Electronic Properties of Curved Carbon Nanostructures

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Abstract

The electronic structure near the Fermi energy of a single carbon layer containing either heptagons or pentagons is investigated within the continuum gauge field-theory model. Two geometries are considered: an upper half of a two-sheet hyperboloid for pentagons included in a graphene sheet, and a one-sheet hyperboloid for circularly situated heptagons in a nanotube. A self-consistent perturbation scheme is developed for numerical calculations of both the eigenfunctions and the local density of states (LDoS) near the pentagonal and heptagonal defects.

1 Introduction

Among the most unique features of carbon nanoparticles are their electronic properties. Electronic states in nanotubes, fullerenes, nanocones, nanohorns as well as in other carbon configurations are the subject of an increasing number of experimental and theoretical studies. They already find a use for the development of modern nanoscale electronic devices: flat panel displays, nano-switches, molecular memory devices, transistors, electron field emitters, etc. Interesting changes in the electronic properties arise from topological defects. The peculiar electronic states due to topological defects (pentagons) have been observed in different kinds of carbon nanoparticles by scanning tunneling microscopy (STM). A pentagon can be inserted in the hexagonal lattice by a cut-and-glue procedure typical for disclination defects. Namely, one has to cut out a 60° sector from a graphene sheet and then glue together the two cut sides of the sheet. Moreover, if the departure from the flat surface is allowed, a cone-like surface with positive Gaussian curvature will be generated (see Fig.1). On the contrary, to produce a heptagon one has to insert a 60° sector into a graphene sheet. This corresponds to a negative disclination and leads to a saddle surface with negative Gaussian curvature. A heptagon included into a nanotube will generate a characteristic saddle configuration with the cone-like asymptotic and the heptagon situated at the saddle point (see Fig.1). Thus, an investigation of the electronic structure requires formulating a theoretical model describing electrons on arbitrary curved surfaces with disclinations taken into account.

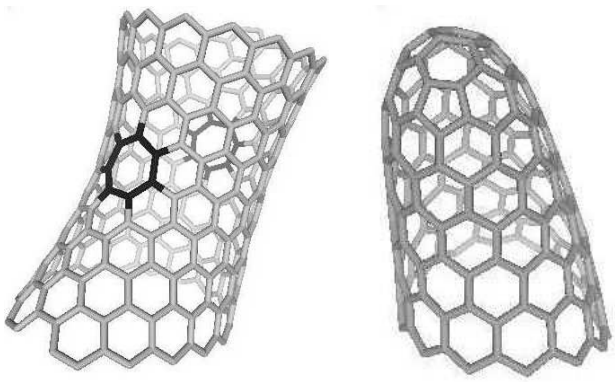

Figure 1: A carbon nanotube with two inserted heptagons (marked), and a carbon nanohorn (on the right).

2 General formalism

Our consideration is based on the effective-mass theory proposed in [1] to study the screening of a single intercalant within a graphite host. A two-dimensional approximation for the description of graphite host was used. Actually, the effective-mass expansion is equivalent to the $\vec{k}\cdot\vec{p}$ expansion of the graphite energy bands about the $\vec{K}$ point in the Brillouin zone when the intercalant potential is zero. In fact, there are two degenerate Bloch eigenstates at $\vec{K}$, so that the wave function can be approximated by

$$\Psi(\vec{k},\vec{r}) = f_1(\vec{\kappa})e^{i\vec{\kappa}\vec{r}}\Psi_1^S(\vec{K},\vec{r}) + f_2(\vec{\kappa})e^{i\vec{\kappa}\vec{r}}\Psi_2^S(\vec{K},\vec{r})$$

where $\vec{k} = \vec{K} + \vec{\kappa}$. Keeping terms of order $\vec{\kappa}$ in the Schrödinger equation one can obtain the secular equation for functions $f_{1,2}(\vec{\kappa})$ and after diagonalization one finally gets the two-dimensional Dirac equation (see details in [1])

$$i\gamma^\mu\partial_\mu\psi(\vec{r}) = E\psi(\vec{r}) \tag{1}$$

where γ^μ are the conventional Pauli matrices, the energy E is accounted from the Fermi energy, and the two-component wave function ψ represents two graphite sublattices. As was mentioned in [1] the essence of the $\vec{k}\cdot\vec{p}$ approximation is to replace the graphite bands by conical dispersions at the Fermi energy. For our purpose, we have to generalize the model (1). First, one has to take into account two independent wave vectors ($\vec{K}$ and $\vec{K}_- = -\vec{K}$) in the carbon lattice, which give the same conical dispersion. A special form of a microscopic electronic wavefunction was suggested in [2]. In the most general case, this wavefunction can be presented as the following:

$$\begin{aligned}\psi(\vec{r}) = \psi_A(\vec{K},\vec{r})F_A^K(\vec{r}) + e^{i\chi_1}\psi_B(\vec{K},\vec{r})F_B^K(\vec{r}) + \\ +e^{i\chi_2}\psi_A(\vec{K}_-,\vec{r})F_A^{K_-}(\vec{r}) + e^{i\chi_3}\psi_B(\vec{K}_-,\vec{r})F_B^{K_-}(\vec{r})\end{aligned} \tag{2}$$

where $\psi_{A,B}(\vec{K},\vec{r})$ are the Bloch functions on A (B) sublattice, respectively. The wavefunction with the Bloch functions depending on both $\vec{K}$ and $\vec{K}_-$ was introduced in [3, 4] where the frame for $\vec{K}_-$ components was rotated through the angle π, so that $F = (F_K(\vec{r})\ F_{K_-}(R(\pi)\vec{r}))^T$.

Let us introduce so-called K-spin matrices τ, which act only on the K-spin (+/-) part of the spinor, while the standard σ (γ) - matrices act on the A/B part. In this case, the Dirac operator does not depend on the K-spin matrices. The microscopic wavefunction which leads to a spinor F can be found from (2) by rotating frame through the angle π for the terms containing K_- (here we define $\vec{R}_{A,B-} = R(\pi)\vec{R}_{B,A}$)

$$\psi(\vec{r}) = \psi_A(\vec{K},\vec{r})F_A^K(\vec{r}) + e^{i\chi_1}\psi_B(\vec{K},\vec{r})F_B^K(\vec{r}) + \\ +e^{i\chi_2}\psi_A(\vec{K},\vec{r}_-)F_A^{K_-}(\vec{r}_-) + e^{i\chi_3}\psi_B(\vec{K},\vec{r}_-)F_B^{K_-}(\vec{r}_-) \quad (3)$$

with $\vec{r}$ being either $\vec{R}_A$ or $\vec{R}_B$. As is seen, (3) does not contain $\vec{K}_-$ in the explicit form. Then the microscopic wavefunction on the sublattices A and B reads

$$\psi_A(\vec{R}_A) = \exp(i\vec{K}\vec{R}_A)F_A^K(\vec{R}_A) + e^{i\chi_3}\exp(i\vec{K}\vec{R}_{B-})F_B^{K_-}(\vec{R}_{B-}) \\ \psi_B(\vec{R}_B) = e^{i\chi_1}\exp(i\vec{K}\vec{R}_B)F_B^K(\vec{R}_B) + e^{i\chi_2}\exp(i\vec{K}\vec{R}_{A-})F_A^{K_-}(\vec{R}_{A-}). \quad (4)$$

When a single $\pi/3$ disclination is inserted into a graphite lattice, one gets the following conditions for the wavefunction (cf. [2])

$$\psi_{A,B}(\vec{R}'_{A,B}) = \psi_{B,A}(\vec{R}_{B,A}), \quad \vec{R}'_{A,B} = R(5\pi/3)(\vec{R}_{B,A} - \vec{R}) + \vec{R}. \quad (5)$$

The presence of a disclination means that a wavefunction obeys discontinious boundary conditions (after the cut-and-paste procedure sublattices A and B become mixed). In this case, one can introduce a gauge field, which makes the wavefunction continuous and carry information about the mixing of sublattices. Due to transformation properties of the Bloch functions, the operator describing boundary conditions is written as $F(\vec{R}') = M_{60}F(\vec{R})$. By appropriate choosing of phases χ_1, χ_2 and χ_3 one gets M_{60} in the form $M_{60} = i\tau_2\exp(-i\pi\sigma_3/6)$ where $\exp(-i\pi\sigma_3/6) = \exp(i\oint\vec{Q}d\vec{r})$ depends on a spin connection term $\vec{Q}$ (see below), which determines the "cut" procedure. The holonomy now is

$$\psi(\varphi + 2\pi) = T\psi(\varphi), \quad T = i\tau_2 = \cos(\pi/2) + i\tau_2\sin(\pi/2) = e^{i\pi\tau_2/2},$$

where T (unlike M) is a holonomy operator (T determines the "paste" procedure). Then the compensating gauge field $\vec{a}$ is determined by a condition

$$\oint\vec{a}d\vec{r} = \frac{\pi}{2}\tau_2, \quad T = \exp(i\oint\vec{a}d\vec{r}).$$

For two or more defects, the operator M is constructed from both M_{60} and the shift operator placing the defect to its position. The shift operator can be written as

$$T(n,m) = \exp(i\frac{2\pi}{3}(n+m)\tau_3). \quad (6)$$

Then an operator describing the defect located at the position (n,m) reads

$$M_{60}(n,m) = T(n,m)M_{60}T(-n,-m) = T(-n,-m)M_{60} \quad (7)$$

where the anti-commutation of different τ- matrices is taken into account. Let us describe the complex defect as two disclinations located at (0,0) and (n,m). Then M takes the following form:

$$M = M_{60}(-n,-m)M_{60} = \exp(i\pi(1 - \frac{2}{3}(n+m))\tau_3)\exp(-i\frac{\pi}{3}\alpha_3), \quad (8)$$

and the gauge field is determined by $\oint \vec{a} d\vec{r} = \pi(1 - \frac{2}{3}(n+m))\tau_3$. For N disclinations located at different points with coordinates (n_i, m_i) the matrix is expressed as

$$M = M_{60}(n_{N-1}, m_{N-1}) M_{60}(n_{N-2}, m_{N-2}) \dots M_{60}(n_1, m_1) M_{60} = \\ = M_{60}(n_{N-1} - n_{N-2} + \dots, m_{N-1} - m_{N-2} + \dots) M_{60}^{N-1}. \quad (9)$$

For odd number of defects, the operator M_{60} ($M_{60} = i\tau_2$) being multiplied by $T(n,m)$ adds finally to the total flux a term proportional to $\pi/2$

$$\exp(i\frac{2\pi}{3}(n+m)\tau_3)(i\tau_2) = i\vec{\tau}\vec{n} = \exp(i\frac{\pi}{2}\vec{\tau}\vec{n}) \quad (10)$$

where $|\vec{n}| = 1$ is the unit vector. By redefining the phases χ_i, the total operator can be easily transformed to $\exp(i\pi\tau_2/2)$. For odd N, the shift operator vanishes and one obtains M_{60}^N. One should mention that the circulation of the gauge field $\vec{a}$ depends only on the lattice topology and is independent of geometry of the structure. For a self-consistent description, one should also include the information about both the disclination itself (its topological nature) and curved background.

A possible way to describe disclinations on arbitrary two-dimensional elastic surfaces is the gauge approach [5]. In accordance with the basic assumption of this approach, disclinations can be incorporated by means of introducing dynamical $SO(2)$ gauge fields (compensating Yang-Mills fields) in the Lagrangian of elasticity theory. What is important, the gauge model was found to admit exact vortex-like solutions for wedge disclinations [5] thus confirming the view of a disclination as a vortex of elastic medium. It is also interesting to note that the elastic flux due to rotational defects (that is directly connected with the Frank vector (see section 3)) is completely determined by the gauge vector fields associated with disclinations. In this context, disclination field can be simply accounted in (1) by using the covariant derivative.

In the linear approximation, the basic field equation which describes the $SO(2)$ gauge field in a curved background reads

$$D_\mu F^{\mu k} = 0, \quad F^{\mu k} = \partial^\mu W^k - \partial^k W^\mu. \quad (11)$$

where covariant derivative $D_\mu := \partial_\mu + \Gamma_\mu$ includes the Levi-Civita (torsion-free, metric compatible) connection

$$\Gamma^k_{\mu\lambda} := (\Gamma_\mu)^k_\lambda = \frac{1}{2} g^{kl} \left(\frac{\partial g_{l\lambda}}{\partial x^\mu} + \frac{\partial g_{\mu l}}{\partial x^\lambda} - \frac{\partial g_{\mu\lambda}}{\partial x^l} \right), \quad (12)$$

with $g_{\mu k}$ being the metric tensor on a Riemannian surface Σ with local coordinates $x^\mu = (x^1, x^2)$. For a single disclination on arbitrary elastic surface a singular solution to (11) is found to be [5]

$$W^k = -\nu \varepsilon^{k\lambda} D_\lambda G(x,y), \quad (13)$$

where

$$D_\mu D^\mu G(x^1, x^2) = 2\pi\delta^2(x^1, x^2)/\sqrt{g}, \quad (14)$$

with $\varepsilon_{\mu k} = \sqrt{g}\epsilon_{\mu k}$ being the fully antisymmetric tensor on Σ, $\epsilon_{12} = -\epsilon_{21} = 1$. It should be mentioned that eqs. (11-14) self-consistently describe a defect located on an arbitrary surface [5].

To incorporate fermions on the curved background we need a set of orthonormal frames $\{e_\alpha\}$ which yield the same metric, $g_{\mu\nu}$, related to each other by the local $SO(2)$ rotation,

$$e_\alpha \to e'_\alpha = \Lambda^\beta_\alpha e_\beta, \quad \Lambda^\beta_\alpha \in SO(2).$$

It then follows that $g_{\mu\nu} = e^{\alpha}_{\mu} e^{\beta}_{\nu} \delta_{\alpha\beta}$ where e^{μ}_{α} is the zweibein, with the orthonormal frame indices being $\alpha, \beta = \{1, 2\}$, and coordinate indices $\mu, \nu = \{1, 2\}$. As usual, to ensure that physical observables be independent of a particular choice of the zweinbein fields, a local $so(2)$ valued gauge field ω_{μ} is to be introduced. The gauge field of the local Lorentz group is known as a spin connection. For a theory to be self-consistent, zweinbein fields must be chosen to be covariantly constant [6]:

$$\mathcal{D}_{\mu} e^{\alpha}_{\nu} := \partial_{\mu} e^{\alpha}_{\nu} - \Gamma^{\lambda}_{\mu\nu} e^{\alpha}_{\lambda} + (\omega_{\mu})^{\alpha}_{\beta} e^{\beta}_{\nu} = 0,$$

which determines the spin connection coefficients explicitly

$$(\omega_{\mu})^{\alpha\beta} = e^{\alpha}_{\nu} D_{\mu} e^{\beta\nu}. \tag{15}$$

Additionally, we should also introduce another gauge field $\vec{a}$, which describes the lattice mixing (see above). Finally, the Dirac equation (1) on a surface Σ in a presence of the $U(1)$ external gauge field W_{μ} is written as

$$i\gamma^{\alpha} e_{\alpha}^{\ \mu} (\nabla_{\mu} - i a_{\mu} - i W_{\mu}) \psi = E\psi, \tag{16}$$

where $\nabla_{\mu} = \partial_{\mu} + \Omega_{\mu}$ with

$$\Omega_{\mu} = -iQ_{\mu} = \frac{1}{8} \omega^{\alpha\ \beta}_{\ \mu} [\gamma_{\alpha}, \gamma_{\beta}] \tag{17}$$

being the spin connection term in the spinor representation. The meaning of the spin connection term, represented as an "external field", results from $\oint Q_{\mu} dx^{\mu} = -\pi n_{\Omega} \sigma_3 / 6$. Here a spinor has the form $\psi = (F^K_A \ F^{K-}_A \ F^K_B \ F^{K-}_B)^T$.

3 Pentagons: two-sheet hyperboloid

An upper half of a hyperboloid can be regarded as an embedding

$$(\chi, \varphi) \to (a \sinh\chi \cos\varphi, a \sinh\chi \sin\varphi, c \cosh\chi)$$

From these one can easily find the metrical tensor and nonvanishing connection coefficients.

In a rotating $SO(2)$ frame the zweibeins become

$$\begin{aligned} e^{1}_{\ \chi} = \sqrt{g_{\chi\chi}} \cos\varphi, \ e^{2}_{\ \chi} = \sqrt{g_{\chi\chi}} \sin\varphi, \\ e^{1}_{\ \varphi} = -a \sinh\chi \sin\varphi, \ e^{2}_{\ \varphi} = a \sinh\chi \cos\varphi, \end{aligned} \tag{18}$$

which in view of eq. (15) gives for the spin connection coefficients

$$\omega^{12}_{\chi} = \omega^{21}_{\chi} = 0, \quad \omega^{12}_{\varphi} = -\omega^{21}_{\varphi} = \frac{1}{2} \left[1 - \frac{a \cosh\chi}{\sqrt{g_{\chi\chi}}} \right] = \omega, \tag{19}$$

so that the spin connection $\Omega_{\varphi} = i\omega\sigma^3$.

External gauge potential in this case is found to be $W_{\chi} = a_{\chi} = 0$, $W_{\varphi} = \nu$, and the Dirac operator on the hyperboloid takes the form

$$\hat{\mathcal{D}} = \begin{bmatrix} 0 & e^{-i\varphi} \left(-\frac{\partial_{\chi}}{\sqrt{g_{\chi\chi}}} + \frac{1}{a \sinh\chi} (i\partial_{\varphi} + \nu + a_{\varphi} + \omega) \right) \\ e^{i\varphi} \left(\frac{\partial_{\chi}}{\sqrt{g_{\chi\chi}}} + \frac{1}{a \sinh\chi} (i\partial_{\varphi} + \nu + a_{\varphi} - \omega) \right) & 0 \end{bmatrix}.$$

The substitution $\tilde{\psi} = \psi\sqrt{\sinh\chi}$ reduces the eigenvalue problem (16) (after diagonalization by the K-spin part) to

$$\begin{aligned} \partial_\chi \tilde{u} - \sqrt{\coth^2\chi + b^2}\,\Phi\tilde{u} &= \tilde{E}\tilde{v}, \\ -\partial_\chi \tilde{v} - \sqrt{\coth^2\chi + b^2}\,\Phi\tilde{v} &= \tilde{E}\tilde{u}, \end{aligned} \tag{20}$$

where $\tilde{E} = \sqrt{g_{\chi\chi}}\,E$, $b = c/a$, and $\Phi = j - n_\Omega/6 + 1/2 \mp (n_\Omega/4 - M/3)$ with $M = -1, 0, 1$ being a factor depending on the morphology of defects. For odd number of defects (and when all the defects are located at the same point), one has $M = 0$ as stated above.

Let us consider the zero-energy modes by setting $E = 0$ in (20). The general solution reads

$$\begin{aligned} \tilde{u}_0(\chi) &= A\left[(k\cosh\chi + \Delta)^{2k}\,\frac{\Delta - \cosh\chi}{\Delta + \cosh\chi}\right]^{\frac{\Phi}{2}}, \\ \tilde{v}_0(\chi) &= A\left[(k\cosh\chi + \Delta)^{2k}\,\frac{\Delta - \cosh\chi}{\Delta + \cosh\chi}\right]^{-\frac{\Phi}{2}}, \end{aligned} \tag{21}$$

where $k = \sqrt{1 + b^2}$, $\Delta = \Delta(\chi) = \sqrt{1 + k^2\sinh^2\chi}$, and A is a normalization factor.

Due to the cone asymptotic, it is quite reasonable to assume a correspondence between the parameter k and the Frank index ν. Namely, like for a cone, one can specify $k = 1/(1 - \nu)$ (see, for example, [7]). In this case, only $\tilde{v}_0$ mode becomes normalized and only for $j = 2$ and $4 < n_\Omega < 6$. Therefore, a true zero-mode solution exists for exactly five disclinations. It is interesting to note that this is the typical nanohorn configuration [8] (see Fig.1). This finding has an important physical consequence. Recall that there are two kinds of sublattice points in a unit cell of the graphene lattice due to degeneracy [1]. Hence the presence of exactly one zero-mode state implies the enhancement of the electron densities only on one sort of points, while for two zero modes both lattice points would have excess densities thus allowing a metallization. Physically, this means that, for example, the field emission properties in the first case are less efficient. This agrees well with the experimental results in [9] where field emission properties of carbon nanohorn films were observed and compared with the best nanotube emitters.

The existence of the zero-mode solutions allows us to formulate a self-consistent approximation procedure to obtain the eigenfunctions near the Fermi level. Namely, the substitution

$$\tilde{u}(\chi) = \tilde{u}_0(\chi)\,\mathcal{U}(\chi), \quad \tilde{v}(\chi) = \tilde{v}_0(\chi)\,\mathcal{V}(\chi)$$

reduces (20) to

$$\partial_\chi \mathcal{U} = \xi\Delta\mathcal{V}\frac{\tilde{v}_0}{\tilde{u}_0}, \quad \partial_\chi \mathcal{V} = -\xi\Delta\mathcal{U}\frac{\tilde{u}_0}{\tilde{v}_0}, \quad \xi = aE \tag{22}$$

Then $\mathcal{U}$ and $\mathcal{V}$ can be found by using the iteration procedure.

Before we proceed, let us discuss asymptotic solutions. At large distances, the hyperboloid geometry becomes nearly the same as the geometry of a cone. For large χ (when $\sqrt{g_{\chi\chi}} \gg a$) (20) is written as

$$\partial_r\tilde{u} - (\Phi k/r)\tilde{u} = Ek\tilde{v}, \; -\partial_r\tilde{v} - (\Phi k/r)\tilde{v} = Ek\tilde{u}, \tag{23}$$

where $r = ae^{\chi}/2 > 0$, which is exactly the polar coordinate r introduced for the cone geometry in [3]. Naturally, when $r \to \infty$ the solution to (23) can be approximated by

$$\tilde{u}_\infty \approx C\cos(Ekr + \varphi_0), \quad \tilde{v}_\infty \approx C\sin(Ekr + \varphi_0). \tag{24}$$

As it follows from (24), $\tilde{u}_\infty^2 + \tilde{v}_\infty^2 \approx C^2 = const$, that is the LDoS tends to a constant. Notice that these solutions are also similar to those for a cone (cf. [3, 7]). Therefore, we may conclude that the influence of the disclination field on the density of states has a local character in the present geometry.

Since only one component in (21) becomes normalizable, one can put $\mathcal{U}^{(0)} = 0$. Then, in the leading approximation one obtains

$$\tilde{u}(\chi) = \xi\tilde{u}_0(\chi)\left(\mathcal{U}^{(1)}(0) + \mathcal{V}^{(0)}\int_0^\chi \Delta(\eta)\frac{\tilde{v}_0(\eta)}{\tilde{u}_0(\eta)}\,d\eta\right),$$
$$\tilde{v}(\chi) = \mathcal{V}^{(0)}\tilde{v}_0(\chi), \tag{25}$$

where the constant $\mathcal{U}^{(1)}(0) = -\mathcal{V}^{(0)}\int_0^\infty \Delta(\eta)(\tilde{v}_0(\eta)/\tilde{u}_0(\eta))\,d\eta$ is chosen in such a way that the normalizing integral with functions (25) converges to a finite value when $\xi \to 0$. This allows us to integrate (20) numerically by using (25) as initial conditions.

4 Heptagons: one-sheet hyperboloid

It was observed in [10] that there exist single-walled nanotube-based structures with the negative curvature. As discussed above, a possible origin of such curvature is the presence of heptagons. We will consider two or more negative disclinations of fixed power (heptagons) situated symmetrically along the ring. In this case, a one-sheet hyperboloid geometry can be realized. Geometrically, the one-sheet hyperboloid can be regarded as an embedding

$$(\chi, \varphi) \to (a\cosh\chi\cos\varphi, a\cosh\chi\sin\varphi, c\,\sinh\chi).$$

The field equations for the one-sheet hyperboloid are similar to (18,19) with the only replacement sinh $\Leftrightarrow$ cosh. Let us solve the first Eq.(13). In our geometry, one obtains $W_\chi = 0$, $W_\varphi = \nu\,\mathrm{sign}\,(\chi)/2$ where sign is a signum function and $\nu = -n_\Omega/6$ is the total Frank index of a defect. This reflects the fact that the disclination sources are distributed continuously along a ring, so that $\rho(\chi, \varphi) = (1/2\pi)\delta(\chi)$ in (14). As for two-sheet hyperboloid, $a_\chi = 0$, and $a_\varphi = \mathrm{sign}\,\chi(6 - n_\Omega/2)\tau_2/4$, if $n_\Omega/2$ is odd, or $a_\varphi = \mathrm{sign}\,\chi\tau_3((6-n_\Omega/2)/4 + M(\mathrm{sign}\,\chi)/3)$ for even $n_\Omega/2$. Notice that the number of defects n_Ω takes only an even value due to the symmetry of the hyperboloid. Then the Dirac operator on the one-sheet hyperboloid takes the same form, but with a_φ depending on $\mathrm{sign}\,\chi$. The substitution $\tilde{\psi} = \psi\sqrt{\cosh\chi}$ together with the linearization procedure reduces the eigenvalue problem (16) to

$$\partial_\chi\tilde{u} - \sqrt{\tanh^2\chi + b^2}\,\Phi\tilde{u} = \tilde{E}\tilde{v},$$
$$-\partial_\chi\tilde{v} - \sqrt{\tanh^2\chi + b^2}\,\Phi\tilde{v} = \tilde{E}\tilde{u} \tag{26}$$

where $\tilde{E} = \sqrt{g_{\chi\chi}}\,E$, $b = c/a$, and $\Phi = \Phi(\mathrm{sign}\,\chi) = j + 1/2 + n_\Omega/12\,\mathrm{sign}\,(\chi) \mp ((6 - n_\Omega/2)/4 + M(\mathrm{sign}\,\chi)/3)\,\mathrm{sign}\,\chi$. Here the morphology factor M depends on $\mathrm{sign}\,\chi$, however, as for the two-sheet hyperboloid, when the

value $n_\Omega/2$ is odd one has $M = 0$. At large distances from a disclination ring ($\chi \to \pm\infty$) the asymptotical solutions from (26) have the same form as (24), and $\tilde{u}^2 + \tilde{v}^2 \approx C^{\pm 2} = const$, that is the LDoS tends to a constant at large distances like for the cone [3, 7] (and like for a plane without disclinations). Therefore, one can conclude that the influence of the disclination field on the density of states has a local character in the present geometry. This allows us to suggest an identical "vacuum" at both ends of hyperboloid which means the same values of the LDoS at $\chi \to \pm\infty$. One can calculate the source equations (26) numerically, using asymptotic solutions to produce initial conditions.

5 Conclusion

In this paper, we have formulated a model to study an influence of graphite sublattice structure, curved geometry and topological defects on the electronic states near the Fermi energy for structures with negative and positive Gaussian curvatures. The departure from the planar graphite lattice is suggested to be entirely due to the presence of negative and positive disclinations, respectively. The studies were carried out within a continuum field-theory gauge model. The electronic fields are described by the massless Dirac equation in two space dimensions. The disclination fields are incorporated by using the external gauge field with either a point-like or continuously distributed source. The curvature is taken into account in Dirac equation via the metrics and spin connection. For two different models, self-consistent perturbation schemes were suggested which allow us to calculate the electronic eigenfunctions near the Fermi energy.

References

[1] D.P. DiVincenzo and E.J. Mele, Phys. Rev. B **29**, 1685 (1984).

[2] H. Matsumura and T. Ando, J. Phys. Soc. Jpn. **67**, 3542 (1998).

[3] P.E. Lammert and V.H. Crespi, Phys. Rev. Lett. **85**, 5190 (2000).

[4] P.E. Lammert and V.H. Crespi, Phys. Rev. B **69**, 035406 (2004).

[5] E.A. Kochetov and V.A. Osipov, J.Phys. A: Math.Gen. **32**, 1961 (1999).

[6] M.B. Green, J.H. Schwartz, and E. Witten, *Superstring theory*, (Cambridge 1988), v. 2.

[7] V. A. Osipov, E. A.Kochetov, and M. Pudlak, JETP **96**, 140 (2003).

[8] J.-C. Charlier and G.-M. Rignanese, Phys. Rev. Lett. **86**, 5970 (2001).

[9] J.-M. Bonard, R. Gaál, S. Garaj, et al., J. Appl. Phys. **91**, 10107 (2002).

[10] S. Iijima, P.M. Ayayan, and T. Ichihashi, Phys. Rev. Lett. **69**, 3100 (1992).