varphi}^\varphi &= (1/2)\partial_\varphi \ln g_{\varphi\varphi}. \end{aligned} \quad (4)$$

The two-folds can be chosen in the form

$$e_r^1 = 1, \quad e_\varphi^2 = \sqrt{g_{\varphi\varphi}}, \quad e_r^1 = e_r^2 = 0. \quad (5)$$

By using the known relation $(\omega_\mu)^{ik} = e_\nu^i D_\mu e^{\beta\nu}$ where an ordinary covariant derivative D_μ includes the metrical connection (4), one finds the spin connection coefficients as

$$(\omega_\varphi)^{12} = -(\omega_\varphi)^{21} = -\frac{g_{\varphi\varphi}}{r}. \quad (6)$$

The model Dirac equation has the form (see [10])

$$-i\sigma^a e_a^\mu (\nabla_\mu - ia_\mu^k - iW_\mu) \psi^k = E\psi^k, \quad (7)$$

where E is measured from the Fermi energy, σ^a ($a = 1, 2$) are the conventional Pauli matrices, a_μ^k ($k = K, K_-$) and W_μ are two gauge fields (non-Abelian and Abelian, respectively), and $\nabla_\mu = \partial_\mu + \Omega_\mu$ ($\mu = r, \varphi$) with

$$\Omega_\mu = \frac{1}{8} \omega_\mu^{ab} [\sigma_a, \sigma_b].$$

In our case, one obtains

$$\Omega_\varphi = -i\sigma_3 \frac{\sqrt{g_{\varphi\varphi}}}{2r}, \quad \Omega_r = 0.$$

To simplify the problem the gauge fields are taken in the same form as for the isotropic case:

$$a_\varphi^k = \pm 1/4, \quad W_\varphi = -1/6, \quad a_r^k = W_r = 0. \quad (8)$$

The Dirac equation (7) can be diagonalized in respect to the K/K_- part (see [10] for detail), so that finally it takes the form

$$-i\sigma_1 (\partial_r + \frac{1}{2r}) \psi - \frac{i\sigma_2}{\sqrt{g_{\varphi\varphi}}} (\partial_\varphi - ia_\varphi - iW_\varphi) \psi = E\psi. \quad (9)$$

One can easily see that for $\alpha = 0$ (9) reduces to the planar Dirac equation in the polar coordinates. Unlike the planar case, in (9) $g_{\varphi\varphi}$ is a function of the polar angle φ . This markedly complicates the analysis. Let us make the separation of variables in (9) assuming

$$\psi(r, \varphi) = \begin{pmatrix} u(r) \\ v(r) \end{pmatrix} \Phi(\varphi).$$

The function Φ should neglect the dependence of the wavefunction on φ in (9). Therefore, we find the equation for Φ in the form

$$\frac{\Phi'}{\Phi} - ia_\varphi - iW_\varphi = ij \sqrt{\sin^2 \theta(\varphi) + \alpha^2 \sin^2(2\varphi)}, \quad (10)$$

where j is a constant. Introducing an auxiliary function

$$G(\varphi) = \int_0^\varphi \sqrt{\sin^2 \theta(\phi) + \alpha^2 \sin^2(2\phi)} d\phi, \quad (11)$$

one can write down Φ in the form $\Phi = \exp(ia_\varphi \varphi + iW_\varphi \varphi) \exp(ijG(\varphi))$. Let us note that $G(2\pi) = 2\pi(7/6)$ due to (2). The boundary condition for the spinor wavefunction has the form $\psi(\varphi + 2\pi) = -\psi(\varphi)$. This allows us to find the constant j as

$$j = j_n = \frac{6}{7} [1/2 + (n - a_\varphi - W_\varphi)], \quad n = 0, \pm 1, \dots \quad (12)$$

and

$$\Phi_n = \exp(i(a_\varphi + W_\varphi)\varphi) \frac{\exp(ij_n G(\varphi))}{\sqrt{2\pi}}, \quad (13)$$

which finally leads to the system of coupled equations for u_n, v_n in the following form:

$$\begin{aligned} -i(\partial_r + \frac{1}{2r} + \frac{j_n}{r})v_n(r) &= Eu_n(r), \\ -i(\partial_r + \frac{1}{2r} - \frac{j_n}{r})u_n(r) &= Ev_n(r). \end{aligned} \quad (14)$$

Notice that this system is equivalent to the planar Dirac equation with the only difference in the values of j_n . The solution to (14) is written as

$$u_n = C J_{|j_n - 1/2|}(|E|r), \quad v_n = \pm i C J_{|j_n + 1/2|}(|E|r), \quad (15)$$

where J are the Bessel functions, and C is the normalization constant. The density of electronic states per unit area (LDoS) can be found from the properly normalized wavefunctions. The normalizing condition

$$C^2 \int r(u^2 + v^2) dr = 1.$$

allows us to find the normalization constant. Taking into account the asymptotical behaviour of the solution (15)

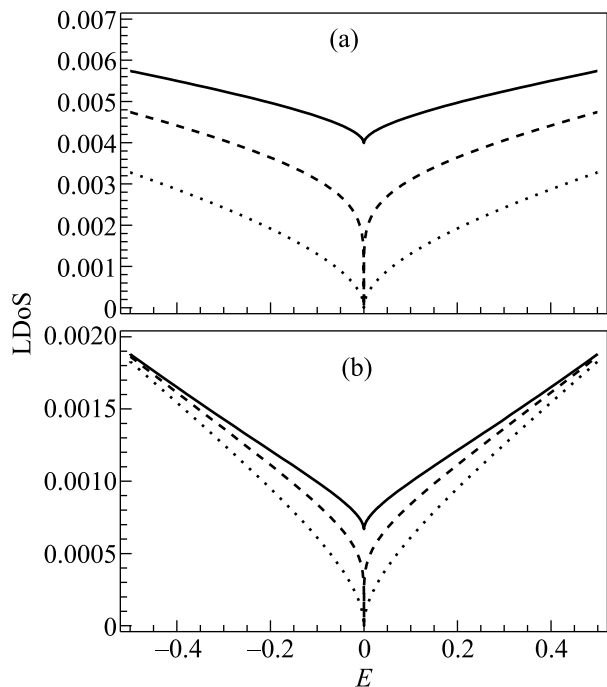


Fig.2. The local density of states per unit area (in the same scale), as a function of the energy near the center (top) and far from the center (bottom)

($[J_{n+1/2}^2(x) + J_{n-1/2}^2(x)]x \simeq 2/\pi$ when $x \rightarrow \infty$) one can find the LDoS in the following form:

$$\text{LDoS}(E, r) = \frac{|E|}{2\pi(1 + \Omega)} \sum_{\epsilon, n} (J_{\epsilon(j_n + 1/2)}(|E|r)^2 + J_{\epsilon(j_n - 1/2)}(|E|r)^2). \quad (16)$$

Here Ω ($\Omega = 1/6$ for a sevenfold) defines a surplus angle of a cone and

$$j_n = 6/7(1/2 + n + 1/6 \pm 1/4). \quad (17)$$

The summation runs over all values of n and $\epsilon = \pm 1$, which satisfies the condition $\epsilon j_n \geq 0$. This restriction comes from the fact that the LDoS should be finite (or zero) in the limit $E \rightarrow 0$. In that way it overrides the

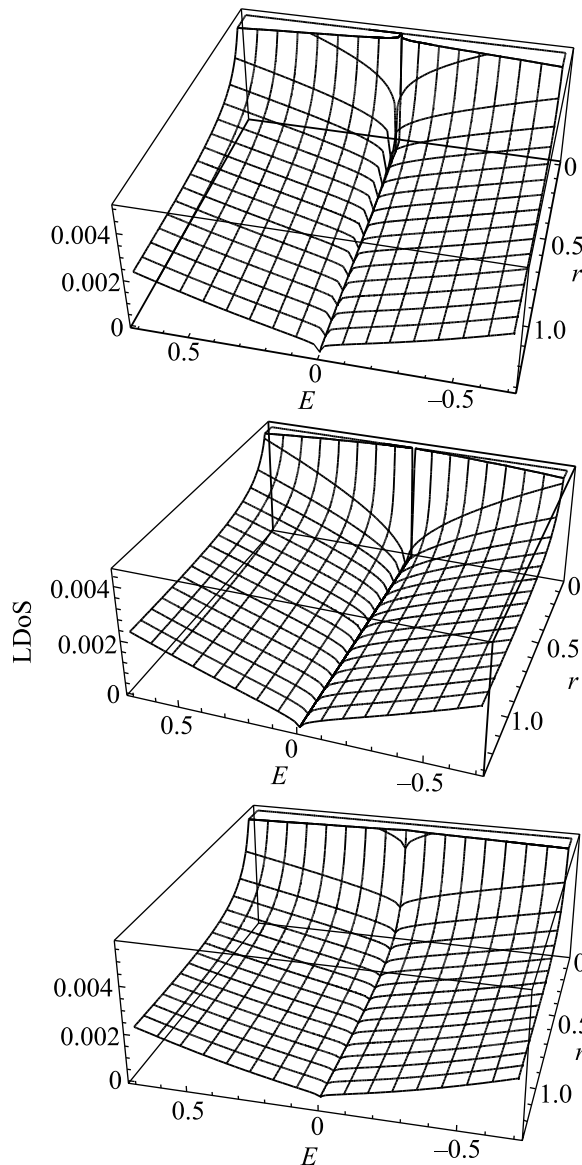


Fig.3. The local density of states per unit area (in the same scale), as a function of the radial coordinate r and the energy E . The cases of a single sevenfold (top), single eightfold or two sevenfolds with $M = 0$ (middle), and two sevenfolds with non-zero M (bottom) are shown

normalization condition for the wavefunction at $r \rightarrow 0$. Notice that the LDoS does not depend on the angle coordinate φ despite the fact that the surface does not possess the axial symmetry. Accordingly, (16) formally looks like the LDoS for a normal (deficit-angle) cone found in [11]. As a result, the only dimensional quantity in the LDoS is r while the energy can be reduced to the dimensionless parameter with respect to the energy unit $\hbar V_F/r$ where V_F is the Fermi velocity.

In the case of two closely situated sevenfolds or one eightfold the LDoS is also described by (16) with $\Omega = 1/3$ and

$$j_n = 6/8(1/2 + n + 1/3 \pm (1/2 + M/3)). \quad (18)$$

The factor M describes the morphology of defects: $M = 0$ for an eightfold or when the shift vector (n, m) from one sevenfold to another satisfies the condition $(n + m) \bmod 3 = 0$, otherwise $M = 1$ (see [10, 11] for detail). The energy dependence of the LDoS near the center and far from the center is presented in Fig.2. As is seen, the LDoS rapidly increases with energy near the sevenfold while far from the defect it has almost linear behavior.

The LDoS as a function of the energy and the coordinate is shown in Fig.3. One can see that at the Fermi energy ($E = 0$) the LDoS is zero for both single defects while a finite value of LDoS is found for two sevenfolds with $M \neq 0$. This is provided by the term with $j_n = 0$ in the LDoS. The LDoS increases near the center ($r \approx 0$) and becomes r -independent at far distances being linear in energy like in the case of planar graphene.

To conclude, we have investigated the electronic structure of the graphene with one and two sevenfolds as well as with one eightfold in the framework of the field-theory approach. The curvature of the surface was taken into account by considering the “negative cone” with infinite and negative Gaussian curvature at the center. The calculations show that near defects the density of states is growing faster in comparison with the planar case. When the energy and/or a distance from the defect increases, the LDoS tends to be almost similar to the planar case. These findings are in general agreement with numerical calculations in [4]. At small distances from the defect an increase of the LDoS (per unit area) was found. Within our approach this increase can be explained by the influence of infinite curvature at the center ($r = 0$). In the case of two sevenfolds with the translational factor $M \neq 0$ the existence of the metal-

lization near the defects was observed. For the eightfold, the metallization in the defect region is absent. This conclusion differs from the results of [4] where near the eightfold a non-zero value of the LDoS was found to vary (highly anisotropic) for different atoms on the same distance from the defect, thus forming local metal states. Such difference can be explained by two reasons: (a) the continual character of our model and (b) an isotropic approximation. Notice that in our study the LDoS does not depend on the angle φ due to excluded radial components of the fields (8). On the other hand, the shape of the surface is properly taken into account in our model, leading to curvature-induced peculiarities which are absent in the planar case [4].

This work has been supported by the Russian Foundation for Basic Research under grant # 08-02-01027.

-
1. S. Iijima, P. M. Ayayan, and T. Ichihashi, *Phys. Rev. Lett.* **69**, 3100 (1992).
 2. H. Terrones and M. Terrones, *New Journ. Phys.* **5**, 126.1 (2005).
 3. A. V. Eletskii, *Phys. Usp.* **40**, 899 (1997).
 4. R. Tamura and M. Tsukada, *Phys. Rev. B* **49**, 7697 (1994).
 5. A. Cortijo and M. A. H. Vozmediano, *Nucl. Phys. B* **763**, 293 (2007).
 6. A. Cortijo and M. A. H. Vozmediano, *EPL* **77**, 47002 (2007).
 7. E. A. Kochetov and V. A. Osipov, *J. Phys. A: Math. Gen.* **32**, 1961 (1999).
 8. V. A. Osipov, E. A. Kochetov, and M. Pudlak, *JETP* **96**, 140 (2003).
 9. D. V. Kolesnikov and V. A. Osipov, *JETP Letters* **79**, 660 (2004).
 10. V. A. Osipov and D. V. Kolesnikov, *Rom. Journ. Phys.* **50**, 435 (2005); D. V. Kolesnikov and V. A. Osipov, *Europhys. J. B* **49**, 465 (2006).
 11. P. E. Lammert and V. H. Crespi, *Phys. Rev. B* **69**, 035406 (2004).