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SOLIDS
Electronic Properties

Electronic Structure of Carbon Nanoparticles¶

V. A. Osipov[a, *], E. A. Kochetov[a, *], and M. Pudlak[b, **]

[a]*Bogolyubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, Moscow oblast, 141980 Russia*

[b]*Institute of Experimental Physics, Slovak Academy of Sciences, Kosice, 043 53 Slovak Republic*

**e-mail: osipov@thsun1.jinr.ru, kochetov@thsun1.jinr.ru*

***e-mail: pudlak@saske.sk*

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Abstract—The electronic structure of graphitic nanoparticles is investigated within a gauge field-theory model. The local and total densities of states (DOS) near the pentagonal defects (disclinations) are calculated for three geometries: sphere, cone, and hyperboloid. It is found that the low-energy electron states have a rather specific dependence on both the energy and the distance from a disclination line. In particular, the low-energy total DOS has a cusp that drops to zero at the Fermi energy for disclinations with the Frank index $\nu < 1/2$, while a region of a nonzero DOS across the Fermi level is formed for $\nu = 1/2$. The true zero-mode fermion state is found for the graphitic hyperboloid. The appearance of an enhanced charge density near the Fermi level for nanocones with a 60° opening angle (180° disclination) is predicted. © *2003 MAIK "Nauka/Interperiodica".*

1. INTRODUCTION

Carbon nanoparticles, which are expected to have important implications for the development of electronic devices, flat panel displays, nanoswitches, etc., have recently received great attention from both experimentalists and theorists (see, e.g., reviews [1, 2]). The high flexibility of carbon allows producing variously shaped carbon nanoparticles: nanotubes, fullerenes, cones, toroids, graphitic onions, and nanohorns. Particular attention has been given to the peculiar electronic states due to topological defects that have been observed in different kinds of carbon nanoparticles by scanning tunneling microscopy (STM). For example, STM images with fivefold symmetry (due to pentagons in the hexagonal graphitic network) have been obtained in the C_{60} fullerene molecule [3]. The peculiar electronic properties at the ends of carbon nanotubes (which include several pentagons) have been probed experimentally in [4, 5]. Recently, the electronic structure of a single pentagon was revealed on an atomic scale by STM in [6], where the enhanced charge density at the pentagon, which was located at the apex of the conical protuberance of the graphitic particle, was experimentally clarified.

By its nature, the pentagon occurring in a graphite sheet is a topological defect. Actually, as mentioned in [7], fivefold coordinated particles are orientational disclination defects in the otherwise sixfold coordinated triangular lattice. Moreover, disclinations are generic defects in closed carbon structures, fullerenes, and nanotubes, because, in accordance with Euler's theorem, these microcrystals can only be formed with the total disclination 4π. According to the geometry of the hexagonal network, this implies the presence of twelve pentagons (60° disclinations) on the closed hexatic surface.

We note that graphitic cones are of special interest because they can contain a single pentagon at the apex, in contrast to twelve pentagons in fullerene molecules and nanotubes. This fact makes nanocones attractive for experimental study of peculiar electronic states due to topological defects that were theoretically predicted in [8, 9]. In particular, analysis within the effective-mass theory shows that a specific $\sqrt{3} \times \sqrt{3}$ superstructure induced by pentagon defects can appear with the wave functions decaying as $r^{-1/5}$ [8]. Recently, this prediction was experimentally verified in [6]. A recent study [10] within both tight-binding and *ab initio* calculations shows the presence of sharp resonant states in the region close to the Fermi energy. The strength and position of these states with respect to the Fermi level were found to depend sensitively on the number and relative positions of the pentagons constituting the conical tip. In particular, a prominent peak occurring just above the Fermi level was found for the nanocone with three symmetric pentagons (which corresponds to a 60° opening angle or, equivalently, to a 180° disclination). On the other hand, the continuum model suggested in [9] predicts apical enhancement of the density of states (DOS) at the Fermi energy (E_F) in the vicinity of the apex for cones with 120° disclinations.

It is interesting to note that the problem of specific electronic states at the Fermi level due to disclinations is similar to that of the fermion zero modes in topologically nontrivial manifolds. In field theory, zero modes

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were found to play an important role in understanding anomalies [11] and charge fractionalization that results in unconventional charge–spin relations (e.g., paramagnetism of charged fermions) [12]. As mentioned in [12], this finding has been experimentally verified in trans-polyacetylene chains for one spatial dimension. The Dirac equation for massless fermions in three-dimensional space–time in the presence of a magnetic field was found to yield $N - 1$ zero modes in the N-vortex background field [13]. As we have shown in [14], the problem of the local electronic structure of fullerene is closely related to Jackiw's analysis [13]. We note that the field-theory models for Dirac fermions in a plane and on a sphere [15, 16] were invoked to describe the variously shaped carbon materials. More recently, the importance of the fermion zero modes was discussed in the context of high-temperature chiral superconductors [17–19] and fullerene molecules [16].

Investigation of the electronic structure requires formulating a theoretical model describing electrons on arbitrary curved surfaces with disclinations taken into account. An important ingredient of this model can be provided by the self-consistent effective-mass theory describing the electron dynamics in the vicinity of an impurity in graphite intercalation compounds [20]. The most important fact found in [20] is that the electronic spectrum of a single graphite plane linearized around the corners of the hexagonal Brillouin zone coincides with that of the Dirac equation in (2 + 1) dimensions. This finding stimulated formulation of some field-theory models for Dirac fermions on hexatic surfaces to describe the electronic structure of variously shaped carbon materials: fullerenes [14, 15], nanotubes [21], and cones [9, 22].

In this paper, we study the problem of electron states in carbon nanostructures for three geometries: sphere, cone, and hyperboloid. We note that, in our approach, the gauge theory of disclinations on fluctuating elastic surfaces [23] is basically used. More specifically, we formulate the Dirac equation on a curved surface with a flux due to a pentagonal apical disclination represented by an Abelian gauge field. Both the local and the total density of states are calculated in each case. Special attention is given to the correct inclusion of the spin connection for fermions. Actually, our analysis shows that the spin connection leads to a redefinition of wave functions but leaves Dirac equations unchanged. In other words, the spin connection does not influence the electron spectrum, but affects the DOS.

The paper is organized as follows. The general formalism for studying electron states in the curved two-dimensional background is presented in Section 2. We formulate a field-theory model for Dirac fermions on hexatic surfaces of an arbitrary geometry with both electrons and disclinations taken into account. The flux due to the pentagonal defect is represented by an Abelian gauge field within a self-consistent gauge model. In Section 3, we apply the model to the problem of electron states in the fullerene molecule. We calculate the local and the total DOS and study zero-energy electronic states. In Section 4, we consider two arbitrary geometries for the description of nanocones, conical and hyperbolical. The results obtained are compared with other approaches. Section 5 is devoted to concluding remarks.

2. GENERAL FORMALISM

Our consideration is based on the effective-mass theory that was applied in [20] to study the screening of a single intercalant within a graphite host, with a two-dimensional approximation used for the description of the graphite host. The effective-mass expansion is equivalent to the $\mathbf{k} \cdot \mathbf{p}$ expansion of the graphite energy bands around the $\mathbf{K}$ point in the Brillouin zone when the intercalant potential is equal to zero. In fact, there are two degenerate Bloch eigenstates, $\Psi_{1,2}(\mathbf{K}, \mathbf{r})$ at $\mathbf{K}$, and the electron wave function on a graphite lattice can therefore be approximated by

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

where $\mathbf{k} = \mathbf{K} + \boldsymbol{\kappa}$. Keeping the terms of the order of $\boldsymbol{\kappa}$ in the Schrödinger equation results in a secular equation for the amplitudes $f_{1,2}(\boldsymbol{\kappa})$, which after diagonalization finally yields the two-dimensional Dirac equation [20]

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

Here, γ^μ are the Dirac matrices that in 2D reduce to the conventional Pauli matrices, the energy E is measured relative to the Fermi energy, and the two-component wave function $\psi \propto (f_1, f_2)^T$ represents two graphite sublattices. As mentioned in [20], the $\mathbf{k} \cdot \mathbf{p}$ approximation essentially amounts to replacing the graphite bands by conical dispersions at the Fermi energy.

For our purpose, we need a generalization of Eq. (1) incorporating both a disclination field and a nontrivial background geometry. A possible description of disclinations on arbitrary two-dimensional elastic surfaces is offered by the gauge approach [23]. In accordance with the basic assumptions of this approach, disclinations can be incorporated in the elasticity theory Lagrangian by introducing a compensating $U(1)$ gauge field W_μ. It is important that the gauge model admits vortexlike solutions for wedge disclinations [23], thus representing a disclination as a vortex of elastic medium. The physical meaning of the gauge field is that the elastic flux due to rotational defect, which is directly related to the Frank vector (see Section 3), is completely determined by the circulation of the W_μ field around the disclination line. In the gauge theory context, the disclination field can be straightforwardly incorporated in (1) by the standard substitution

$$\partial_\mu \longrightarrow \partial_\mu - iW_\mu.$$

Within the linear approximation to gauge theory of disclinations (which amounts to the conventional elasticity theory with linear defects), the basic field equation that describes the $U(1)$ gauge field in a curved background is given by

$$D_\mu F^{\mu k} = 0, \quad F^{\mu k} = \partial^\mu W^k - \partial^k W^\mu, \tag{2}$$

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

$$\Gamma^k_{\mu\lambda} := (\Gamma_\mu)^k_\lambda = \frac{1}{2} g^{kl}\left(\frac{\partial g_{l\lambda}}{\partial x^\mu} + \frac{\partial g_{\mu l}}{\partial x^\lambda} - \frac{\partial g_{\mu\lambda}}{\partial x^l}\right), \tag{3}$$

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 an arbitrary elastic surface, a singular solution to (2) is found to be [23]

$$W^k = -\nu \varepsilon^{k\lambda} D_\lambda G(x, y), \tag{4}$$

where

$$D_\mu D^\mu G(x^1, x^2) = \frac{2\pi\delta^2(x^1, x^2)}{\sqrt{g}}, \tag{5}$$

with $\varepsilon_{\mu k} = \sqrt{g}\,\epsilon_{\mu k}$ being the totally antisymmetric tensor on Σ, $\epsilon_{12} = -\epsilon_{21} = 1$. We note that Eqs. (2)–(5) self-consistently describe a defect located on an arbitrary surface [23].

To describe fermions in a curved background, we need a set of orthonormal frames $\{e_\alpha\}$ for the metric $g_{\mu\nu}$; local $SO(2)$ rotations act on the frames as

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

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 the coordinate indices $\mu, \nu = \{1, 2\}$. As usual, to ensure that physical observables are independent of a particular choice of the zweibein fields, a local $so(2)$-valued gauge field ω_μ must be introduced. The gauge field of the local Lorentz group is known as the spin connection. For the theory to be self-consistent, the zweibein fields must be chosen to be covariantly constant [24],

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

which determines the spin connection coefficients explicitly,

$$(\omega_\mu)^{\alpha\beta} = e^\alpha_\nu D_\mu e^{\beta\nu}. \tag{6}$$

Finally, Dirac equation (1) on a surface Σ in the presence of the U(1) external gauge field W_μ is written as

$$i\gamma^\alpha e^\mu_\alpha (\nabla_\mu - iW_\mu)\psi = E\psi, \tag{7}$$

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

$$\Omega_\mu = \frac{1}{8}(\omega_\mu)^{\alpha\beta}[\gamma_\alpha, \gamma_\beta] \tag{8}$$

being the spin connection term in the spinor representation.

3. SPHERICAL FULLERENE MOLECULES

Variously shaped fullerene molecules appear in the process of graphite vaporization. The more spherical of them is the C_{60} molecule, also nicknamed the "bucky ball." Others are either slightly (as C_{70}, whose shape is more like an elliptical deformation) or remarkably deformed. We are interested here in the C_{60} molecule and in its spherical generalizations like the C_{240} and C_{540} molecules.

3.1. The Model

To describe a sphere, we use the polar projective coordinates

$$x^1 = r \quad x^2 = \varphi; \quad 0 \le r < \infty, \quad 0 \le \varphi < 2\pi,$$

where R is the radius of the sphere. In these coordinates, the metric tensor becomes

$$g_{rr} = \frac{4R^4}{(R^2 + r^2)^2}, \quad g_{\varphi\varphi} = \frac{4R^4 r^2}{(R^2 + r^2)^2}, \tag{9}$$
$$g_{r\varphi} = g_{\varphi r} = 0,$$

and therefore,

$$\sqrt{g} := \sqrt{\det\|g_{\mu\nu}\|} = \frac{4R^4 r}{(R^2 + r^2)^2}.$$

Nonvanishing coefficients of connection (3) are given by

$$\Gamma^r_{rr} = -\frac{2r}{R^2 + r^2}, \quad \Gamma^r_{\varphi\varphi} = -r\frac{R^2 - r^2}{R^2 + r^2},$$

$$\Gamma^\varphi_{r\varphi} = \frac{1}{r}\frac{R^2 - r^2}{R^2 + r^2},$$

and the general representation for the zweibeins is

$$e^1_r = e^2_\varphi = \frac{2R^2\cos\varphi}{R^2 + r^2}, \quad e^1_\varphi = -e^2_r = -\frac{2R^2\sin\varphi}{R^2 + r^2},$$

which in view of Eq. (6) gives

$$\omega_r^{12} = \omega_r^{21} = 0, \quad \omega_\varphi^{12} = -\omega_\varphi^{21} = \frac{2r^2}{R^2 + r^2} =: 2\omega. \quad (10)$$

The following solution to Eqs. (4) and (5) can be easily found:

$$G = \ln r, \quad W_r = 0, \quad W_\varphi = \nu, \quad r \neq 0.$$

Locally, it describes a topological vortex on the Euclidean plane, which confirms the observation that disclinations can be viewed as vortices in elastic media.

The elastic flow through a surface on the sphere is given by the circular integral

$$\frac{1}{2\pi}\oint \mathbf{W} d\mathbf{r} = \nu.$$

Generally, there are no restrictions on the value of the winding number ν apart from $\nu > -1$ for topological reasons. But if we take the symmetry group of the underlying crystal lattice into account, the possible values of ν become "quantized" in accordance with the group structure (e.g., $\nu = 1/6, 1/3, 1/2, \ldots$ for the hexagonal lattice). We note that the elastic flux is characterized by the Frank vector $\boldsymbol{\omega}$, $|\boldsymbol{\omega}| = 2\pi\nu$, with ν being the Frank index. Thus, the elastic flux is "classical" in its origin; i.e., there is no quantization (in contrast to the magnetic vortex). In some physically interesting applications, however, vortices with a fractional winding number have already been considered (see, e.g., the discussion in [17]). We also note that a detailed theory of magnetic vortices on the sphere has been presented in [25].

In 2D, the Dirac matrices can be chosen as the Pauli matrices, $\gamma^1 = -\sigma^2$ and $\gamma^2 = \sigma^1$; Eq. (8) then reduces to

$$\Omega_\varphi = i\omega\sigma^3. \quad (11)$$

As a result, the Dirac operator

$$\hat{\mathcal{D}} := i\gamma^\alpha e_\alpha^\mu (\nabla_\mu + iW_\mu)$$

on the two-sphere becomes

$$\hat{\mathcal{D}} = \hat{\mathcal{D}}^\dagger = \frac{r^2 + R^2}{2R^2}\begin{Bmatrix} 0 & e^{-i\varphi}\left(-\partial_r + \dfrac{i\partial_\varphi + \nu}{r} + \dfrac{\omega}{r}\right) \\ e^{i\varphi}\left(\partial_r + \dfrac{i\partial_\varphi + \nu}{r} - \dfrac{\omega}{r}\right) & 0 \end{Bmatrix}. \quad (12)$$

In proving that the operator $\hat{\mathcal{D}}$ is Hermitian, we use that in the presence of a metric,

$$\partial_r^\dagger = -\partial_r - \frac{1}{2}\partial_r \ln g.$$

For massless fermions, σ^3 serves as a conjugation matrix, and the energy eigenmodes are symmetric with respect to $E = 0$:

$$\sigma^3 \psi_E = \psi_{-E}.$$

The generator of the local Lorentz transformations $\Lambda_\alpha^\beta \in SO(2)$ takes the form $-i\partial_\varphi$, and the generator of the Dirac spinor transformations $\rho(\Lambda)$ is

$$\Sigma_{12} = \frac{i}{4}[\gamma_1, \gamma_2] = \frac{1}{2}\sigma^3.$$

The total angular momentum of the 2D Dirac system is therefore given by

$$L_z = -i\partial_\varphi + \frac{1}{2}\sigma^3,$$

which commutes with operator (12). Consequently, the eigenfunctions are classified with respect to the eigenvalues of $J_z = j + 1/2$, $j = 0, \pm 1, \pm 2, \ldots$ and are to be taken in the form

$$\psi = \begin{pmatrix} u(r)e^{i\varphi j} \\ v(r)e^{i\varphi(j+1)} \end{pmatrix}. \quad (13)$$

As follows from Eq. (12), the spin connection term can be taken into account by redefining the wave function as

$$\psi = \tilde{\psi}\sqrt{R^2 + r^2}, \quad (14)$$

which reduces eigenvalue problem (7) to

$$\begin{aligned} \partial_r \tilde{u} - \frac{(j - \nu)}{r}\tilde{u} &= \tilde{E}\tilde{v}, \\ -\partial_r \tilde{v} - \frac{(j + 1 - \nu)}{r}\tilde{v} &= \tilde{E}\tilde{u}, \end{aligned} \quad (15)$$

where

$$\tilde{E} = \frac{2R^2 E}{R^2 + r^2}.$$

3.2. Extended Electron States

The general solution to (15) is not available, unfortunately. But because we are mainly interested in electronic states near the disclination line, we can restrict our consideration to the case of small r. In this case, a solution to (15) (with (14) taken into account) is found to be

$$\begin{pmatrix} u \\ v \end{pmatrix} = A\begin{pmatrix} J_\eta(2Er) \\ \pm J_{\bar\eta}(2Er) \end{pmatrix}, \tag{16}$$

where

$$\eta = \pm(j-\nu), \quad \bar\eta = \pm(j-\nu+1),$$

and A is a normalization factor. Therefore, there are two independent solutions with $\eta(\bar\eta) > 0$ and $\eta(\bar\eta) < 0$. We note that the respective signs "±" in (16) correspond to states with $E > 0$ and $E < 0$. As already noted, σ^3 serves as the conjugation matrix for massless fermions and the energy eigenmodes are symmetric with respect to $E = 0$. We can therefore consider either case, for instance, $E > 0$.

The important restrictions come from the normalization condition

$$\int(|u|^2 + |v|^2)\sqrt{g}dx^1dx^2 = 1. \tag{17}$$

From (16), it follows that $A^2 \propto E$. On the other hand, the integrand in (17) must be nonsingular at small Er. This imposes a restriction on possible values of j. Namely, for $\eta, \bar\eta > 0$, we obtain $j - \nu > -1/2$, and for $\eta, \bar\eta < 0$, we have $j - \nu < -1/2$. It follows that possible values of j do not overlap at any ν.

In the vicinity of a pentagon, the electron wave function is given by

$$\begin{pmatrix} u \\ v \end{pmatrix} \propto \begin{pmatrix} E^{1/2+\eta}r^\eta, \\ E^{1/2+\bar\eta}r^{\bar\eta} \end{pmatrix}. \tag{18}$$

In particular, in the leading order, we obtain

$$\Psi \propto \begin{cases} \sqrt{E}, & \nu = 0, \\ E^{1/3}r^{-1/6}, & \nu = 1/6, \\ E^{1/6}r^{-1/3}, & \nu = 1/3. \end{cases}$$

Because the local density of states diverges as $r \longrightarrow 0$, it is more appropriate to consider the total density of states on a patch $0 < r \le \delta$ for small δ, rather than the local quantities. For this, we must integrate the electron density over a small disk $|r| < \delta$. (We recall that r and φ are stereographically projected coordinates on the sphere.) The result is

$$D(E,\delta) \propto \begin{cases} (E\delta)\delta, & \nu = 0, \\ (E\delta)^{2/3}\delta, & \nu = 1/6, 5/6, \\ (E\delta)^{1/3}\delta, & \nu = 1/3, 2/3, \\ \delta, & \nu = 1/2. \end{cases} \tag{19}$$

For the defect-free case ($\nu = 0$), we obtain the well-known behavior of the total DOS in the δ disk given by $D(E,\delta) \propto E\delta^2$ (in accordance with the previous analysis [20]). For $\nu = 1/6, 1/3, 2/3, 5/6$, the low-energy total DOS has a cusp that drops to zero at the Fermi energy. Most intriguing is the case where $\nu = 1/2$ and a region of a nonzero DOS across the Fermi level is formed. This implies local metallization of graphite in the presence of a 180° disclination. In the fullerene molecule, however, there are twelve 60° disclinations, and therefore, the case $\nu = 1/6$ is actually realized.

3.3. Zero-Energy Modes

An interesting issue to be addressed is the existence of zero-energy modes. For the two-sphere, this problem can be solved exactly (see [13, 14]). Namely, for $E = 0$, Eq. (15) reduces to

$$\begin{aligned} \partial_r\tilde u_0 - \frac{(j-\nu)}{r}\tilde u_0 &= 0, \\ -\partial_r\tilde v_0 - \frac{(j+1-\nu)}{r}\tilde v_0 &= 0. \end{aligned} \tag{20}$$

We can construct self-conjugate solutions $\begin{pmatrix} \tilde u_0 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ \tilde v_0 \end{pmatrix}$, where

$$\tilde u_0 = Ar^{j-\nu}, \quad \tilde v_0 = Ar^{-(j-\nu+1)}. \tag{21}$$

The normalization condition

$$\int|\psi_0|^2\sqrt{g}drd\varphi = 1 \tag{22}$$

yields

$$2\pi A^2\int_0^\infty \frac{4R^4r^{2l}}{R^2+r^2}rdr = 1, \tag{23}$$

where $l = j - \nu$ for u_0 and $l = -(j - \nu + 1)$ for v_0. Finally,

$$A^2 = \frac{\sin\pi\bar\eta}{4\pi^2R^{2(1+\bar\eta)}},$$

for u_0 and

$$A^2 = -\frac{\sin\pi\eta}{4\pi^2 R^{2(1-\eta)}}$$

for v_0. We note that the restriction $-1 < j - \nu < 0$ serves to avoid divergence in (22). In the defect-free case ($\nu = 0$), this yields no zero modes on the sphere. We note that this agrees with the general observation that the Dirac operator can have no zero modes on a manifold with an everywhere positive Ricci scalar curvature $\mathcal{R}$. Indeed, we easily find that $\hat{\mathcal{D}}^2 = \Delta + \mathcal{R}/4$, where the Laplace–Beltrami operator Δ has nonnegative eigenvalues [26]. For the two-sphere, $\mathcal{R} = 1/R^2$, and therefore, $\hat{\mathcal{D}}^2 > 0$.

In the case where $\nu = 1/6$, in which we are interested here, the only possible value of j is $j = 0$, and therefore, $u_0 \propto r^{-1/6}$ and $v_0 \propto r^{-5/6}$ near the disclination line. Thus, our analysis shows that two normalizable zero modes can exist on the sphere in the presence of a disclination vortex. We note that this conclusion agrees with [15] (where a different continuum model was formulated) and differs from [13, 14], where either u_0 or v_0 was found to be normalizable. The reason is that, in [13, 14], the external gauge field was assumed to be well-behaved at the origin. In this paper, we admit singular solutions as well.

The total density of states on the patch $0 < r \le \delta$ becomes

$$D(\delta) \propto \begin{cases} \delta^{1/3}, & \nu = 1/6, 5/6, \\ \delta^{2/3}, & \nu = 1/3, 2/3, \\ \delta, & \nu = 1/2. \end{cases} \quad (24)$$

It follows that this behavior differs from (19) and therefore allows recognizing the zero-eigenvalue states in experiment.

4. NANOCONES

A conelike structure (an exposed surface) is formed when a pentagon is introduced into a graphite sheet. There are two possible scenarios for modeling nanocones. First, the cut-and-paste procedure can be accomplished in which the pentagon is constructed in the hexagonal network by cutting out a 60° sector from the graphene sheet (a single layer of graphite). In this case, we have a real cut with the consequent departure from the flat surface. Pentagonal defects in cones can therefore be considered as apical disclinations, and the opening angle is directly connected to the Frank index of the disclination. Because of the symmetry of the graphite sheet, only five types of cones can be created from a continuous sheet of graphite. The total disclinations of all these cones are multiples of 60°, corresponding to the presence of a given number (n) of pentagons at the apices. It is important to mention that carbon nanocones with the cone angles of 19°, 39°, 60°, 85°, and 113° have been observed in a carbon sample [27]. We note that these angles might correspond to 300°, 240°, 180°, 120°, and 60° disclinations in graphite, respectively. Disks ($n = 0$) and one-open-end nanotubes ($n = 6$) have also been observed in the same sample [27]. This case was theoretically studied in [9, 10, 22]. At the same time, cones with the apex angles of 30°, 50°, and 70° have also been found [28, 29]. These angles are forbidden within the above scenario. In [28, 29], the appearance of such cones was explained in terms of the open cone model.

Second, a single disclination on a finite graphite sheet is known to be buckled to screen its energy, thus leading to a curved hexagonal network [7]. In this context, the pentagon in graphene can result in a curved conelike structure. The most appropriate conelike figure is the hyperboloid. We note that this agrees with a suggestion made in [1] that nonsymmetric fullerenes of a special form can serve as nucleating centers for the nanocone. We consider both these scenarios below.

4.1. Cone Geometry

4.1.1. The model. In the polar coordinates $(r, \varphi) \in R^2$, a cone can be regarded as the embedding

$$(r, \varphi) \longrightarrow (ar\cos\varphi, ar\sin\varphi, cr),$$
$$0 < r < 1, \quad 0 \le \varphi < 2\pi,$$

with a and c being the cone parameters. From this, the components of the induced metric can easily be obtained as

$$g_{rr} = a^2 + c^2, \quad g_{\varphi\varphi} = a^2 r^2, \quad g_{r\varphi} = g_{\varphi r} = 0. \quad (25)$$

The opening angle of the cone, θ, is determined by

$$\sin(\theta/2) = a/\sqrt{a^2 + c^2}.$$

Because the cone itself appears when one or more sectors are removed from graphene, all possible angles are divisible by $\pi/3$. Therefore, the Frank index of the apical disclination can be specified by

$$\nu = 1 - \sin(\theta/2).$$

At $\nu = 0$, we obtain a flat graphene sheet ($\theta = \pi$). For convenience, we introduce the parameter

$$\xi = 1 + c^2/a^2$$

such that

$$\sin(\theta/2) = 1/\sqrt{\xi}$$

and

$$1/\sqrt{\xi} = 1 - \nu.$$

Nonvanishing coefficients of connection (3) are now given by

$$\Gamma^r_{\varphi\varphi} = -\frac{r}{\xi}, \quad \Gamma^\varphi_{r\varphi} = \Gamma^\varphi_{\varphi r} = \frac{1}{r}.$$

The general representation for the zweibeins is found to be

$$e_r^1 = \sqrt{a^2+c^2}\cos\varphi, \quad e_\varphi^1 = -ar\sin\varphi,$$
$$e_r^2 = \sqrt{a^2+c^2}\sin\varphi, \quad e_\varphi^2 = ar\cos\varphi,$$

which in view of Eq. (6) gives

$$\omega_r^{12} = \omega_r^{21} = 0,$$
$$\omega_\varphi^{12} = -\omega_\varphi^{21} = 1 - 1/\sqrt{\xi} =: 2\omega. \tag{26}$$

The external gauge potential is then $W_r = 0$, $W_\varphi = \nu$, and the Dirac operator on the cone takes the form

$$\hat{\mathcal{D}} = \hat{\mathcal{D}}^\dagger = \begin{bmatrix} 0 & e^{-i\varphi}\left(-\dfrac{\partial_r}{\sqrt{a^2+c^2}} + \dfrac{1}{ar}(i\partial_\varphi + \nu + \omega)\right) \\ e^{i\varphi}\left(\dfrac{\partial_r}{\sqrt{a^2+c^2}} + \dfrac{1}{ar}(i\partial_\varphi + \nu - \omega)\right) & 0 \end{bmatrix}.$$

Making the substitution

$$\psi = \tilde{\psi} r^\alpha, \quad \alpha = \sqrt{\xi}\omega,$$

we reduce the eigenvalue problem in Eq. (7) to

$$\partial_r \tilde{u} - \frac{\sqrt{\xi}}{r}(j-\nu)\tilde{u} = \tilde{E}\tilde{v},$$
$$-\partial_r \tilde{v} - \frac{\sqrt{\xi}}{r}(j+1-\nu)\tilde{v} = \tilde{E}\tilde{u}, \tag{27}$$

where $\tilde{E} = \sqrt{\xi}\, aE$.

4.1.2. Electron states. In contrast to the previous case of the two-sphere, the cone is essentially a flat manifold (the scalar curvature $\mathcal{R} = 0$ everywhere on the cone, except at the origin), and as a result, (27) allows an exact solution. Namely, the general solution to (27) is found to be [22]

$$\begin{pmatrix} \tilde{u} \\ \tilde{v} \end{pmatrix} = Ar^{-\alpha}\begin{pmatrix} J_\eta(\tilde{E}r) \\ \pm J_{\bar{\eta}}(\tilde{E}r) \end{pmatrix}, \tag{28}$$

where

$$\eta = \pm(\sqrt{\xi}(j-\nu+1/2) - 1/2),$$
$$\bar{\eta} = \pm(\sqrt{\xi}(j-\nu+1/2) + 1/2).$$

As earlier, we consider the case where $E > 0$. Normalization condition (17) now becomes

$$2\pi\sqrt{\xi}a^2A^2\int_0^1 (J_\eta^2(\tilde{E}r) + J_{\bar{\eta}}^2(\tilde{E}r))rdr = 1. \tag{29}$$

The normalization factor can be extracted from the asymptotic formula for Bessel functions at large arguments. Indeed, $\bar{\eta} - \eta = 1$ in our case, and therefore,

$$J_\eta^2 + J_{\bar{\eta}}^2 \longrightarrow 2/\pi\tilde{E}r \quad \text{for} \quad \tilde{E}r \gg 1.$$

Substituting this in (29) yields

$$A^2 = \frac{E}{4a}.$$

Clearly, (29) must be nonsingular at small r. This imposes a restriction on possible values of j. For $\eta, \bar{\eta} > 0$, we obtain $j > -1$ (i.e., $j = 0, 1, 2, \ldots$), and for $\eta, \bar{\eta} < 0$, we have $j < -2\nu$ ($j = -1, -2, \ldots$ at $\nu < 1/2$).

We are interested in the electron states near the apex of the cone. As follows directly from (28), the wave functions behave as

$$\begin{pmatrix} u \\ v \end{pmatrix} \propto \begin{pmatrix} E^{1/2+\eta}r^\eta, \\ E^{1/2+\bar{\eta}}r^{\bar{\eta}} \end{pmatrix} \tag{30}$$

for small r. In the leading order, we obtain

$$\Psi \propto E^{(1-2\nu)/2(1-\nu)}r^{-\nu/(1-\nu)}.$$

In particular, we obtain

$$\Psi \propto \begin{cases} \sqrt{E}, & \nu = 0, \\ E^{2/5}r^{-1/5}, & \nu = 1/6, \\ E^{1/4}r^{-1/2}, & \nu = 1/3. \end{cases}$$

Finally, the total density of states on the patch $0 <$

$r \le \delta$ is given by

$$D(E, \delta) \propto \begin{cases} E^{(1+2\nu)/(1-\nu)}\delta^{(\nu+2)/(1-\nu)}, & \eta, \bar{\eta} > 0, \\ E^{(1-2\nu)/(1-\nu)}\delta^{(2-3\nu)/(1-\nu)}, & \eta, \bar{\eta} < 0. \end{cases} \quad (31)$$

It should be stressed that, according to (31), a specific behavior of $D(E, \delta)$ occurs only for $\nu = 1/2$, where $D \propto E^0\delta$. This prediction of our model agrees with a finding in [10], where the prominent peak just above the Fermi level was found for the nanocone with three symmetric pentagons (180° disclination). In the leading order, it follows from (31) that

$$D(E, \delta) \propto \begin{cases} E\delta^2, & \nu = 0, \\ E^{4/5}\delta^{9/5}, & \nu = 1/6, \\ E^{1/2}\delta^{3/2}, & \nu = 1/3, \\ \delta, & \nu = 1/2. \end{cases} \quad (32)$$

As can be seen, the extended states with a nonzero density of states at E_F appear only at $\nu = 1/2$. This conclusion disagrees with the results obtained in [9], where a nonzero DOS at E_F was found to occur at $\nu = 1/3$. We now comment on this disagreement briefly. There is an important point where our consideration differs from [9]. Our model is based on the gauge-theory approach where defects on an elastic curved surface are described by an Abelian gauge field. As a result, the flux due to pentagonal apical disclination (elastic vortex) is explicitly incorporated into the Dirac equation. On the other hand, the model in [9] treats the appropriate boundary conditions for electron states resulting from the cut-and-paste procedure. In that approach, the gauge field carries information about the boundary conditions. In fact, both models are similar but not identical, which is exemplified by the different predictions.

To examine the electron states at the Fermi energy, we return to (27) and set $E = 0$. The solution reads

$$u_0 = Ar^{-1/2+\tilde{j}\sqrt{\xi}}, \quad v_0 = Br^{-1/2-\tilde{j}\sqrt{\xi}}, \quad (33)$$

where $\tilde{j} = j - \nu + 1/2$. A simple analysis shows that, for $j = 0$, both u_0 and v_0 are normalizable on the cone of a finite size. Both solutions are singular. For $\nu = 1/6$, we obtain

$$|u_0|^2 \propto r^{-1/5}/a^2, \quad |v_0|^2 \propto r^{-9/5}/a^2.$$

For any other j, either u_0 or v_0 is found to be normalizable and the solutions become nonsingular. As before, the total DOS can be considered for singular states. It is easy to find that $D \propto \delta^{1/5}$ for u_0 and $D \propto \delta^{9/5}$ for v_0. This result differs from [8], where, although in a different framework, the states on a finite cone with a single-pentagon defect have been found at the Fermi energy (these states decay away from the apex as $|\psi|^2 \propto r^{-2/5}$). At the same time, our study confirms the principal conclusion in [8, 30] that the states contributing to the nonzero DOS at the Fermi energy exhibit a power-law behavior for a single-pentagon defect. We also note that there are no zero-energy electronic states on a single disclination in monolayer graphite of an infinite length ($a \longrightarrow \infty$). We emphasize that this conclusion agrees with the results of numerical calculations in [30], where the local density of states at the Fermi level was found to be zero for five-membered rings (pentagons). We also note that, for $\nu = 1/2$, $D \propto \delta$ for both u_0 and v_0.

4.2. Hyperboloid Geometry

4.2.1. The model. The upper half of a hyperboloid can be regarded as the embedding

$$(\chi, \varphi) \longrightarrow (a\sinh\chi\cos\varphi, a\sinh\chi\sin\varphi, c\cosh\chi),$$
$$0 \le \chi < \infty, \quad 0 \le \varphi < 2\pi.$$

From this, the components of the induced metric can be obtained as

$$g_{\chi\chi} = a^2\cosh^2\chi + c^2\sinh^2\chi, \quad g_{\varphi\varphi} = a^2\sinh^2\chi, \quad g_{\varphi\chi} = g_{\chi\varphi} = 0, \quad (34)$$

which yields

$$\Gamma^{\chi}_{\chi\chi} = \frac{(a^2 + c^2)\sinh 2\chi}{2g_{\chi\chi}},$$
$$\Gamma^{\chi}_{\varphi\varphi} = -\frac{a^2\sinh 2\chi}{2g_{\chi\chi}}, \quad \Gamma^{\varphi}_{\varphi\chi} = \Gamma^{\varphi}_{\chi\varphi} = \coth\chi \quad (35)$$

for the nonvanishing coefficients of the connection. In a rotating $SO(2)$ frame, the zweibeins become

$$e^1_\chi = \sqrt{g_{\chi\chi}}\cos\varphi, \quad e^2_\chi = \sqrt{g_{\chi\chi}}\sin\varphi,$$
$$e^1_\varphi = -a\sinh\chi\sin\varphi, \quad e^2_\varphi = a\sinh\chi\cos\varphi, \quad (36)$$

which, in view of Eq. (6), gives the spin connection coefficients

$$\omega^{12}_\chi = \omega^{21}_\chi = 0,$$
$$\omega^{12}_\varphi = -\omega^{21}_\varphi = \frac{1}{2}\left[1 - \frac{a\cosh\chi}{\sqrt{g_{\chi\chi}}}\right] =: \omega, \quad (37)$$

and therefore,

$$\Omega_\varphi = i\omega\sigma^3. \quad (38)$$

The external gauge potential is then $W_\chi = 0$, $W_\varphi = \nu$, and the Dirac operator on the hyperboloid takes the form

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

It can be verified that $\hat{\mathcal{D}} = \hat{\mathcal{D}}^\dagger$.

The substitution

$$\tilde{\psi} = \psi\sqrt{\sinh\chi}$$

reduces the eigenvalue problem in Eq. (7) to

$$\begin{aligned} \partial_\chi\tilde{u} - \sqrt{\coth^2\chi + b^2}\,\tilde{j}\tilde{u} &= \tilde{E}\tilde{v}, \\ -\partial_\chi\tilde{v} - \sqrt{\coth^2\chi + b^2}\,\tilde{j}\tilde{v} &= \tilde{E}\tilde{u}, \end{aligned} \tag{39}$$

where

$$\tilde{E} = \sqrt{g_{\chi\chi}}E, \quad b = c/a, \quad \tilde{j} = j - \nu + 1/2.$$

4.2.2. Electron states. To study electronic states on the hyperboloid, we must analyze Eqs. (39). Because of the nonvanishing scalar curvature, the general solution to the Dirac equation on the hyperboloid (as well as on the sphere) is not available and we are forced to simplify the problem. Fortunately, we are interested in the behavior of the electron states near the apex and can therefore consider only the case of small χ. We then obtain

$$\begin{aligned} \partial_\chi\tilde{u} - \frac{\tilde{j}}{\chi}\tilde{u} &= Ea\tilde{v}, \\ -\partial_\chi\tilde{v} - \frac{\tilde{j}}{\chi}\tilde{v} &= Ea\tilde{u}, \end{aligned} \tag{40}$$

with the obvious solutions

$$\begin{aligned} \tilde{u} &= A\sqrt{Ea\chi}J_{|j-\nu|}(Ea\chi), \\ \tilde{v} &= A\sqrt{Ea\chi}J_{|j-\nu+1|}(Ea\chi). \end{aligned}$$

As can be seen, this is exactly the case of a sphere, which should not be surprising, because these two manifolds are locally diffeomorphic. Evidently, the total DOS on a finite hyperboloid is the same as on the sphere (see (19)).

We now consider the zero-energy modes, setting $E = 0$ in (39). The general solution is found to be

$$\begin{aligned} \tilde{u}(\chi) &= A\left[(k\cosh\chi + \Delta)^{2k}\frac{\Delta - \cosh\chi}{\Delta + \cosh\chi}\right]^{\tilde{j}/2}, \\ \tilde{v}(\chi) &= A\left[(k\cosh\chi + \Delta)^{2k}\frac{\Delta - \cosh\chi}{\Delta + \cosh\chi}\right]^{-\tilde{j}/2}, \end{aligned} \tag{41}$$

where

$$k = \sqrt{1 + b^2}, \quad \Delta = \sqrt{1 + k^2\sinh^2\chi}.$$

An important restriction comes from the normalization condition (see (17)) which on a finite hyperboloid yields $\tilde{j} > -1/2$ for $u(\chi)$ and $\tilde{j} < 1/2$ for $v(\chi)$. We see that, for $-1/2 < \tilde{j} < 1/2$, both $u(\chi)$ and $v(\chi)$ are normalizable simultaneously. For the zero-energy mode, the total DOS on a finite hyperboloid is found to be the same as on the sphere (see (24)).

Although the local electronic structures are similar on the hyperboloid and the sphere, there is a principal global distinction. We consider an unbounded hyperboloid (full locus). In this case, additional restrictions at the upper limit of the integral in (17) must be taken into account. We obtain $-1/2 < \tilde{j} < -1/2k$ for $u(\chi)$ and $1/2k < \tilde{j} < 1/2$ for $v(\chi)$. Therefore, either $u(\chi)$ or $v(\chi)$ becomes normalizable on the hyperboloid of infinite volume. We see that, as $c/a \longrightarrow 0$, a normalizable solution does not exist. In fact, the hyperboloid then becomes a plane. Consequently, our results are in accordance with the planar case. The total density of states on an infinite hyperboloid for a variety of defects is as follows:

$$D(\delta) \propto \begin{cases} \delta^{1/3}, & \nu = 1/6, \quad c/a > \sqrt{5}/2, \\ \delta^{2/3}, & \nu = 1/3, \quad c/a > 2\sqrt{2}, \\ \delta^{2/3}, & \nu = 2/3, \quad c/a > 2\sqrt{2}, \\ \delta^{1/3}, & \nu = 5/6, \quad c/a > \sqrt{5}/2. \end{cases} \tag{42}$$

We note that normalizable zero-energy states do not exist for the defect with $\nu = 1/2$ nor for the defect-free case $\nu = 0$. The most important conclusion from our consideration is that there is a possibility for the true zero-mode fermion state on the hyperboloid. As we have shown, the normalized zero-mode states on both the sphere and the cone exist only for a finite system size and disappear in the infinite-size limit. For an infinite hyperboloid, a normalized zero-energy electron state can exist in the presence of a disclination flux.

5. CONCLUSIONS

We have formulated a gauge field-theory model describing electron states on graphitic nanoparticles. The topological nature of the pentagonal defect is found to markedly modify the low-energy electronic

structure. In particular, the total density of extended states has a rather specific dependence on both the energy and the distance from the disclination line. We have found that the low-energy total DOS has a characteristic cusp at the Fermi energy for any disclinations with $\nu < 1/2$. In particular, this finding suppresses the extended electron states with a nonzero DOS at E_F in the fullerene molecule with $\nu = 1/6$. For zero-mode states, the total DOS on the patch $0 < r < \delta$ behaves as $\delta^{1/3}$. A similar behavior is found for a graphitic hyperboloid. There is, however, a principal distinction due to the possibility for the true zero-mode fermion state to occur on the hyperboloid. Namely, the normalized zero-energy electron state can exist even on an infinite-size hyperboloid.

We have shown that the local and the total DOS at the apices of nanocones are strongly dependent on the pentagon concentration. In particular, our model predicts anomalous behavior of $D(E, \delta)$ only for $\nu = 1/2$ (three pentagons at the apex), where $D \propto E^0\delta$; that is, the enhanced charge density at E_F is located at the apex of the cone at a 60° opening angle. This implies local metallization, thus suggesting some important applications of nanocone-based structures in microelectronic devices. First of all, such a remarkable increase of the DOS must provoke the corresponding enhancement of the field emission current, thereby decreasing the threshold voltage for emitted electrons. We note that this conclusion agrees well with the results in [10], where the prominent peak appearing just above the Fermi level was established in a nanocone with three pentagons at the apex. It was proposed that such peculiar nanocones are good candidates for nanoprobes in scanning probe microscopy and excellent candidates for field-emission devices. As was also mentioned in [10], the nanocones with free pentagons at the tip have the highest probability of nucleation and are frequently observed [27]. It is expected that localized states at the Fermi level may give rise to materials with novel electronic and magnetic properties. We hope that our predictions will motivate further measurements of electronic properties of graphitic nanoparticles.

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