

Properties of the ground state of electronic excitations in carbon-like nanocones

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On the basis of the continuum model for long-wavelength charge carriers, originating in the tight-binding approximation for the nearest-neighbour interaction of atoms in the crystalline lattice, we consider quantum ground-state effects of electronic excitations in Dirac materials with two-dimensional monolayer honeycomb structures warped into nanocones by a disclination; the nonzero size of the disclination is taken into account, and a boundary condition at the edge of the disclination is chosen to ensure self-adjointness of the Dirac–Weyl Hamiltonian operator. We show that the quantum ground-state effects are independent of the disclination size and find circumstances when they are independent of a parameter of the boundary condition. The magnetic flux circulating in the angular direction around the nanocone apex and the pseudomagnetic flux directed orthogonally to the nanocone surface are shown to be induced in the ground state.

Keywords: Dirac materials; nanocones; ground state; quantum effects in monolayer crystals.

1. Introduction

A wealth of new phenomena in micro- and nanophysics, suggesting possible applications to technology and industry, is promised by a synthesis in this century of strictly two-dimensional atomic crystals (for instance, a monolayer of carbon atoms, graphene, [1,2]). The electronic states near the Fermi level in these crystals are characterized by the linear and isotropic dispersion relation, with the density of states at the Fermi level being strictly zero. Condensed matter systems with such a behavior of electronic excitations are known as the two-dimensional Dirac materials comprising a diverse set ranging from honeycomb crystalline structures (graphene [1], silicene and germanene [3], phosphorene [4]) to high-temperature d -wave superconductors, superfluid phases of helium-3 and topological insulators, see review in [5]. Using the tight-binding approximation for the nearest-neighbour interaction in the crystalline lattice, an effective long-wavelength description of electronic excitations can be given in terms of a continuum model which is based on the Dirac–Weyl equation for massless electrons in 2+1-dimensional space-time, with the role of velocity of light c played by Fermi velocity $v \approx c/300$ [6,7].

Freely suspended samples of crystalline monolayers are not exactly plane surfaces, but possess ripples which are due to the appearance of topological defects in a crystalline lattice: disclinations and disclination dipoles (dislocations). A single disclination warps a sheet of the crystalline lattice, giving it the shape of a cone. The squared length element of the conical surface is

$$ds^2 = dr^2 + v^{-2}r^2 d\varphi^2, \quad 0 \leq \varphi < 2\pi, \quad (1)$$

where $v = (1 - \eta)^{-1}$, and $2\pi\eta$ is the deficit angle. Conical spaces (i.e., 3-dimensional spaces with a 2-dimensional section given by (1)) emerge in a field rather different from condensed matter physics — in cosmology. The early universe in the process of its cosmological expansion is likely to undergo a series of phase transitions with spontaneous breakdown of continuous symmetries, and a vortex-like topological defect which is formed in the aftermath of such a transition is known under the name of a cosmic string, see reviews in [8,9]. Starting with a random tangle, the cosmic string network evolves into two distinct sets: the stable one which consists of several long, approximately straight strings spanning the horizon volume and the unstable one which consists of a variety of string loops decaying by gravitational radiation. A straight infinitely long cosmic string in its rest

frame is characterized by an outer space with the transverse section given by (1). Parameter η is related to the mass per unit length of the cosmic string, hence it is positive, and the present-day astrophysical observations restrict its values to range $0 < \eta < 10^{-6}$ (see, e.g., [10]).

On the contrary, in the case of conically-shaped crystalline monolayers, parameter η takes both positive and negative discrete values of order 1 and even larger: a disclination obtained by deleting atoms from the crystalline lattice results in the positive deficit angle, whereas a disclination obtained by adding atoms into the crystalline lattice results in the negative deficit (i.e., proficit) angle. For instance, in the case of the honeycomb lattice of graphene, silicene, germanene or phosphorene, a natural way of producing the apex of a nanocone is by substituting some of hexagons by pentagons (positive deficit angle) or heptagons (negative deficit angle); thus, $\eta = N_d / 6$, where N_d is an integer which is smaller than 6. A general disclination in the honeycomb lattice is obtained by substituting a hexagon by a polygon with $6 - N_d$ sides; polygons with $N_d > 0$ ($N_d < 0$) induce locally positive (negative) curvature at the apex, whereas the crystalline sheet is locally flat away from the disclination, as is the conical surface away from the apex. In the case of nanocones with $N_d > 0$, the value of N_d is related to apex angle δ , $\sin \delta / 2 = 1 - N_d / 6$, and N_d counts the number of sectors of the value of $\pi/3$ which are removed from the crystalline sheet. If $N_d < 0$, then $-N_d$ counts the number of such sectors which are inserted into the crystalline sheet. Certainly, polygonal defects with $N_d > 1$ and $N_d < -1$ are mathematical abstractions, as are cones with a pointlike apex. In reality, the defects are smoothed, and $N_d > 0$ counts the number of the pentagonal defects which are tightly clustered producing a conical shape; carbon nanocones with the apex angles $\delta = 112.9^\circ, 83.6^\circ, 60.0^\circ, 38.9^\circ, 19.2^\circ$, which correspond to the values $N_d = 1, 2, 3, 4, 5$, were observed experimentally, see [11] and references therein. Theory also predicts an infinite series of the saddle-like nanocones with quantity $-N_d$ counting the number of the heptagonal defects which are tightly clustered forming the saddle centre. Saddle-like nanocones serve as an element which is necessary for joining parts of carbon nanotubes of different radii.

Another distinction from the case of cosmic strings is in the intertwinement of valleys, as well as sublattices, in the case of disclinations corresponding to odd values of N_d . It seems reasonable to identify a matrix exchanging both the sublattice and valley indices with γ^5 . Hence, the relevant bundle connection corresponding to the gauge axial vector field appears, describing the pseudomagnetic vortex with flux related to the deficit angle. This is in contrast to the case of cosmic strings, where the relevant bundle connection correspond to the gauge vector field describing the vortex with flux unrelated to the deficit angle.

In the present paper, we consider the quantum ground-state effects of electronic excitations in honeycomb crystal-

line monolayer structures with disclinations corresponding to $N_d = \pm 1, \pm 2, \pm 3, 4, 5, -6$. A crucial point is a choice of the boundary condition at the location of the disclination. The previous consideration [12–14] was neglecting the transverse size of the disclination, treating it as a pointlike one. We are now tackling the problem more carefully by taking into account the finite size of the disclination, imposing the most general boundary condition at the disclination edge, and then going to the physically sensible limit of the nanocone size exceeding considerably the disclination size. This more physical approach allows us to specify the boundary condition with more definiteness. We find out that the pseudomagnetic field directed orthogonally to the nanocone surface is induced in the ground state, whereas the electric charge is not; the magnetic field circulating in the angular direction around the nanocone apex is induced in the ground state in cases $N_d = \pm 2, -6$ only.

2. Continuum model description of electronic excitations in monolayer atomic crystals with a disclination

Electronic excitations in a plane sheet of the honeycomb crystalline lattice are described in terms of a four-component wave function,

$$\psi = \left(\psi_A^{(I)}, \psi_B^{(I)}, \psi_A^{(II)}, \psi_B^{(II)} \right)^T, \quad (2)$$

where subscripts A and B correspond to two sublattices and superscripts (I) and (II) correspond to two valleys (inequivalent Fermi points). As was noted in Introduction, in the framework of the long-wavelength continuum model, the wave function of electronic excitations satisfies the Dirac–Weyl equation,

$$(i\partial_0 - H)\psi = 0, \quad H = -i\hbar v \left(\alpha^1 \partial_1 + \alpha^2 \partial_2 \right). \quad (3)$$

The generating elements of the Clifford algebra of anticommuting matrices in 3+1-dimensional space-time can be chosen as

$$\gamma^0 = \tau^0 \sigma^3, \quad \alpha^1 = -\tau^0 \sigma^2, \quad \alpha^2 = \tau^3 \sigma^1, \quad \alpha^3 = \tau^1 \sigma^1, \quad (4)$$

where σ^0 and σ^j (τ^0 and τ^j) are the unity and Pauli matrices with the sublattice (valley) indices, and $j = 1, 2, 3$. Defining $\gamma^5 = -i\alpha^1 \alpha^2 \alpha^3$, one gets

$$\gamma^5 = -\tau^2 \sigma^2. \quad (5)$$

A rotation by angle ϑ in the plane of a honeycomb lattice sheet is implemented by operator $\exp(i\vartheta\Sigma)$, where

$$\Sigma = \frac{1}{2i} \alpha^1 \alpha^2 = \frac{1}{2} \tau^3 \sigma^3 \quad (6)$$

is the pseudospin playing here the role of the operator of spin component which is orthogonal to the plane. The honeycomb lattice is invariant under a rotation by 2π , but is not invariant under a rotation by π . The parity transformation

can be introduced as a rotation by π , which is simultaneously supplemented by the exchange of both the sublattice and valley indices [15],

$$P\psi = \left(\psi_B^{(II)}, \psi_A^{(II)}, \psi_B^{(I)}, \psi_A^{(I)} \right)^T \quad (7)$$

with

$$P = 2\Sigma R, \quad [P, H]_+ = [R, H]_- = 0; \quad (8)$$

in representation (4) we obtain

$$P = \alpha^3, \quad R = \gamma^5. \quad (9)$$

The wave function is chosen as a section of a bundle with spin connection -2Σ , i.e., it obeys condition

$$\psi(\varphi + 2\pi) = -\psi(\varphi). \quad (10)$$

If a defect with $N_d = \pm 1$ is inserted at the origin, then condition (10) is changed to the Möbius-strip-type condition:

$$\psi(\varphi + 2\pi) = \pm iR\psi(\varphi), \quad \psi(\varphi + 4\pi) = -\psi(\varphi). \quad (11)$$

For a general defect with $N_d < 6$, the condition takes form

$$\psi(\varphi + 2\pi) = -\exp\left(-i\frac{\pi}{2}N_d R\right)\psi(\varphi), \quad (12)$$

while the Hamiltonian operator for electronic excitations in a conical surface with the squared length element given by (1) takes form

$$H = -i\hbar v \left[\alpha^r \left(\partial_r + \frac{1}{2r} \right) + \alpha^\varphi \partial_\varphi \right], \quad (13)$$

where

$$\alpha^r = \alpha_r = -\tau^0 \sigma^2, \quad \alpha^\varphi = \frac{v}{r} \tau^3 \sigma^1, \quad \alpha_\varphi = \frac{r^2}{v^2} \alpha^\varphi. \quad (14)$$

By performing a singular gauge transformation, we arrive at the wave function obeying condition (10) and the Hamiltonian operator involving bundle connection $\Phi(2\pi\hbar v)^{-1}$ [12]:

$$H = -i\hbar v \left[\alpha^r \left(\partial_r + \frac{1}{2r} \right) + \alpha^\varphi \left(\partial_\varphi - i \frac{\Phi}{2\pi\hbar v} \right) \right], \quad (15)$$

where

$$\Phi = 3\pi\hbar v(1 - v^{-1})R, \quad v = (1 - N_d/6)^{-1}; \quad (16)$$

note that in the case of cosmic strings quantity Φ is the flux of a gauge vector field corresponding to the generator of a spontaneously broken continuous symmetry.

Next, by performing in addition a unitary transformation, we arrive at the representation with both R and P diagonal,

$$\gamma^5 = R = \tau^3 \sigma^0, \quad \alpha^3 = P = \tau^0 \sigma^3, \quad \gamma^0 = \tau^1 \sigma^1, \quad (17)$$

while relations (6) and (14) are maintained. The initial representation with diagonal γ^0 , see (4), can be denoted as the

standard one, and it has been chosen to be diagonal in both the sublattice and the valley indices, see (2). The final representation with diagonal γ^5 , see (17), can be denoted as the chiral one, and it mixes up sublattices, as well as valleys.

Using the chiral representation, we decompose the solution to the stationary Dirac–Weyl equation, $H\psi_E(\mathbf{x}) = E\psi_E(\mathbf{x})$, with H given by (15) and (16) as

$$\psi_E(\mathbf{x}) = \sum_{n \in \mathbb{Z}} \begin{pmatrix} f_{n,+}(r, E) e^{i(n+1/2)\varphi} \\ g_{n,+}(r, E) e^{i(n+1/2)\varphi} \\ f_{n,-}(r, E) e^{i(n-1/2)\varphi} \\ g_{n,-}(r, E) e^{i(n-1/2)\varphi} \end{pmatrix}, \quad (18)$$

where the radial functions satisfy the system of first-order differential equations

$$\left\{ \begin{array}{l} \hbar v \left[-\partial_r + \frac{1}{r}(\pm v n - v + 1) \right] f_{n,\pm}(r, E) = E g_{n,\pm}(r, E) \\ \hbar v \left[\partial_r + \frac{1}{r}(\pm v n - v + 2) \right] g_{n,\pm}(r, E) = E f_{n,\pm}(r, E) \end{array} \right\}; \quad (19)$$

thus a component of definite chirality, + or –, is a superposition of components with definite sublattice and valley indices.

Quantum effects in the ground state of electronic excitations comprise the induced electric charge density:

$$q(\mathbf{x}) = -\frac{e}{2} \int_{-\infty}^{\infty} \frac{dE E}{\hbar^2 v^2} \psi_E^\dagger(\mathbf{x}) \psi_E(\mathbf{x}), \quad (20)$$

the induced electric current density:

$$\mathbf{j}(\mathbf{x}) = -\frac{e}{2} \int_{-\infty}^{\infty} \frac{dE E}{\hbar^2 v} \psi_E^\dagger(\mathbf{x}) \boldsymbol{\alpha} \psi_E(\mathbf{x}); \quad (21)$$

the induced parity-breaking condensate density:

$$\rho(\mathbf{x}) = -\frac{1}{2} \int_{-\infty}^{\infty} \frac{dE E}{\hbar^2 v^2} \psi_E^\dagger(\mathbf{x}) P \psi_E(\mathbf{x}), \quad (22)$$

and the induced R -current density:

$$\mathbf{j}^R(\mathbf{x}) = -\frac{1}{2} \int_{-\infty}^{\infty} \frac{dE E}{\hbar^2 v} \psi_E^\dagger(\mathbf{x}) \boldsymbol{\alpha} R \psi_E(\mathbf{x}). \quad (23)$$

The magnetic field strength, $\mathbf{B}(\mathbf{x})$, is also induced in the ground state, as a consequence of the Maxwell equation,

$$\partial \times \mathbf{B}(\mathbf{x}) = \frac{1}{v} \mathbf{j}(\mathbf{x}), \quad (24)$$

as well as does the pseudomagnetic field strength, $\mathbf{B}^R(\mathbf{x})$, which is a consequence of the analogue of the Maxwell equation,

$$\partial \times \mathbf{B}^R(\mathbf{x}) = \frac{1}{v} \mathbf{j}^R(\mathbf{x}); \quad (25)$$

the use of term “pseudomagnetic” is justified because R coincides with γ^5 ; due to this, also the R -current can be regarded as an axial current.

Using (14), (17) and (18), one gets $j_r^R = 0$ immediately and, with more careful analysis (see the beginning of Section 4), $j_3^R = 0$, where

$$j_3^R(r) = -\frac{1}{2} \int_{-\infty}^{\infty} \frac{dEE}{\hbar^2 v} \sum_{n \in \mathbb{Z}} [f_{n,+}^2(r, E) - g_{n,+}^2(r, E) - f_{n,-}^2(r, E) + g_{n,-}^2(r, E)]. \quad (26)$$

Thus, the only component of the induced ground-state R -current,

$$j_\varphi^R(r) = -\frac{r}{v} \int_{-\infty}^{\infty} \frac{dEE}{\hbar^2 v} \sum_{n \in \mathbb{Z}} [f_{n,+}(r, E)g_{n,+}(r, E) + f_{n,-}(r, E)g_{n,-}(r, E)], \quad (27)$$

is independent of the angular variable. The induced ground-state pseudomagnetic field strength is also independent of the angular variable, being directed orthogonally to the conical surface,

$$B_3^R(r) = \frac{v}{v} \int_r^{r_{\max}} \frac{dr'}{r'} j_\varphi^R(r') + B_3^R(r_{\max}), \quad (28)$$

with total flux

$$\Phi_1^R = \frac{2\pi}{v} \int_{r_0}^{r_{\max}} dr r B_3^R(r), \quad (29)$$

where it is assumed without a loss of generality that a nanocone is of a rotationally invariant shape with r_{\max} being its radius and r_0 being the radius of a disclination, $r_{\max} \gg r_0$ in the physically sensible case.

Turning to the induced ground-state electric charge and parity-breaking condensate, their densities are also independent of the angular variable:

$$q(r) = -\frac{e}{2} \int_{-\infty}^{\infty} \frac{dEE}{\hbar^2 v^2} \sum_{n \in \mathbb{Z}} [f_{n,+}^2(r, E) + g_{n,+}^2(r, E) + f_{n,-}^2(r, E) + g_{n,-}^2(r, E)] \quad (30)$$

and

$$\rho(r) = -\frac{1}{2} \int_{-\infty}^{\infty} \frac{dEE}{\hbar^2 v^2} \sum_{n \in \mathbb{Z}} [f_{n,+}^2(r, E) - g_{n,+}^2(r, E) + f_{n,-}^2(r, E) - g_{n,-}^2(r, E)]. \quad (31)$$

Appropriately, one can define total charge

$$Q = \frac{2\pi}{v} \int_{r_0}^{r_{\max}} dr r q(r) \quad (32)$$

and total P -condensate

$$C = \frac{2\pi}{v} \int_{r_0}^{r_{\max}} dr r \rho(r). \quad (33)$$

Note that the induced ground-state condensate of pseudospin Σ (6) is proportional to j_3^R (26) and, thus, is vanishing.

As to the induced ground-state electric current, note an evident relation, $j_r = 0$, and a less evident one (substantiated in the beginning of Sec. 4), $j_\varphi = 0$, where

$$j_\varphi(r) = -\frac{er}{v} \int_{-\infty}^{\infty} \frac{dEE}{\hbar^2 v} \sum_{n \in \mathbb{Z}} [f_{n,+}(r, E)g_{n,+}(r, E) - f_{n,-}(r, E)g_{n,-}(r, E)]; \quad (34)$$

hence, the only nonvanishing component is directed orthogonally to the conical surface and is related to the P -condensate:

$$j_3(r) = ev\rho(r). \quad (35)$$

The total electric current,

$$J_3 = \frac{2\pi}{v} \int_{r_0}^{r_{\max}} dr r j_3(r), \quad (36)$$

is appropriately related to the total P -condensate:

$$J_3 = evC. \quad (37)$$

The induced ground-state magnetic field strength is also independent of the angular variable, being directed in the conical surface along a circle with an apex in its center,

$$B_\varphi(r) = -\frac{1}{v\vartheta} \int_r^{r_{\max}} dr' r' j_3(r') + B_\varphi(r_{\max}). \quad (38)$$

Its total flux is

$$\Phi_1 = \int_{r_0}^{r_{\max}} dr B_\varphi(r). \quad (39)$$

Concluding this Section, note that we are considering the ground-state characteristics which are diagonal in chiralities. The nondiagonal ones (for instance, the γ^0 -condensate) are proportional, as follows from (18), either to $\cos \varphi$ or to $\sin \varphi$ and, thus, vanish upon averaging over the angular variable.

3. Self-adjointness and choice of boundary conditions

Let us note first, that (15) is not enough to define the Hamiltonian operator rigorously in a mathematical sense. To define an operator in a unambiguous way, one has to specify its domain of definition. Let the set of functions ψ be the domain of definition of operator H , and the set of functions $\tilde{\psi}$ be the domain of definition of its adjoint, op-

erator H^\dagger . Then the operator is Hermitian (or symmetric in mathematical parlance),

$$\int_X d^2x \sqrt{g} \tilde{\psi}^\dagger (H\psi) = \int_X d^2x \sqrt{g} (H^\dagger \tilde{\psi})^\dagger \psi, \quad (40)$$

if relation

$$-i \int_{\partial X} dl \tilde{\psi}^\dagger \alpha \psi = 0 \quad (41)$$

is valid; here functions $\psi(\mathbf{x})$ and $\tilde{\psi}(\mathbf{x})$ are defined in space X with boundary ∂X . It is evident that condition (41) can be satisfied by imposing different boundary conditions for ψ and $\tilde{\psi}$. But, a nontrivial task is to find a possibility that a boundary condition for $\tilde{\psi}$ is the same as that for ψ ; then the domain of definition of H^\dagger coincides with that of H , and operator H is self-adjoint (for a review of the Weyl-von Neumann theory of self-adjoint operators see [16,17]). The action of a self-adjoint operator results in functions belonging to its domain of definition only, and a multiple action and functions of such an operator, for instance, the resolvent and evolution operators, can be consistently defined. Thus, in the case of a surface of radius r_{\max} with a deleted central disc of radius r_0 , we have to ensure the validity of relations

$$\tilde{\psi}^\dagger \alpha^r \psi \Big|_{r=r_0} = 0, \quad \tilde{\psi}^\dagger \alpha^r \psi \Big|_{r=r_{\max}} = 0, \quad (42)$$

meaning that the quantum matter excitations do not penetrate outside. It is implied that functions ψ and $\tilde{\psi}$ are differentiable and square-integrable. As $r_{\max} \rightarrow \infty$, they conventionally turn into differentiable functions corresponding to the continuum, and the condition at $r = r_{\max}$ yields no restriction at $r_{\max} \rightarrow \infty$, whereas the condition at $r = r_0$ yields

$$\psi \Big|_{r=r_0} = K \psi \Big|_{r=r_0}, \quad \tilde{\psi} \Big|_{r=r_0} = K \tilde{\psi} \Big|_{r=r_0}, \quad (43)$$

where K is a matrix (element of the Clifford algebra in 2+1-dimensional space-time) which obeys condition

$$K^2 = I \quad (44)$$

and without a loss of generality can be chosen to be Hermitian; in addition, it has to obey either condition

$$[K, \alpha^r]_+ = 0, \quad (45)$$

or condition

$$[K, \alpha^r]_- = 0. \quad (46)$$

One can simply go through four linearly independent elements of the Clifford algebra in 2+1-dimensional space-time and find that two of them satisfy (45) and two other satisfy (46). However, if one chooses

$$K = c_1 I + c_2 \alpha^r \quad (47)$$

to satisfy (46), then (44) is violated. There remains the only possibility to choose

$$K = c_1 \gamma^0 + c_2 i \gamma^0 \alpha^r \quad (48)$$

with real coefficients obeying condition

$$c_1^2 + c_2^2 = 1; \quad (49)$$

then both (44) and (45) are satisfied. Using obvious parameterization

$$c_1 = \sin \theta, \quad c_2 = \cos \theta,$$

we finally obtain

$$K = i \gamma^0 \alpha^r e^{-i\theta \alpha^r}. \quad (50)$$

Thus, boundary condition (43) with K given by (50) is the most general boundary condition ensuring self-adjointness of the Hamiltonian operator on a surface with a deleted disc of radius r_0 , and parameter θ can be interpreted as the self-adjoint extension parameter. Value $\theta = 0$ corresponds to the MIT bag boundary condition which was proposed as the condition ensuring the confinement of the matter field, that is, the absence of the matter flux across the boundary [18]. However, it should be comprehended that a condition with an arbitrary value of θ is motivated equally as well as that with $\theta = 0$.

Imposing the boundary condition (43) with matrix K (50) on the solution to the Dirac–Weyl equation, $\psi_E(x)$ (18), we obtain the condition for the modes:

$$\cos\left(\frac{\theta}{2} + \frac{\pi}{4}\right) f_{n,\pm}(r_0, E) = -\sin\left(\frac{\theta}{2} + \frac{\pi}{4}\right) g_{n,\pm}(r_0, E). \quad (51)$$

Let us consider nanocones with $N_d = 1, 2, 3, 4, 5$ ($1 < \nu < 7$), as well as with $N_d = -1, -2, -3$ ($\frac{3}{5} < \nu < 1$),

and introduce positive quantity

$$F = \frac{3}{2} \nu - \frac{1}{2} \nu \operatorname{sgn}(\nu - 1) - 1, \quad (52)$$

which exceeds 1 at $N_d = 3, 4, 5$ ($2 \leq \nu < 7$) only; here $\operatorname{sgn}(u)$ is the sign function, $\operatorname{sgn}(u) = 1$ at $u > 0$ and $\operatorname{sgn}(u) = -1$ at $u < 0$. Define also

$$n_c = \pm \frac{1}{2} [\operatorname{sgn}(\nu - 1) - 1], \quad (53)$$

as well as

$$\begin{pmatrix} f_{n_c} \\ g_{n_c} \end{pmatrix} = \frac{1}{2} \frac{\sqrt{\nu}}{\pi} \frac{1}{\sqrt{1 + \sin(2\mu_{1-F}) \cos(F\pi)}} \begin{pmatrix} [\sin(\mu_{1-F}) J_{-F}(kr) + \cos(\mu_{1-F}) J_F(kr)] \\ \operatorname{sgn}(E) [\sin(\mu_{1-F}) J_{1-F}(kr) - \cos(\mu_{1-F}) J_{-1+F}(kr)] \end{pmatrix}, \quad (54)$$

$$\begin{pmatrix} f_n^{(\wedge)} \\ g_n^{(\wedge)} \end{pmatrix} = \frac{1}{2} \sqrt{\frac{\nu}{\pi}} \begin{pmatrix} \left[\sin(\mu_{\nu l+1-F}^{(\wedge)}) J_{\nu l-F}(kr) + \cos(\mu_{\nu l+1-F}^{(\wedge)}) Y_{\nu l-F}(kr) \right] \\ \text{sgn}(E) \left[\sin(\mu_{\nu l+1-F}^{(\wedge)}) J_{\nu l+1-F}(kr) + \cos(\mu_{\nu l+1-F}^{(\wedge)}) Y_{\nu l+1-F}(kr) \right] \end{pmatrix}, \quad (55)$$

where $l = n - n_c$, and

$$\begin{pmatrix} f_n^{(\vee)} \\ g_n^{(\vee)} \end{pmatrix} = \frac{1}{2} \sqrt{\frac{\nu}{\pi}} \begin{pmatrix} \left[\sin(\mu_{\nu l'+F}^{(\vee)}) J_{\nu l'+F}(kr) + \cos(\mu_{\nu l'+F}^{(\vee)}) Y_{\nu l'+F}(kr) \right] \\ -\text{sgn}(E) \left[\sin(\mu_{\nu l'+F}^{(\vee)}) J_{\nu l'-1+F}(kr) + \cos(\mu_{\nu l'+F}^{(\vee)}) Y_{\nu l'-1+F}(kr) \right] \end{pmatrix}, \quad (56)$$

where $l' = -n + n_c$; here $J_\lambda(u)$ and $Y_\lambda(u)$ are the Bessel and Neumann functions of order λ .

In the case of $2 \leq \nu < 7$ ($F = \nu - 1$, $N_d = 3, 4, 5$), the complete set of solutions to (19) is given by

$$\begin{pmatrix} f_{n,\pm} \\ g_{n,\pm} \end{pmatrix} \Big|_{n \geq n_c+1} = \begin{pmatrix} f_n^{(\wedge)} \\ g_n^{(\wedge)} \end{pmatrix}, \quad \begin{pmatrix} f_{n,\pm} \\ g_{n,\pm} \end{pmatrix} \Big|_{n \leq n_c} = \begin{pmatrix} f_n^{(\vee)} \\ g_n^{(\vee)} \end{pmatrix}. \quad (57)$$

In the case of $\frac{3}{5} < \nu < 2$ ($0 < F < 1$, $N_d = 2, 1, -1, -2, -3$), the complete set of solutions to (19) is given by

$$\begin{pmatrix} f_{n,\pm} \\ g_{n,\pm} \end{pmatrix} \Big|_{n \geq n_c+1} = \begin{pmatrix} f_n^{(\wedge)} \\ g_n^{(\wedge)} \end{pmatrix}, \quad \begin{pmatrix} f_{n,\pm} \\ g_{n,\pm} \end{pmatrix} \Big|_{n=n_c} = \begin{pmatrix} f_{n_c} \\ g_{n_c} \end{pmatrix}, \\ \begin{pmatrix} f_{n,\pm} \\ g_{n,\pm} \end{pmatrix} \Big|_{n \leq n_c-1} = \begin{pmatrix} f_n^{(\vee)} \\ g_n^{(\vee)} \end{pmatrix}. \quad (58)$$

$$\lim_{r \rightarrow 0} \left(\frac{r}{r_{\max}} \right)^F \cos \left(\frac{\Theta}{2} + \frac{\pi}{4} \right) f_{n_c,\pm}(r, E) = -\lim_{r \rightarrow 0} \left(\frac{r}{r_{\max}} \right)^{1-F} \sin \left(\frac{\Theta}{2} + \frac{\pi}{4} \right) g_{n_c,\pm}(r, E), \quad (59)$$

where Θ is the self-adjoint extension parameter, F is given by (52) for $N_d = 2, 1, -1, -2, -3$ and $F = 1/2$ for $N_d = -6$, while n_c is given by (53) for $N_d = 2, 1, -1, -2, -3$ and $n_c = \mp 2$ for $N_d = -6$. As follows from the present section, in the case of a disclination of nonzero size, when the boundary condition is imposed at its edge, the total Hamiltonian operator is self-adjoint extended with the use of one parameter, see (51).

Value Θ of the self-adjoint extension parameter in the case of a pointlike disclination can be fixed by the limiting procedure $r_0 \rightarrow 0$ in the case of a nonzero-size disclination. Namely in this way, the condition of minimal irregularity [19,20] is obtained:

$$\Theta = \begin{cases} \frac{\pi}{2}, & 0 < F < \frac{1}{2}, \\ \theta, & F = \frac{1}{2}, \\ -\frac{\pi}{2}, & \frac{1}{2} < F < 1. \end{cases} \quad (60)$$

It should be noted that, in the case of $\nu = \frac{1}{2}$ ($N_d = -6$), the complete set of solutions to (19) is also given by (58) with $F = 1/2$ and $n_c = \mp 2$.

Let us compare this with the case of an infinitely thin (pointlike) disclination which was considered in detail in [12–14]. In the latter case several partial Hamiltonian operators are self-adjoint extended, and the deficiency index can be (0,0) (no need for extension, all partial operators are essentially self-adjoint), (1,1) (one partial operator is extended with one parameter), (2,2) (two partial operators are extended with four parameters), etc. In particular, in the case of carbon-like nanocones, there is no need for self-adjoint extension for $N_d = 3, 4, 5$, there is one self-adjoint extension parameter for $N_d = 2, 1, -1, -2, -3, -6$, there are four and more self-adjoint extension parameters for $N_d = -4, -5$ and $N_d \leq -7$. For the deficiency index equal to (1,1), the boundary condition at the location of a pointlike disclination ($r = 0$) takes form

It should be noted that scale invariance is broken (condition (59) depends on r_{\max}) unless $\Theta = \pm\pi/2$ at $F \neq 1/2$ and $F = 1/2$ at arbitrary Θ . Thus condition (60) is the only one that is consistent with scale invariance.

4. Induced ground-state effects

Using the explicit form of modes $f_{n,\pm}$ and $g_{n,\pm}$, satisfying (19) and (51), we can calculate the induced ground-state effects of electronic excitations in carbon-like nanocones. Concerning the R -current component which is orthogonal to the conical surface, j_3^R (26), and the electric current angular component, j_ϕ (35), they vanish due to the cancellation between modes with + and – subscripts. The calculation of the R -current angular component (27) and the pseudomagnetic field strength (28) in the case of $\frac{3}{5} < \nu < 2$ ($0 < F < 1$) and $\nu = \frac{1}{2}$ ($F = 1/2$) yields:

$$j_{\varphi}^R(r) \Big|_{F < \frac{1}{2}, \theta \neq \frac{\pi}{2}} = -\frac{v}{(2\pi)^2} \frac{1}{r} \left\{ \int_0^{\infty} \frac{du}{\cosh^2(u/2)} \frac{\sin(F\pi) \cosh \left[\left(F + v - \frac{1}{2} \right) u \right] - \sin[(F+v)\pi] \cosh \left[\left(F - \frac{1}{2} \right) u \right]}{\cosh(vu) - \cos(v\pi)} + \right. \\ \left. + 8 \int_0^{\infty} dw w \left[\sum_{l=0}^{\infty} C_{vl+1-F}^{(\wedge)} \left(w \frac{r_0}{r} \right) K_{vl+1-F}(w) K_{vl-F}(w) - \sum_{l=1}^{\infty} C_{vl+F}^{(\vee)} \left(w \frac{r_0}{r} \right) K_{vl+F}(w) K_{vl-1+F}(w) \right] \right\}, \quad (61)$$

$$j_{\varphi}^R(r) \Big|_{F > \frac{1}{2}, \theta \neq \frac{\pi}{2}} = \frac{v}{(2\pi)^2} \frac{1}{r} \left\{ \int_0^{\infty} \frac{du}{\cosh^2(u/2)} \frac{\sin(F\pi) \cosh \left[\left(F - v - \frac{1}{2} \right) u \right] - \sin[(F-v)\pi] \cosh \left[\left(F - \frac{1}{2} \right) u \right]}{\cosh(vu) - \cos(v\pi)} - \right. \\ \left. - 8 \int_0^{\infty} dw w \left[\sum_{l=1}^{\infty} C_{vl+1-F}^{(\wedge)} \left(w \frac{r_0}{r} \right) K_{vl+1-F}(w) K_{vl-F}(w) - \sum_{l=0}^{\infty} C_{vl+F}^{(\vee)} \left(w \frac{r_0}{r} \right) K_{vl+F}(w) K_{vl-1+F}(w) \right] \right\}, \quad (62)$$

$$j_{\varphi}^R(r) \Big|_{F \neq \frac{1}{2}, \theta = \pm \frac{\pi}{2}} = \mp \frac{v}{2(2\pi)^2} \frac{1}{r} \left\{ \int_0^{\infty} \frac{du}{\cosh^2(u/2)} \frac{\sin(F\pi) \cosh \left[\left(F - \frac{1}{2} \pm v \right) u \right] - \sin[(F \pm v)\pi] \cosh \left[\left(F - \frac{1}{2} \right) u \right]}{\cosh(vu) - \cos(v\pi)} + \right. \\ \left. + 8 \int_0^{\infty} dw w \left[\frac{I_{\frac{1}{2} \mp (F - \frac{1}{2})} \left(w \frac{r_0}{r} \right)}{K_{\frac{1}{2} \mp (F - \frac{1}{2})} \left(w \frac{r_0}{r} \right)} K_F(w) K_{1-F}(w) + \right. \right. \\ \left. \left. + \sum_{l=1}^{\infty} \left(\frac{I_{vl-F + \frac{1}{2} \pm \frac{1}{2}} \left(w \frac{r_0}{r} \right)}{K_{vl-F + \frac{1}{2} \pm \frac{1}{2}} \left(w \frac{r_0}{r} \right)} K_{vl+1-F}(w) K_{vl-F}(w) + \frac{I_{vl+F - \frac{1}{2} \mp \frac{1}{2}} \left(w \frac{r_0}{r} \right)}{K_{vl+F - \frac{1}{2} \mp \frac{1}{2}} \left(w \frac{r_0}{r} \right)} K_{vl+F}(w) K_{vl-1+F}(w) \right) \right] \right\}, \quad (63)$$

$$j_{\varphi}^R(r) \Big|_{F = \frac{1}{2}} = -\frac{v \sin \theta}{2\pi^2} \left[\frac{1}{r - r_0} + \frac{8}{r} \int_0^{\infty} dw w \sum_{l=1}^{\infty} \tilde{C}_{vl + \frac{1}{2}} \left(w \frac{r_0}{r} \right) K_{vl + \frac{1}{2}}(w) K_{vl - \frac{1}{2}}(w) \right], \quad (64)$$

$$B_3^R(r) \Big|_{F < \frac{1}{2}, \theta \neq \frac{\pi}{2}} = -\frac{v}{(2\pi)^2} \frac{1}{r} \left\{ \int_0^{\infty} \frac{du}{\cosh^2(u/2)} \frac{\sin(F\pi) \cosh \left[\left(F + v - \frac{1}{2} \right) u \right] - \sin[(F+v)\pi] \cosh \left[\left(F - \frac{1}{2} \right) u \right]}{\cosh(vu) - \cos(v\pi)} + \right. \\ \left. + 8r \int_r^{r_{\max}} \frac{dr'}{r'^2} \int_0^{\infty} dw w \left[\sum_{l=0}^{\infty} C_{vl+1-F}^{(\wedge)} \left(w \frac{r_0}{r'} \right) K_{vl+1-F}(w) K_{vl-F}(w) - \sum_{l=1}^{\infty} C_{vl+F}^{(\vee)} \left(w \frac{r_0}{r'} \right) K_{vl+F}(w) K_{vl-1+F}(w) \right] \right\}, \quad (65)$$

$$B_3^R(r) \Big|_{F > \frac{1}{2}, \theta \neq \frac{\pi}{2}} = \frac{v}{(2\pi)^2} \frac{1}{r} \left\{ \int_0^{\infty} \frac{du}{\cosh^2(u/2)} \frac{\sin(F\pi) \cosh \left[\left(F - v - \frac{1}{2} \right) u \right] - \sin[(F-v)\pi] \cosh \left[\left(F - \frac{1}{2} \right) u \right]}{\cosh(vu) - \cos(v\pi)} - \right. \\ \left. - 8r \int_r^{r_{\max}} \frac{dr'}{r'^2} \int_0^{\infty} dw w \left[\sum_{l=1}^{\infty} C_{vl+1-F}^{(\wedge)} \left(w \frac{r_0}{r'} \right) K_{vl+1-F}(w) K_{vl-F}(w) - \sum_{l=0}^{\infty} C_{vl+F}^{(\vee)} \left(w \frac{r_0}{r'} \right) K_{vl+F}(w) K_{vl-1+F}(w) \right] \right\}, \quad (66)$$

$$\begin{aligned}
 B_3^R(r) \Big|_{F \neq \frac{1}{2}, \theta = \pm \frac{\pi}{2}} = & \mp \frac{\nu}{(2\pi)^2} \frac{1}{r} \left\{ \int_0^\infty \frac{du}{\cosh^2(u/2)} \frac{\sin(F\pi) \cosh \left[\left(F - \frac{1}{2} \pm \nu \right) u \right] - \sin[(F \pm \nu)\pi] \cosh \left[\left(F - \frac{1}{2} \right) u \right]}{\cosh(\nu u) - \cos(\nu\pi)} + \right. \\
 & + 8r \int_r^{r_{\max}} \frac{dr'}{r'^2} \int_0^\infty dw w \left[\frac{I_{\frac{1}{2} \mp (F - \frac{1}{2})} \left(w \frac{r_0}{r'} \right)}{K_{\frac{1}{2} \mp (F - \frac{1}{2})} \left(w \frac{r_0}{r'} \right)} K_F(w) K_{1-F}(w) + \right. \\
 & \left. \left. + \sum_{l=1}^\infty \left(\frac{I_{\nu l - F + \frac{1}{2} \pm \frac{1}{2}} \left(w \frac{r_0}{r'} \right)}{K_{\nu l - F + \frac{1}{2} \pm \frac{1}{2}} \left(w \frac{r_0}{r'} \right)} K_{\nu l + 1 - F}(w) K_{\nu l - F}(w) + \frac{I_{\nu l + F - \frac{1}{2} \mp \frac{1}{2}} \left(w \frac{r_0}{r'} \right)}{K_{\nu l + F - \frac{1}{2} \mp \frac{1}{2}} \left(w \frac{r_0}{r'} \right)} K_{\nu l + F}(w) K_{\nu l - 1 + F}(w) \right) \right] \right\} \quad (67)
 \end{aligned}$$

and

$$B_3^R(r) \Big|_{F = \frac{1}{2}} = \frac{\nu \sin \theta}{2\pi^2} \left[\frac{1}{r_0} \ln \left(1 - \frac{r_0}{r} \right) - 8 \int_r^{r_{\max}} \frac{dr'}{r'^2} \int_0^\infty dw w \sum_{l=1}^\infty \tilde{C}_{\nu l + \frac{1}{2}} \left(w \frac{r_0}{r'} \right) K_{\nu l + \frac{1}{2}}(w) K_{\nu l - \frac{1}{2}}(w) \right], \quad (68)$$

where

$$C_\rho^{(\wedge)}(y) = \left\{ I_\rho(y) K_\rho(y) \tan \left(\frac{\theta}{2} + \frac{\pi}{4} \right) - I_{\rho-1}(y) K_{\rho-1}(y) \cot \left(\frac{\theta}{2} + \frac{\pi}{4} \right) \right\} \times \left[K_\rho^2(y) \tan \left(\frac{\theta}{2} + \frac{\pi}{4} \right) + K_{\rho-1}^2(y) \cot \left(\frac{\theta}{2} + \frac{\pi}{4} \right) \right]^{-1}, \quad (69)$$

$$C_\rho^{(\vee)}(y) = \left\{ I_\rho(y) K_\rho(y) \cot \left(\frac{\theta}{2} + \frac{\pi}{4} \right) - I_{\rho-1}(y) K_{\rho-1}(y) \tan \left(\frac{\theta}{2} + \frac{\pi}{4} \right) \right\} \left[K_\rho^2(y) \cot \left(\frac{\theta}{2} + \frac{\pi}{4} \right) + K_{\rho-1}^2(y) \tan \left(\frac{\theta}{2} + \frac{\pi}{4} \right) \right]^{-1} \quad (70)$$

and

$$\tilde{C}_{\nu l + \frac{1}{2}}(y) = \frac{2}{y} \frac{K_{\nu l + \frac{1}{2}}(y) K_{\nu l - \frac{1}{2}}(y)}{\cos^2 \theta \left[K_{\nu l + \frac{1}{2}}^2(y) + K_{\nu l - \frac{1}{2}}^2(y) \right]^2 + 4 \sin^2 \theta K_{\nu l + \frac{1}{2}}^2(y) K_{\nu l - \frac{1}{2}}^2(y)}; \quad (71)$$

$I_\lambda(y)$ and $K_\lambda(y)$ are the modified Bessel functions with the exponential increase and decrease, respectively, at large real positive values of their argument.

In the case of $2 \leq \nu < 7$ ($F = \nu - 1$) we obtain

$$\begin{aligned}
 j_\Phi^R(r) = & -\frac{\nu}{(2\pi)^2} \frac{1}{r} \left\{ \frac{2\pi}{\nu} \sum_{p=1}^{\lfloor \nu/2 \rfloor} \frac{\sin(3p\pi/\nu)}{\sin^2(p\pi/\nu)} - \frac{\pi}{\nu} \delta_{\nu, 2N} + \sin(\nu\pi) \int_0^\infty \frac{du}{\cosh^2(u/2)} \times \right. \\
 & \times \frac{\cosh \left(\frac{3}{2} u \right)}{\cosh(\nu u) - \cos(\nu\pi)} + 8 \int_0^\infty dw w \left[\sum_{l=1}^\infty C_{\nu(l-1)+2}^{(\wedge)} \left(w \frac{r_0}{r} \right) K_{\nu(l-1)+2}(w) K_{\nu(l-1)+1}(w) - \sum_{l=0}^\infty C_{\nu(l+1)-1}^{(\vee)} \left(w \frac{r_0}{r} \right) K_{\nu(l+1)-1}(w) K_{\nu(l+1)-2}(w) \right] \Big\} \quad (72)
 \end{aligned}$$

and

$$\begin{aligned}
 B_3^R(r) = & -\frac{\nu}{(2\pi)^2} \frac{1}{r} \left\{ \frac{2\pi}{\nu} \sum_{p=1}^{\lfloor \nu/2 \rfloor} \frac{\sin(3p\pi/\nu)}{\sin^2(p\pi/\nu)} - \frac{\pi}{\nu} \delta_{\nu, 2N} + \sin(\nu\pi) \int_0^\infty \frac{du}{\cosh^2(u/2)} \times \right. \\
 & \times \frac{\cosh \left(\frac{3}{2} u \right)}{\cosh(\nu u) - \cos(\nu\pi)} + 8r \int_r^{r_{\max}} \frac{dr'}{r'^2} \int_0^\infty dw w \left[\sum_{l=1}^\infty C_{\nu(l-1)+2}^{(\wedge)} \left(w \frac{r_0}{r'} \right) K_{\nu(l-1)+2}(w) K_{\nu(l-1)+1}(w) - \right. \\
 & \left. \left. - \sum_{l=0}^\infty C_{\nu(l+1)-1}^{(\vee)} \left(w \frac{r_0}{r'} \right) K_{\nu(l+1)-1}(w) K_{\nu(l+1)-2}(w) \right] \right\}, \quad (73)
 \end{aligned}$$

where $[|u|]$ is the integer part of quantity u (i.e., the integer which is less than or equal to u), p and N denote positive integers, $\delta_{\omega, \omega'}$ is the Kronecker symbol ($\delta_{\omega, \omega'} = 0$ at $\omega' \neq \omega$ and $\delta_{\omega, \omega} = 1$).

It should be noted that the integral over the w variable in (61)–(64) and (72) vanishes in the limit of $r_0 \rightarrow 0$. Moreover, in the limit of $r \rightarrow \infty$, it decreases as $(r_0/r)^{2\lambda}$, where

$$\lambda = 1 - F, \quad \frac{3}{5} < \nu < 2, \quad \left\{ \begin{array}{l} 0 < F < \frac{1}{2}, \quad \theta \neq -\frac{\pi}{2} \\ \frac{1}{2} < F < 1, \quad \theta = \frac{\pi}{2} \end{array} \right\}, \quad (74)$$

$$\lambda = F, \quad \frac{3}{5} < \nu < 2, \quad \left\{ \begin{array}{l} \frac{1}{2} < F < 1, \quad \theta \neq \frac{\pi}{2} \\ 0 < F < \frac{1}{2}, \quad \theta = -\frac{\pi}{2} \end{array} \right\}, \quad (75)$$

$$\left\{ \begin{array}{l} \lambda = \nu + \frac{1}{2}, \quad \theta \neq \pm \frac{\pi}{2} \\ \lambda = \nu - \frac{1}{2}, \quad \theta = \pm \frac{\pi}{2} \end{array} \right\}, \quad \frac{3}{5} < \nu < 2, \quad F = \frac{1}{2}, \quad (76)$$

$$\left\{ \begin{array}{l} \lambda = 1, \quad \theta \neq \pm \frac{\pi}{2} \\ \lambda = \frac{1}{2} \ln \ln(r/r_0), \quad \theta = \pm \frac{\pi}{2} \end{array} \right\}, \quad \nu = \frac{1}{2}, \quad F = \frac{1}{2}, \quad (77)$$

$$\left\{ \begin{array}{l} \lambda = \frac{\ln \ln(r/r_0)}{2 \ln(r/r_0)}, \quad \nu = 2 \\ \lambda = \nu - 2, \quad 2 < \nu < 7 \end{array} \right\}, \quad F = \nu - 1. \quad (78)$$

The latter circumstance has far-reaching consequences, when we turn to the total flux of the induced ground-state pseudomagnetic field strength, see (29). Namely, the contribution of the w -integral to Φ_1^R is damped and the field strength is proportional to the current in the physically sensible case, i.e. at $r_{\max} \gg r_0$:

$$j_\varphi^R(r) = \frac{\nu \Phi_1^R}{2\pi r_{\max}} \frac{1}{r}, \quad B_3^R(r) = \frac{\nu \Phi_1^R}{2\pi r_{\max}} \frac{1}{r}, \quad (79)$$

where

$$\begin{aligned} \Phi_1^R \Big|_{0 < F < \frac{1}{2}, \theta \neq -\frac{\pi}{2}} &= \Phi_1^R \Big|_{\frac{1}{2} < F < 1, \theta = \frac{\pi}{2}} = -\frac{1}{2\pi} r_{\max} \int_0^\infty \frac{du}{\cosh^2(u/2)} \times \\ &\times \frac{\sin(F\pi) \cosh\left[\left(F + \nu - \frac{1}{2}\right)u\right] - \sin[(F + \nu)\pi] \cosh\left[\left(F - \frac{1}{2}\right)u\right]}{\cosh(\nu u) - \cos(\nu\pi)}, \quad \frac{3}{5} < \nu < 2, \end{aligned} \quad (80)$$

$$\begin{aligned} \Phi_1^R \Big|_{\frac{1}{2} < F < 1, \theta \neq \frac{\pi}{2}} &= \Phi_1^R \Big|_{0 < F < \frac{1}{2}, \theta = -\frac{\pi}{2}} = \frac{1}{2\pi} r_{\max} \int_0^\infty \frac{du}{\cosh^2(u/2)} \times \\ &\times \frac{\sin(F\pi) \cosh\left[\left(F - \nu - \frac{1}{2}\right)u\right] - \sin[(F - \nu)\pi] \cosh\left[\left(F - \frac{1}{2}\right)u\right]}{\cosh(\nu u) - \cos(\nu\pi)}, \quad \frac{3}{5} < \nu < 2, \end{aligned} \quad (81)$$

$$\Phi_1^R \Big|_{F = \frac{1}{2}} = -\frac{\sin \theta}{\pi} r_{\max} \quad (82)$$

and

$$\Phi_1^R \Big|_{F = \nu - 1} = -\frac{1}{2\pi} r_{\max} \left[\frac{2\pi}{\nu} \sum_{p=1}^{[|\nu/2|]} \frac{\sin(3p\pi/\nu)}{\sin^2(p\pi/\nu)} - \frac{\pi}{\nu} \delta_{\nu, 2N} + \sin(\nu\pi) \int_0^\infty \frac{du}{\cosh^2(u/2)} \frac{\cosh\left(\frac{3}{2}u\right)}{\cosh(\nu u) - \cos(\nu\pi)} \right], \quad 2 \leq \nu < 7. \quad (83)$$

The analysis of the induced ground-state electric charge and P -condensate is performed in a similar way. Basing on the acquired experience, the results in the physically sensible case ($r_{\max} \gg r_0$) can be immediately obtained by employing the condition of minimal irregularity, see (60), in the case of a pointlike disclination. Note that in the latter case the contribution of modes (55) and (56) is canceled upon summation over the energy sign, thus

$$q(r) = \rho(r) = 0, \quad F = \nu - 1 \quad (2 \leq \nu < 7). \quad (84)$$

Otherwise, at $0 < F < 1$ ($\frac{3}{5} < \nu < 2$ and $\nu = \frac{1}{2}$), only mode (54) contributes, and the appropriate results for arbitrary Θ were first obtained in [21,22] and later generalized to $\nu \neq 1$ in [12–14]:

$$q(r) = -\frac{ev \sin(F\pi)}{\pi^3 r^2} \times \int_0^\infty dw w \frac{K_F^2(w) - K_{1-F}^2(w)}{\cosh\left[(2F-1)\ln\left(w\frac{r_{\max}}{r}\right) + \ln \tan\left(\frac{\Theta}{2} + \frac{\pi}{4}\right)\right]} \quad (85)$$

and

$$\rho(r) = -\frac{v \sin(F\pi)}{\pi^3 r^2} \times \int_0^\infty dw w \frac{K_F^2(w) + K_{1-F}^2(w)}{\cosh\left[(2F-1)\ln\left(w\frac{r_{\max}}{r}\right) + \ln \tan\left(\frac{\Theta}{2} + \frac{\pi}{4}\right)\right]} \quad (86)$$

By applying (60) to (85) and (86) we obtain

$$q(r) = 0, \quad 0 < F < 1, \quad (87)$$

$$\rho(r) = 0, \quad \left\{ \begin{array}{l} 0 < F < \frac{1}{2} \\ \frac{1}{2} < F < 1 \end{array} \right\} \quad (88)$$

and

$$\rho(r) = -\frac{v \cos \theta}{2\pi^2 r^2}, \quad F = \frac{1}{2}. \quad (89)$$

Thus, the electric charge is not induced at all, while the P -condensate is induced at $F = 1/2$ only, with the total value equal to

$$C|_{F=1/2} = -\frac{\cos \theta}{\pi} \ln(r_{\max} / r_0). \quad (90)$$

Recalling the relation between the P -condensate and the electric current, see (35) and (37), we get that the induced ground-state electric current density is nonvanishing at $F = 1/2$ only, being directed orthogonally to the conical surface:

$$j_3(r)|_{F=1/2} = \frac{v J_3|_{F=1/2}}{2\pi \ln(r_{\max} / r_0)} r^{-2}, \quad (91)$$

where

$$J_3|_{F=1/2} = -ev \frac{\cos \theta}{\pi} \ln(r_{\max} / r_0) \quad (92)$$

is the total electric current. The induced ground-state magnetic field circulating in the angular direction around the apex of the conical surface, see (38), is presented as

$$\begin{aligned} B_\varphi(r)|_{F=1/2} - B_\varphi(r_{\max})|_{F=1/2} &= -\frac{eC|_{F=1/2}}{2\pi \ln(r_{\max} / r_0)} \ln(r_{\max} / r) = \\ &= -\frac{J_3|_{F=1/2}}{2\pi v \ln(r_{\max} / r_0)} \ln(r_{\max} / r) = e \frac{\cos \theta}{2\pi^2} \ln(r_{\max} / r), \end{aligned} \quad (93)$$

where it is plausible to put the constant of integration equal to zero, $B_\varphi(r_{\max})|_{F=1/2} = 0$. Then the total magnetic flux, see (39), is

$$\Phi_I|_{F=1/2} = e \frac{\cos \theta}{2\pi^2} r_{\max}. \quad (94)$$

5. Conclusions

On the basis of the continuum model for long-wavelength charge carriers, originating in the tight-binding approximation for the nearest-neighbour interaction of the lattice atoms, we have studied quantum ground-state effects of electronic excitations in crystalline monolayers warped into nanocones by a disclination; the nonzero size of the disclination at the apex of a nanocone has been taken into account. Our main finding is that the physically sensible limit of the nanocone size exceeding considerably the disclination size fixes a boundary condition at the nanocone apex as the scale invariant one ensuring the minimal irregularity of the modes; consequently, quantum ground-state effects are independent of the disclination size.

Restricting ourselves to the carbon-like nanocones, we have considered all disclinations resulting in the conventional nanocones, $N_d = 1, 2, 3, 4, 5$, and several disclinations resulting in the saddle-like nanocones, $N_d = -1, -2, -3, -6$. As we have proved, the results obtained earlier in [12–14] for the case of a zero-size disclination should be reduced to the case obtained by imposing condition (60). In particular, the ground-state electric charge is not induced at all. As to the local density of states, it is defined as

$$\Delta(\mathbf{x}; E') = \int_{-\infty}^{\infty} \frac{dE|E|}{\pi \hbar^2 v^2} \psi_E^\dagger(\mathbf{x}) \text{Im}(E - E' - i0)^{-1} \psi_E(\mathbf{x}). \quad (95)$$

The density of the induced ground-state electric charge is related to (95) as

$$q(\mathbf{x}) = -\frac{e}{2} \int_{-\infty}^{\infty} dE' \Delta(\mathbf{x}; E') \text{sgn}(E'), \quad (96)$$

and only the odd in E' piece of $\Delta(\mathbf{x}; E')$ contributes to $q(\mathbf{x})$. In the case of planar crystalline monolayer ($v = 1$), one immediately gets

$$\Delta(\mathbf{x}, E') = \frac{|E'|}{\pi \hbar^2 v^2}, \quad (97)$$

and, as follows from the nullification of the charge, disclinations leave relation (97) unchanged; this also follows from expression (55) in [12] for the total density of states (when condition (60) is imposed).

As to the nonvanishing ground-state effects which are induced in carbon-like nanocones, they comprise two sets. One includes the magnetic field circulating in the angular direction around the nanocone apex, the electric current directed orthogonally to the nanocone surface and the parity-breaking condensate. In terms of the sublattice and valley indices, this set corresponds to bilinear form

$$\begin{pmatrix} (I) \\ A \end{pmatrix} \begin{pmatrix} (II) \\ B \end{pmatrix} + \begin{pmatrix} (I) \\ B \end{pmatrix} \begin{pmatrix} (II) \\ A \end{pmatrix}$$

and emerges at $F = 1/2$ only, i.e. at $N_d = \pm 2, -6$. Another set includes the pseudomagnetic field directed orthogonally to the nanocone surface and the R -current circulating in the angular direction around the nanocone apex. In terms of the sublattice and valley indices, this set corresponds to bilinear form

$$\begin{pmatrix} (I) \\ A \end{pmatrix} \begin{pmatrix} (II) \\ A \end{pmatrix} - \begin{pmatrix} (I) \\ B \end{pmatrix} \begin{pmatrix} (II) \\ B \end{pmatrix}$$

and emerges in all considered cases except $v = 3$, i.e. $N_d = 4$. We summarize our results by presenting expressions for the total magnetic and pseudomagnetic fluxes Φ_I and Φ_I^R :

$$\Phi_I^R \Big|_{\theta \neq -\frac{\pi}{2}} = -\frac{1}{2\pi} r_{\max} \int_0^\infty \frac{du}{\cosh^2(u/2)} \frac{\sin\left(\frac{1}{5}\pi\right) \cosh\left(\frac{9}{10}u\right) - \sin\left(\frac{7}{5}\pi\right) \cosh\left(\frac{3}{10}u\right)}{\cosh\left(\frac{6}{5}u\right) - \cos\left(\frac{6}{5}\pi\right)}, \quad N_d = 1, \quad (98)$$

$$\Phi_I^R \Big|_{\theta = -\frac{\pi}{2}} = \frac{1}{2\pi} r_{\max} \sin\left(\frac{1}{5}\pi\right) \int_0^\infty \frac{du}{\cosh^2(u/2)} \frac{\cosh\left(\frac{3}{2}u\right)}{\cosh\left(\frac{6}{5}u\right) - \cos\left(\frac{6}{5}\pi\right)}, \quad N_d = 1, \quad (99)$$

$$\Phi_I^R \Big|_{\theta \neq \frac{\pi}{2}} = \frac{1}{2\pi} r_{\max} \int_0^\infty \frac{du}{\cosh^2(u/2)} \frac{\sin\left(\frac{5}{7}\pi\right) \cosh\left(\frac{9}{14}u\right) + \sin\left(\frac{1}{7}\pi\right) \cosh\left(\frac{3}{14}u\right)}{\cosh\left(\frac{6}{7}u\right) - \cos\left(\frac{6}{7}\pi\right)}, \quad N_d = -1, \quad (100)$$

$$\Phi_I^R \Big|_{\theta = \frac{\pi}{2}} = -\frac{1}{2\pi} r_{\max} \int_0^\infty \frac{du}{\cosh^2(u/2)} \frac{\sin\left(\frac{5}{7}\pi\right) \cosh\left(\frac{15}{14}u\right) - \sin\left(\frac{11}{7}\pi\right) \cosh\left(\frac{3}{14}u\right)}{\cosh\left(\frac{6}{7}u\right) - \cos\left(\frac{6}{7}\pi\right)}, \quad N_d = -1, \quad (101)$$

$$\Phi_I = e \frac{\cos \theta}{2\pi^2} r_{\max}, \quad \Phi_I^R = -\frac{\sin \theta}{\pi} r_{\max}, \quad N_d = \pm 2, -6, \quad (102)$$

$$\Phi_I^R \Big|_{\theta \neq -\frac{\pi}{2}} = -\frac{\sqrt{3}}{4\pi} r_{\max} \int_0^\infty \frac{du}{\cosh(u/2)} \frac{1}{\cosh\left(\frac{2}{3}u\right) - \cos\left(\frac{2}{3}\pi\right)}, \quad N_d = -3, \quad (103)$$

$$\Phi_I^R \Big|_{\theta = -\frac{\pi}{2}} = \frac{\sqrt{3}}{4\pi} r_{\max} \int_0^\infty \frac{du}{\cosh^2(u/2)} \frac{\cosh\left(\frac{5}{6}u\right) + \cosh\left(\frac{1}{6}u\right)}{\cosh\left(\frac{2}{3}u\right) - \cos\left(\frac{2}{3}\pi\right)}, \quad N_d = -3, \quad (104)$$

$$\Phi_I^R = \frac{1}{4} r_{\max}, \quad N_d = 3, \quad (105)$$

$$\Phi_I^R = -\frac{7}{12} r_{\max}, \quad N_d = 5. \quad (106)$$

We conclude that the induced ground-state effects change drastically as N_d changes. The effects are absent in the case of the four-heptagonal defect ($N_d = 4$), whereas they appear of opposite signs as a heptagon is removed from ($N_d = 3$) or added to ($N_d = 5$) this defect, see (105) and (106). These cases are independent of the boundary parameter, θ ; note that namely these cases correspond to that situation with the zero-size defect when there is no need for self-adjoint extension (the deficiency index is (0,0)). In all other cases the results depend on θ . The most distinct depend-

ence is characteristic for the cases of two-pentagonal, two- and six-heptagonal defects, when the results coincide, see (102). In the cases of one-pentagonal, one- and three-heptagonal defects, the results are almost independent of θ unless $\theta = -\frac{\pi}{2}$ for $N_d = 1, -3$ and $\theta = \frac{\pi}{2}$ for $N_d = -1$, see (98)–(101), (103) and (104).

Effective magnetic and pseudomagnetic fields which appear in corrugated crystalline monolayers produce strains and scattering of electronic excitations in a sample [23]. As

follows from our consideration, the ground-state magnetic and pseudomagnetic fields can be induced in the locally flat regions out of disclinations, and this may have observable consequences in experimental measurements, likely with the use of scanning tunnel and transmission electron microscopy.

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Властивості основного стану електронних збуджень у вуглецевоподібних наноконусах

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На основі континуальної моделі для довгохвильових зарядових носіїв, що побудована в наближенні сильного зв'язку у взаємодії найближчих сусідніх атомів кристалічної ґратки, розглянуто квантові ефекти основного стану електронних збуджень в діракових матеріалах із двовимірними одношаровими сотовими структурами, скрученими дисклинацією у наноконуси; враховується ненульовий розмір дисклинації, а гранична умова на краю дисклинації вибирається такою, що забезпечує самосполучення гамільтонова оператора Дірака–Вейля. Показано, що квантові ефекти основного стану не залежать від розміру дисклинації, та знайдено обставини, коли вони не залежать від параметра граничної умови. Показано, що в основному стані індукуються магнітний потік, котрий циркулює в кутовому напрямку навколо вершини наноконуса, та псевдомагнітний потік, який спрямований ортогонально до поверхні наноконуса.

Ключові слова: діраківські матеріали, наноконуси, основний стан, квантові ефекти в одношарових кристалах.

Свойства основного состояния электронных возмущений в углеродоподобных наноконусах

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Исходя из континуальной модели для длинноволновых зарядовых носителей, построенной в приближении сильной связи для взаимодействия ближайших соседних атомов в кристаллической решетке, рассмотрены квантовые эффекты основного состояния электронных возмущений в дираковских материалах с двумерными однослойными сотовыми структурами, скрученными дисклинацией в наноконусы; учитывается ненулевой размер дисклинации, а граничное условие на краю дисклинации выбирается так, что обеспечивается самосопряженность гамильтонова оператора Дирака–Вейля. Показано, что квантовые эффекты основного состояния не зависят от размера дисклинации, и найдены обстоятельства, при которых они не зависят от параметра граничного условия. Показано, что в основном состоянии индуцируются магнитный поток, циркулирующий в угловом направлении вокруг вершины наноконуса, и псевдомагнитный поток, направленный ортогонально к поверхности наноконуса.

Ключевые слова: дираковские материалы, наноконусы, основное состояние, квантовые эффекты в однослойных кристаллах.