ELECTRONIC PROPERTIES OF GRAPHITIC NANOCONES

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A graphitic sheet (graphene), which is characterized in the long-wave approximation by a linear spectrum of quasiparticle excitations, represents a unique example of a really two-dimensional "relativistic" electron system. This system can manifest rather unusual properties in the presence of topological defects. We have demonstrated that a disclination that rolls up the graphitic sheet into a nanocone can be described by a pseudomagnetic vortex, the flux of which is related to the deficit angle of the cone. Analytic expressions for both the density of states and a charge of the ground state of some graphitic nanocones have been obtained.

1. Introduction

The experimental and theoretical researches of carbon nanostructures become more and more urgent owing to their possible implications in novel technologies. The recent synthesis of rigorously two-dimensional atomic crystals of carbon (a single-layered graphite film – graphene) [1] promises a plenty of new interesting effects. This discovery provides an opportunity to replace silicon microcircuits by carbon nano-sized ones, which allows graphite films to be regarded as a more perspective material – in comparison with carbon nanotubes – from the viewpoint of its applications in electronics [2–5]. On the basis of graphene, the first transistors not thicker than an atom and not longer than 50 atoms have already been fabricated.

Graphene is a complex crystal lattice consisting of regular hexagons with carbon atoms in their vertices. The rhombic elementary cell of such a crystal contains two atoms. A characteristic feature of electron quasiparticle excitations in graphene is a linear isotropic dispersion relation between the energy and the momentum in the vicinity of the Fermi points, where the valence and conduction bands come in touch with each other. As a result, the low-energy electron excitations are described by the massless Dirac–Weyl equation, where the role of the speed of light is played by the Fermi velocity of about 10^6 m/s [6, 7]. The availability of four components of the fermionic field in this approach stems from the presence of two sublattices in the crystal and two nonequivalent Fermi points.

Topological defects in graphene are various disclinations which result in the convolution of the graphite sheets into cones. Three-dimensional conical spaces have been known for rather a long time, and the first among physicists who paid attention to them and pointed out their interesting properties was M. Fierz (unpublished; see a footnote in work [8]). Detailed researches of the physical properties of conical spaces were carried out by L. Marder [9]. The interest in such spaces became considerably enhanced when it had been found that they are associated with cosmic strings – linear topological defects that arise owing to phase transitions with the spontaneous violation of continuous symmetries at the early stages of the Universe evolution [10, 11]. Cosmic strings can play a certain role in the formation of a large-scale Universe structure and serve as gravitational lenses which generate the double images of astrophysical objects. The scattering of classical and quantum-mechanical particles in the field of a cosmic string was studied in works [12–16] (see also work [17]). In the general case, the cosmic string is characterized by two parameters, namely, the flux of magnetic vortex, which corresponds to the violated gauge symmetry, and the deficit angle, which is connected with the linear mass of the string. The possible values of the deficit angle for cosmic strings are confined by a rather small value of the order of $(10^{-4} \div 10^{-3})^\circ$. On the contrary, the deficit angle for two-dimensional graphitic nanocones can acquire both positive and negative values which are multiples of 60°. We shall demonstrate that the graphitic nanocone, as well as the cosmic string, is characterized by an additional parameter, which, however, is not independent; it is the flux of pseudo-magnetic vortex, which acquires discrete values related to the values of deficit angle.

In this work, we use the theory of vacuum polarization by singular external fields [18–21] in order to calculate the charge of the ground state of some graphitic nanocones.

2. Continuous Model for Low-energy Electron Excitations

The crystal lattice of a graphite sheet is made up of two sublattices Λ_A and Λ_B. The elementary cell is rhombic and contains two atoms of carbon, which are located from each other at the distance d equal to one third of the large diagonal of the elementary cell. Three of four electrons of the external shell of carbon atom hybridize to form three σ-orbitals directed along the atomic bonds with three nearest atoms, while the fourth electron forms a π-orbital, which is orthogonal to the lattice plane and is responsible for the conductive properties of graphene. Three radius-vectors, which are directed from an atom in one sublattice towards three nearest neighbor ones that belong to the other sublattice, are chosen in the form

$$\begin{aligned} \Lambda_A \to \Lambda_B: \quad & \mathbf{u}_1 = (-d, 0), \quad \mathbf{u}_2 = \left(\tfrac{1}{2}d, \tfrac{\sqrt{3}}{2}d\right), \\ & \mathbf{u}_3 = \left(\tfrac{1}{2}d, -\tfrac{\sqrt{3}}{2}d\right), \\ \Lambda_B \to \Lambda_A: \quad & \mathbf{v}_1 = (d, 0), \quad \mathbf{v}_2 = \left(-\tfrac{1}{2}d, -\tfrac{\sqrt{3}}{2}d\right), \\ & \mathbf{v}_3 = \left(-\tfrac{1}{2}d, \tfrac{\sqrt{3}}{2}d\right). \end{aligned} \tag{1}$$

The motions of a conduction electron over the crystal lattice, which occur by electron hopping with the amplitude t onto the next atoms, are described by a Hamiltonian in the approximation of tightly bound electrons

$$\mathcal{H} = -t \sum_{i\in\Lambda_A} \sum_{j=1}^{3} a^\dagger(\mathbf{r}_i) b(\mathbf{r}_i + \mathbf{u}_j) -$$

$$-t \sum_{i\in\Lambda_B} \sum_{j=1}^{3} b^\dagger(\mathbf{r}_i) a(\mathbf{r}_i + \mathbf{v}_j), \tag{2}$$

where the operators of creation $a^\dagger(\mathbf{r}_i)$ $(b^\dagger(\mathbf{r}_i))$ and annihilation $a(\mathbf{r}_i)$ $(b(\mathbf{r}_i))$, which are relevant to the sublattice $\Lambda_A(\Lambda_B)$, satisfy the anticommutation relations

$$[a(\mathbf{r}_i),\ a^\dagger(\mathbf{r}_{i'})]_+ = [b(\mathbf{r}_i),\ b^\dagger(\mathbf{r}_{i'})]_+ = \delta_{ii'}.$$

Using the notation

$$|\Psi\rangle = C_A \sum_{i'\in\Lambda_A} e^{i\mathbf{k}\mathbf{r}_{i'}} a^\dagger(\mathbf{r}_{i'})|0\rangle + C_B \sum_{i'\in\Lambda_B} e^{i\mathbf{k}\mathbf{r}_{i'}} b^\dagger(\mathbf{r}_{i'})|0\rangle$$

for the eigenstate of Hamiltonian (2) and taking the relation

$$\mathcal{H}|\Psi\rangle = -t\sum_{j=1}^{3} e^{i\mathbf{k}\mathbf{u}_j} C_B \sum_{i'\in\Lambda_A} e^{i\mathbf{k}\mathbf{r}_{i'}} a^\dagger(\mathbf{r}_{i'})|0\rangle -$$

$$-t\sum_{j=1}^{3} e^{i\mathbf{k}\mathbf{v}_j} C_A \sum_{i'\in\Lambda_B} e^{i\mathbf{k}\mathbf{r}_{i'}} b^\dagger(\mathbf{r}_{i'})|0\rangle$$

into account, the equation for eigenvalues, $\mathcal{H}|\Psi\rangle = E|\Psi\rangle$, can be reduced to the form

$$\begin{pmatrix} 0 & -t \sum\limits_{j=1}^{3} e^{i\mathbf{k}\mathbf{u}_j} \\ -t \sum\limits_{j=1}^{3} e^{i\mathbf{k}\mathbf{v}_j} & 0 \end{pmatrix} \begin{pmatrix} C_A \\ C_B \end{pmatrix} =$$

$$= E \begin{pmatrix} C_A \\ C_B \end{pmatrix}, \tag{3}$$

the corresponding eigenvalues are

$$E = \pm t \sqrt{\sum_{j=1}^{3} e^{i\mathbf{k}\mathbf{u}_j} \sum_{j'=1}^{3} e^{i\mathbf{k}\mathbf{v}_{j'}}} =$$

$$= \pm t \sqrt{1 + 4\cos\left(\frac{\sqrt{3}}{2}k_y d\right)\left[\cos\left(\frac{3}{2}k_x d\right) + \cos\left(\frac{\sqrt{3}}{2}k_y d\right)\right]}. \tag{4}$$

As is evident from expression (4), the one-particle energy spectrum of the graphite sheet in the approximation of tightly bound electrons consists of two surfaces (corresponding to $E_k > 0$ and $E_k < 0$), which touch at six conical points

$$\begin{aligned} & k_x = 0, && k_y = \pm 4\pi(3\sqrt{3}d)^{-1}, \\ & k_x = \pm 2\pi(3d)^{-1}, && k_y = \pm 2\pi(3\sqrt{3}d)^{-1}; \end{aligned} \tag{5}$$

so that the Fermi level becomes degenerate into six points. The first Brillouin zone in the momentum space is a regular hexagon, the vertices of which coincide with the corresponding Fermi points, only two of which are nonequivalent; in particular, two mutually opposite points can be chosen as such.

Near the Fermi level, the one-electron spectrum of the graphite sheet is linear. Therefore, it is convenient to consider long-wave – or low-energy – electron excitations by passing to the continuous limit ($d \to 0$) in the

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vicinity of nonequivalent Fermi points. Choosing the pair of nonequivalent points $\mathbf{K}_\pm = \left(0, \pm 4\pi \left(3\sqrt{3}d\right)^{-1}\right)$, we obtain – in the continuous limit – the one-particle Hamiltonian in the linear approximation with respect to $\mathbf{k} - \mathbf{K}_\pm$:

$$H_\pm = \lim_{d\to 0} d^{-1} \left(\begin{array}{cc} 0 & -t\sum_{j=1}^{3} e^{i\mathbf{k}\mathbf{u}_j} \\ -t\sum_{j=1}^{3} e^{i\mathbf{k}\mathbf{v}_j} & 0 \end{array} \right)\Bigg|_{\mathbf{k}=\mathbf{K}_\pm+\boldsymbol{\kappa}} =$$

$$= \frac{3}{2}t \left(\begin{array}{cc} 0 & i\kappa_x \pm \kappa_y \\ -i\kappa_x \pm \kappa_y & 0 \end{array} \right) =$$

$$= \hbar v(-\sigma^2\kappa_x \pm \sigma^1\kappa_y), \qquad (6)$$

where $v = \frac{3}{2}t\hbar^{-1}$ is the Fermi velocity, and σ^1 and σ^2 are the off-diagonal Pauli matrices. Combining the contributions from $\mathbf{K}_+$ and $\mathbf{K}_-$ and carrying out the Fourier transformation $\boldsymbol{\kappa} \to -i\boldsymbol{\partial}$, we obtain

$$H = -i\hbar v(\alpha^1\partial_x + \alpha^2\partial_y), \qquad (7)$$

where

$$\alpha^1 = -\left(\begin{array}{cc} \sigma^2 & 0 \\ 0 & \sigma^2 \end{array} \right), \quad \alpha^2 = \left(\begin{array}{cc} \sigma^1 & 0 \\ 0 & -\sigma^1 \end{array} \right). \qquad (8)$$

Hamiltonian (7) acts on the four-component wave function

$$\psi = (\psi_{A+}, \psi_{B+}, \psi_{A-}, \psi_{B-})^T, \qquad (9)$$

where the subscripts A and B correspond to two sublattices, while the subscripts + and − to two nonequivalent Fermi points. Hence, the electronic processes in graphene are effectively described in the low-energy approximation in the framework of the continuous model which is based on the Dirac–Weyl equation for zero-mass electrons in the $(2 + 1)$-dimensional space-time, where the speed of light c is replaced by a corresponding Fermi velocity $v \approx c/300$ [6, 7].

In the graphite sheet plane, the rotation by an angle ϑ is carried out by the operator $\exp(i\vartheta\Sigma)$, where

$$\Sigma = \frac{1}{2i}\alpha^1\alpha^2 = \frac{1}{2}\left(\begin{array}{cc} \sigma^3 & 0 \\ 0 & -\sigma^3 \end{array} \right) \qquad (10)$$

is the pseudo-spin, which plays the role of the operator of the spin component that is orthogonal to the sheet plane. The crystal lattice of graphene is invariant with respect to a rotation by 360°, i.e.

$$\exp(i2\pi\Sigma)\psi = -\psi, \qquad (11)$$

but non-invariant with respect to a rotation by 180°, $\exp(i\pi\Sigma)\psi = 2i\Sigma\psi$, i.e. at the replacement $(x \to -x,\ y \to -y)$. The symmetry of graphite sheet allows the rotation by 180° to be appended by a simultaneous mutual exchange of two sublattices and two nonequivalent Fermi points. Such a combined transformation,

$$\Big(\psi_{A+}(x,y),\, \psi_{B+}(x,y),\, \psi_{A-}(x,y),\, \psi_{B-}(x,y)\Big)^T \to i\Big(\psi_{B-}(-x,-y),\, \psi_{A-}(-x,-y),\, \psi_{B+}(-x,-y),\, \psi_{A+}(-x,-y)\Big)^T$$

leaves the lattice unchanged and can be considered as a parity transformation for graphene. Let us choose a representation of the Clifford algebra, where the γ^5-matrix is diagonal:

$$\gamma^0 = \left(\begin{array}{cc} 0 & \sigma^1 \\ \sigma^1 & 0 \end{array} \right), \quad \gamma^3 = -i\left(\begin{array}{cc} 0 & \sigma^2 \\ \sigma^2 & 0 \end{array} \right),$$

$$\gamma^5 = \left(\begin{array}{cc} -I & 0 \\ 0 & I \end{array} \right), \qquad (12)$$

where $\gamma^5 = i\alpha^1\alpha^2\alpha^3$ and $\gamma^k = \gamma^0\alpha^k$. Then, the parity transformation for graphene is carried out by means of the operator $i\gamma^0$:

$$i\gamma^0 (\psi_{A+}, \psi_{B+}, \psi_{A-}, \psi_{B-})^T =$$

$$= i(\psi_{B-}, \psi_{A-}, \psi_{B+}, \psi_{A+})^T. \qquad (13)$$

3. Graphitic Nanocones

Topological defects in graphene are disclinations in its hexagonal lattice, when some of hexagons become substituted by pentagons or heptagons; with the graphite film surface becoming deformed at that. In the general case, a hexagon is replaced by a polygon with $6 - N_d$ vertices, where N_d is an integer less than 6. Polygons with $N_d > 0$ ($N_d < 0$) induce a film curvature,

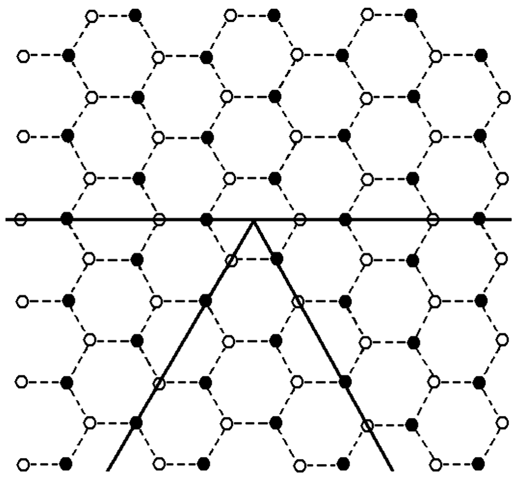

Fig. 1. Creation of a conical surface: one, two, or three 60°-sectors are removed from the graphite lattice

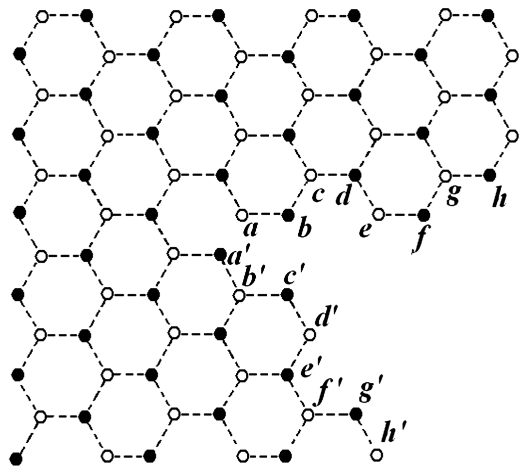

Fig. 2. Creation of a graphitic nanocone by removal of a 60°-sector: atoms belonging to different sublattices are identified (a with a', b with b', c with c', *etc.*)

which is locally positive (negative), while the graphite film remains flat far from the defect − in the same manner as a conical surface is flat far from its vertex. In the case of nanocones with positive N_d, the value of the latter represents the number of 60°-sectors that were removed from the graphite sheet (see Fig. 1) and is connected with the value of the apex angle of the conical surface δ by the relation

$$\sin\frac{\delta}{2} = 1 - \frac{N_d}{6}. \qquad (14)$$

If $N_d < 0$, the value of $-N_d$ corresponds to the number of sectors additionally inserted into the graphite sheet. Certainly, polygonal defects with $N_d > 1$ and $N_d < -1$ are mathematical abstraction, as well as cones with point-like vertices. Actually, defects are smoothed out, and the value of $N_d > 1$ corresponds to the number of pentagonal defects, which are crowded in the smoothed vertex of the cone; graphitic cones about a micron in linear dimensions and with the apex angles $\delta = 112.9, 83.6, 60.0, 38.9,$ and $19.2°$ − which correspond to the values $N_d = 1, 2, 3, 4,$ and 5 − were observed experimentally [22].

The theory also predicts the existence of saddle-shaped cones, for which the value of $-N_d$ is the number of heptagonal defects which are crowded in their central regions. We should emphasize that, as numerical simulations of molecular dynamics demonstrated [23], in the case $N_d \leq -4$, the surface with a polygonal defect turns out more stable than the surface having the same profile but with a smoothed defect in the form of corresponding number of heptagons.

The metric of the conical surface is determined by the relationship

$$ds^2 = dr^2 + (1-\eta)^2 r^2 d\varphi, \qquad (15)$$

where the polar coordinates r and φ are reckoned from the cone's vertex, and $-\infty < \eta < 1$. In terms of the angular variable $\varphi' = (1-\eta)\varphi$, the metric in the (r, φ')-coordinates coincides with the metric of a plane; but, in this case, $0 < \varphi' < 2\pi(1-\eta)$. Therefore, the quantity $2\pi\eta$ at $0 < \eta < 1$ is a deficit angle which measures the magnitude of the sector removed. In the case of a negative deficit angle, the value of $-2\pi\eta$ measures the magnitude of the added sector. The Dirac–Weyl Hamiltonian on the conical surface (15) reads

$$H = -i\hbar v \left\{ \alpha^1 \partial_r + \alpha^2 r^{-1} \left[(1-\eta)^{-1} \partial_\varphi - i\Sigma \right] \right\}. \qquad (16)$$

For graphitic nanocones, the parameter η is discrete: $\eta = N_d/6$.

Consider a nanocone with a pentagonal defect in its vertex, i.e. the cone which can be obtained from a graphite sheet by cutting-off a 60°-sector and identifying the atoms lying on two borders of the remaining sector (see Fig. 2). While going around the vertex of this nanocone, the sublattices, as well as the nonequivalent Fermi points, exchange. A double path tracing around the pentagonal defect is analogous to a single path tracing around a hexagon in a plane graphene. Hence, in the case of a nanocone with one pentagonal defect, the electron wave function has to satisfy a boundary condition of the Möbius-strip type, which demands for a double path tracing to be done to come back to the initial point. Note that the parity transformation for graphene includes, besides the rotation by 180°, the exchange of both the sublattices and the Fermi points. Taking into account the relation

$$i\gamma^0 = -2i\Sigma\gamma^3\gamma^5 \tag{17}$$

and the fact that the rotation by 180° is carried out by the operator $2i\Sigma$, we find that the exchange of the sublattices and the Fermi points is fulfilled by the operator $-\gamma^3\gamma^5$. Hence, the boundary condition for the electron wave function on a graphitic nanocone with a pentagonal defect can be selected in the form

$$\psi(r,\, \varphi+2\pi) = -i\gamma^3\gamma^5\psi(r,\varphi). \tag{18}$$

Then, for a double path tracing around the vertex, we have

$$\psi(r,\, \varphi+4\pi) = -\psi(r,\, \varphi), \tag{19}$$

because $(\gamma^3\gamma^5)^2 = I$. It is easy to prove that the sublattices (and the Fermi points) become entangled in the case of odd N_d and do not become entangled in the case of even N_d. Therefore, the boundary condition for an arbitrary graphitic nanocone looks like

$$\psi(r,\, \varphi+2\pi) = -\exp\left(i\frac{\pi}{2}N_d\gamma^3\gamma^5\right)\psi(r,\, \varphi). \tag{20}$$

Carrying out the singular gauge transformation

$$\psi' = e^{i\Omega}\psi, \quad \Omega = -\frac{\varphi}{4}N_d\gamma^3\gamma^5, \tag{21}$$

we pass to the wave function that satisfies the condition

$$\psi'(r,\, \varphi+2\pi) = -\psi'(r,\, \varphi). \tag{22}$$

At the same time, Hamiltonian (16) is transformed in the following way:

$$H' = e^{i\Omega}He^{-i\Omega} =$$

$$= -i\hbar v\left[\alpha^1\partial_r + \alpha^2 r^{-1}\left(\frac{\partial_\varphi + i\frac{3}{2}\eta\gamma^3\gamma^5}{1-\eta} - i\Sigma\right)\right], \tag{23}$$

where the relation between η and N_d for graphitic nanocones has been taken into account. Thus, the topological defect, which corresponds to the convolution of the graphite sheet into a cone, is represented by a pseudo-magnetic vortex with the flux $\pi N_d/2$ through the vertex of the cone with the deficit angle $\pi N_d/3$.

Let us fulfill the unitary transformation

$$\psi'' = U\psi', \quad H'' = UH'U^{-1}, \tag{24}$$

where

$$U = U^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} I & i\sigma^2 \\ -i\sigma^2 & -I \end{pmatrix}. \tag{25}$$

Then

$$U\gamma^3\gamma^5U^{-1} = \begin{pmatrix} -I & 0 \\ 0 & I \end{pmatrix} \tag{26}$$

and the Hamiltonian acquires a block-diagonal form,

$$H'' = \begin{pmatrix} H_1 & 0 \\ 0 & H_{-1} \end{pmatrix}, \tag{27}$$

where

$$H_s = \hbar v\left[i\sigma^2\partial_r - \sigma^1 r^{-1}\left(\frac{is\partial_\varphi + \frac{3}{2}\eta}{1-\eta} + \frac{1}{2}\sigma^3\right)\right],$$

$$s = \pm 1. \tag{28}$$

It is worth noting that the definite sublattice (A or B) and Fermi-point ($+$ or $-$) subscripts are attributed to the components of ψ-function (9), whereas transformations (21) and (24) bring about the ψ''-function, the components of which contain both entangled sublattices and entangled Fermi points.

4. Ground State Charge

The density of states is determined as follows:

$$\tau(E) = \frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}(H - E - i0)^{-1}, \tag{29}$$

where the notation Tr means the trace of the integro-differential operator in the functional space,

$$\mathrm{Tr}\; O = \int d^2r\; \mathrm{tr}\langle \mathbf{r}|O|\mathbf{r}\rangle,$$

and tr means the trace operator with respect to spinor indices only.

In the case of a plane graphene, where electron excitations are described by the Dirac–Weyl equation with Hamiltonian (7), we have

$$\tau(E) = \frac{S|E|}{\pi\hbar^2v^2}, \tag{30}$$

where S is the area of the graphite sheet. The charge of the ground state,

$$Q = -\frac{e}{2} \int\limits_{-\infty}^{\infty} dE\, \tau(E)\, \mathrm{sgn}(E), \tag{31}$$

vanishes in this case, because dependence (30) is the even function of the energy.

In order to determine the density of states in the case of a graphitic nanocone, it is necessary to find the complete system of solutions for the Dirac–Weyl equation $H\psi = E\psi$, where H is given by relation (16) and ψ satisfies condition (20). Since the result of calculations of the functional trace in Eq. (29) does not depend on the representation used, it is convenient, after carrying out transformations (21) and (24), to pass to a representation, where the Hamiltonian is block-diagonal (Eq. (27)) and the wave function looks like

$$\psi''(r, \varphi) = \sum_{n\in Z} \begin{pmatrix} f_{n,1}(r)\, e^{i(n+\frac{1}{2})\varphi} \\ g_{n,1}(r)\, e^{i(n+\frac{1}{2})\varphi} \\ f_{n,-1}(r)\, e^{i(n-\frac{1}{2})\varphi} \\ g_{n,-1}(r)\, e^{i(n-\frac{1}{2})\varphi} \end{pmatrix}, \tag{32}$$

where Z is the set of integer numbers. Taking Eqs. (27) and (28) into account, we reduce the Dirac–Weyl equation to the system of equations for radial functions,

$$\begin{pmatrix} 0 & D^{\dagger}_{n,s} \\ D_{n,s} & 0 \end{pmatrix} \begin{pmatrix} f_{n,s}(r) \\ g_{n,s}(r) \end{pmatrix} = E \begin{pmatrix} f_{n,s}(r) \\ g_{n,s}(r) \end{pmatrix}, \tag{33}$$

where

$$D_{n,s} = \hbar v \left[-\partial_r + r^{-1}(1-\eta)^{-1}(sn-\eta)\right],$$
$$D^{\dagger}_{n,s} = \hbar v \left[\partial_r + r^{-1}(1-\eta)^{-1}(sn+1-2\eta)\right]. \tag{34}$$

Two linearly independent solutions of Eq. (33) are expressed through cylindrical functions. In the cases $N_d = 3, 4,$ and 5, the condition of function regularity at $r = 0$ is equivalent to the condition of its square-integrability at this point; and it is this condition that defines a physically comprehensible solution. It can be demonstrated that the density of states is an even function of the energy; moreover, in the case $N_d = 3$, it coincides with Eq. (30), and, in the cases $N_d = 4$ and 5, differs from Eq. (30) by an insignificant summand which does not include the area factor. Thus, in all those cases, as well as in the case of plane graphene ($N_d = 0$), the charge of the ground state is equal to zero.

In all other cases of nanocones, there emerge the modes, for which the condition of regularity is not equivalent to the condition of square-integrability: both linearly independent solutions for these modes are simultaneously irregular and square-integrable at $r = 0$. We confine ourselves to the consideration of those cases, where there is only one such mode: $n = n_c$.

In the cases $N_d = 2, 1, -1, -2,$ and -3, we have $n_c = s[\mathrm{sgn}(N_d) - 1]/2$, and, in the case $N_d = -6$, $n_c = -2s$. The partial Hamiltonian, which corresponds to this mode, is not essentially self-adjoint, so that there arises a problem of its self-adjoint extension. Making use of the Weyl–von Neumann theory of self-adjoint operators (see, e.g., [24]) allows one to solve this problem and find a condition which must be satisfied by the irregular mode:

$$\frac{\lim\limits_{r\to 0}(rMv/\hbar)^F f_{n_c,s}(r)}{\lim\limits_{r\to 0}(rMv/\hbar)^{1-F} g_{n_c,s}(r)} =$$
$$= -2^{2F-1}\frac{\Gamma(F)}{\Gamma(1-F)}\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right), \tag{35}$$

where Θ is the parameter of self-adjoint extension, M is the parameter with a mass dimension, $\Gamma(u)$ is the Euler gamma-function, and

$$F = \begin{cases} \frac{3-3\mathrm{sgn}(N_d)+N_d}{6-N_d}, & N_d = 2,\ 1,\ -1,\ -2,\ -3, \\ 1/2, & N_d = -6. \end{cases} \tag{36}$$

The density of states in a plane graphene and the density of states in a graphitic nanocone differ from each other by a contribution made by an irregular mode which arises owing to the circumstance that the flux of a pseudo-magnetic vortex is fractional. Using the theory of vacuum polarization by singular external fields [18–21], it can be shown that the irregular mode is responsible for the appearance of a term in the density of states, which is odd with respect to the energy:

$$\tau(E) = \frac{2(2F-1)\sin(F\pi)\left[\left(\frac{|E|}{Mv^2}\right)^{2F-1}\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)+\left(\frac{|E|}{Mv^2}\right)^{1-2F}\cot\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)\right]}{\pi E\left[\left(\frac{|E|}{Mv^2}\right)^{2(2F-1)}\tan^2\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)-2\cos(2F\pi)+\left(\frac{|E|}{Mv^2}\right)^{2(1-2F)}\cot^2\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)\right]}. \tag{37}$$

Substituting the latter relation into Eq. (31) and fulfilling the integration, we obtain the charge of a graphitic nanocone in the ground state:

$$Q = e\,\mathrm{sgn}_0[(1-2F)\cos\Theta], \qquad (38)$$

where

$$\mathrm{sgn}_0(u) = \left\{ \begin{array}{cc} \mathrm{sgn}(u), & u \neq 0 \\ 0, & u = 0 \end{array} \right\}.$$

5. Conclusions

Hence, the charge of the ground state in graphene with a disclination is equal to zero in the cases $N_d = 2, -2,$ and -6, because $F = 1/2$ at that. Taking into account that $F = 1/5$ at $N_d = 1$, $F = 5/7$ at $N_d = -1$, and $F = 1/3$ at $N_d = -3$, we attain the conclusion that

$$Q|_{N_d=1} = -Q|_{N_d=-1} = Q|_{N_d=-3} = e\,\mathrm{sgn}_0(\cos\Theta). \qquad (39)$$

Thus, the theory predicts the dependence of the charge in the ground state on the parameter of self-adjoint extension Θ in the case of a graphite film with a defect in the form of a pentagon, a heptagon, or three heptagons. The task for future experiments can be to elucidate whether the quantity $\cos\Theta$ gets values different from zero. In the case of the positive answer, it would mean that there occurs the induction of the charge in the ground state of graphitic nanocones.

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ЕЛЕКТРОННІ ВЛАСТИВОСТІ ГРАФІТОВИХ НАНОКОНУСІВ

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Р е з ю м е

Графітовий лист (графен), що в довгохвильовому наближенні характеризується лінійним спектром квазічастинкових збуджень, є унікальним прикладом справді двовимірної "релятивістської" електронної системи, котра за наявності топологічних дефектів може мати досить незвичні властивості. Показано, що дисклінація, яка приводить до скручування графітового листа у наноконус, описується псевдомагнітним вихором з потоком, що пов'язаний з дефіцитом кута конуса. Отримано аналітичні вирази для щільності станів та заряду основного стану деяких графітових наноконусів.