Fizika Nizkikh Temperatur, 2008, v. 34, No. 10, p. 1049–1057

Vacuum polarization in graphene with a topological defect

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Received January 31, 2008

The influence of a topological defect in graphene on the ground state of electronic quasiparticle excitations is studied in the framework of the long-wavelength continuum model originating in the tight-binding approximation for the nearest neighbour interaction in the graphitic lattice. A topological defect that rolls up a graphitic sheet into a nanocone is represented by a pointlike pseudomagnetic vortex with a flux which is related to the deficit angle of the cone. The method of self-adjoint extensions is employed to define the set of physically acceptable boundary conditions at the apex of the nanocone. The electronic system on a graphitic nanocone is found to acquire the ground state condensate and current of special type, and we determine the dependence of these quantities on the deficit angle of the nanocone, continuous parameter of the boundary condition at the apex, and the distance from the apex.

PACS: **11.10.–z** Field theory;
73.43.Cd Theory and modeling;
73.61.Wp Fullerenes and related materials;
81.05.Uw Carbon, diamond, graphite.

Keywords: graphitic nanocones, Dirac–Weyl equation, self-adjoint extension, ground state polarization.

1. Introduction

Topological phenomena are of great interest and importance because of their universal nature connected with general properties of the space. Topological defects in the quasirelativistic fermionic matter can induce vacuum quantum numbers. A general theory of the vacuum polarization by a pointlike topological defect of the vortex type in two-dimensional quantum systems of massless Dirac fermions was elaborated in Refs. 1,2. In the present paper we apply this theory to the study of the ground state polarization in graphene with a topological defect (see also Refs. 3,4).

Carbon atoms in graphene compose a planar honeycomb lattice with one valence electron per each site. The primitive cell is rhombic and contains two atoms, thus the graphene lattice consists of two rhombic sublattices. The first Brillouin zone is a regular hexagon with corners corresponding to the Fermi points; among six of them, the two oppositely located ones are inequivalent. Electronic quasiparticle excitations in graphene are characterized by a linear and isotropic dispersion relation between the energy and the momentum in the vicinity of the Fermi points, where the valence and conduction bands touch each other. Using the tight-binding approximation for the nearest neighbour interaction in the honeycomb lattice, an effective long-wavelength description of electronic states in graphene can be written in terms of a continuum model which is based on the Dirac–Weyl equation for masless electrons in 2 + 1-dimensional space-time with the role of speed of light c played by Fermi velocity $v \approx c/300$ [5–7]. The one-particle Hamiltonian operator of the model takes form

$$H^{(0)} = -i\hbar v (\alpha^1_{(0)}\partial_1 + \alpha^2_{(0)}\partial_2), \qquad (1)$$

where $\alpha^1_{(0)}$ and $\alpha^2_{(0)}$ are the 4×4 matrices belonging to a reducible representation composed as a direct sum of two inequivalent irreducible representations of the Clifford algebra in 2 + 1-dimensional space-time. The one-particle wave function possesses 4 components, which reflects the existence of 2 sublattices and 2 inequivalent Fermi points (valleys).

Unlike the conventional case of spinor electrodynamics in 2 + 1-dimensional space-time (see, e.g., Ref. 8), the parity transformation in the continuum model of graphene implies the inversion of both spatial axes and the exchange of both sublattices and valleys [9],

$$\Psi(vt, x^1, x^2) \to P\Psi(vt, -x^1, -x^2), \qquad (2)$$

where

$$PH^{(0)} = -H^{(0)}P, \; P^2 = I. \qquad (3)$$

The time reversal implies the exchange of valleys [10],

$$\Psi(vt, x^1, x^2) \to T\Psi(-vt, x^1, x^2), \qquad (4)$$

where

$$T(H^{(0)})^* = H^{(0)}T, \quad T^2 = -I. \qquad (5)$$

The matrix of the spatial inversion can be presented as

$$P = 2\Sigma R, \qquad (6)$$

where

$$\Sigma = \frac{1}{2i}\alpha^1_{(0)}\alpha^2_{(0)} \qquad (7)$$

is the pseudospin, and R satisfies commutation relations

$$[R, \alpha^1_{(0)}]_- = [R, \alpha^2_{(0)}]_- = 0 \qquad (8)$$

and exchanges the sublattice indices, as well as the valley indices.

In the second quantization picture, one can consider ground state expectation values:
the P-condensate

$$\rho(x) = \langle \text{vac}|\Psi^+(x)P\Psi(x)|\text{vac}\rangle \qquad (9)$$

and the R-current

$$\mathbf{j}(x) = \langle \text{vac}|\Psi^+(x)\boldsymbol{\alpha}R\Psi(x)|\text{vac}\rangle, \qquad (10)$$

where $x = (vt, x^1, x^2)$, $\boldsymbol{\alpha} = (\alpha^1, \alpha^2)$, and $|\text{vac}\rangle$ denotes the ground state (vacuum). Evidently, quantities (9) and (10) are vanishing in the case of Hamiltonian given by $H^{(0)}$ (1), which corresponds to the idealized strictly planar graphene with all interactions neglected. In reality, the layers of graphene are corrugated at mesoscopic scales [11–13], and namely the effects of curvature in graphene samples are addressed in the present paper. Therefore, our starting point is the ground state expectation value of the time-ordered product of fermion fields in the form

$$\langle \text{vac}|T\Psi(x)\overline{\Psi}(y)|\text{vac}\rangle = \langle x|(\hbar v\gamma^\mu\nabla_\mu)^{-1}|y\rangle, \qquad (11)$$

where $\overline{\Psi} = \Psi^+\gamma^0$, and ∇_μ $(\mu = 0, 1, 2)$ is the covariant derivative in curved $2+1$-dimensional space-time. Restricting ourselves to static backgrounds ($\nabla_0 = \partial_0$) and using Eq. (11), we get

$$\rho(x) = -i\,\text{tr}\langle x|P(i\hbar v\partial_0 - H)^{-1}|x\rangle \qquad (12)$$

and

$$\mathbf{j}(x) = -i\,\text{tr}\langle x|\boldsymbol{\alpha}R(i\hbar v\partial_0 - H)^{-1}|x\rangle, \qquad (13)$$

where

$$H = -i\hbar v\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} \qquad (14)$$

is the Dirac–Weyl Hamiltonian on a curved surface,

$$[\alpha^j, \alpha^{j'}]_+ = 2g^{jj'}I, \qquad (15)$$

and $g_{jj'}$ is the metric of this surface. Further, using the Wick rotation of the time axis, Eqs. (12) and (13) are recast into the form which exhibits explicitly their time independence,

$$\rho(\mathbf{x}) = -\frac{1}{2}\text{tr}\langle \mathbf{x}|P\,\text{sgn}(H)|\mathbf{x}\rangle \qquad (16)$$

$$\mathbf{j}(\mathbf{x}) = -\frac{1}{2}\text{tr}\langle \mathbf{x}|\boldsymbol{\alpha}R\,\text{sgn}(H)|\mathbf{x}\rangle. \qquad (17)$$

In the present paper we compute the P-condensate and the R-current in graphene with a topological defect.

2. Topological defects

Topological defects in graphene are disclinations in the honeycomb lattice, resulting from the substitution of a hexagon by, say, a pentagon or a heptagon; such a disclination rolls up the graphitic sheet into a cone. More generally, a hexagon is substituted by a polygon with $6 - N_d$ sides, where N_d is an integer which is smaller than 6. Polygons with $N_d > 0$ ($N_d < 0$) induce locally positive (negative) curvature, whereas the graphitic sheet is flat away from the defect, 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,

$$\sin\frac{\delta}{2} = 1 - \frac{N_d}{6},$$

and N_d counts the number of sectors of the value of $\pi/3$ which are removed from the graphitic sheet. If $N_d < 0$, then $-N_d$ counts the number of such sectors which are inserted into the graphitic 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; graphitic 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 [14]. Theory predicts also an infinite series of the saddle-like nanocones with $-N_d$ counting the number of the heptagonal defects which are clustered in their central regions. Saddle-like nanocones serve as an element which is necessary for joining parts of carbon nanotubes of differing radii and for creating Schwarzite [15], a structure appearing in many forms of carbon nanofoam [16]. As it was shown by using molecular-dynamics simulations [17], in the case of $N_d \le -4$, a surface with a polygonal defect is more stable than a similarly shaped surface containing a multiple number of heptagons; a screw dislocation can be presented as the $N_d \to -\infty$ limit of a $6-N_d$-gonal defect.

The metric of a conical surface with a pointlike apex has the form

$$g_{rr} = 1, \; g_{\varphi\varphi} = (1-\eta)^2 r^2, \tag{18}$$

where r and φ are polar coordinates centred at the apex, and $-\infty < \eta < 1$. The intrinsic curvature of the cone possesses a $\delta^2(\mathbf{x})$-singularity at its apex, vanishing at $\mathbf{x} \neq 0$, and parameter η enters the coefficient before this singularity term. Quantity $2\pi\eta$ for $0 < \eta < 1$ is the deficit angle measuring the magnitude of the removed sector, and quantity $-2\pi\eta$ for $-\infty < \eta < 0$ is the proficit angle measuring the magnitude of the inserted sector. In the case of graphitic nanocones, parameter η takes discrete values:

$$\eta = \frac{N_d}{6}. \tag{19}$$

Using Eqs. (15) and (18), one gets

$$\alpha^r = \alpha^1_{(0)}, \quad \alpha^\varphi = (1-\eta)^{-1} r^{-1} \alpha^2_{(0)}, \tag{20}$$

and the Dirac–Weyl Hamiltonian on the cone takes form

$$H = -i\hbar v \{\alpha^1_{(0)}\partial_r + \alpha^2_{(0)} r^{-1}[(1-\eta)^{-1}\partial_\varphi - i\Sigma]\}. \tag{21}$$

The second-quantized fermion field operator is presented as

$$\Psi(x) = \sum_{n\in Z}\int_0^\infty \frac{dE|E|}{\hbar^2 v^2} \exp[-iEx^0(\hbar v)^{-1}]\psi_{En}(\mathbf{x}) a_{En} + $$
$$+ \sum_{n\in Z}\int_{-\infty}^0 \frac{dE|E|}{\hbar^2 v^2} \exp[-iEx^0(\hbar v)^{-1}]\psi_{En}(\mathbf{x}) b^+_{En}, \tag{22}$$

where $\mathbb{Z}$ is the set of integer numbers, a^+_{En} and a_{En} (b^+_{En} and b_{En}) are the fermion (antifermion) creation and destruction operators satisfying anticommutation relations

$$[a_{En}, a^+_{En}]_+ = [b_{En}, b^+_{En}]_+ = \frac{\delta(E-\tilde{E})}{\sqrt{E\tilde{E}}}\delta_{n\tilde{n}}, \tag{23}$$

and $\psi_{En}(\mathbf{x})$ is the solution to the stationary Dirac–Weyl equation

$$H\psi_{En}(\mathbf{x}) = E\psi_{En}(\mathbf{x}). \tag{24}$$

The ground state is defined conventionally as

$$a_{En}|\text{vac}\rangle = b_{En}|\text{vac}\rangle = 0. \tag{25}$$

Solutions to the Dirac–Weyl equation form a complete set and are orthonormalized in a way which is usual for the case of the continuum

$$\int_0^{2\pi} d\varphi \int_0^\infty \delta r \sqrt{g}\, \psi^+_{En}(\mathbf{x})\psi_{\tilde{E}\tilde{n}}(\mathbf{x}) = 2\hbar^2 v^2 \frac{\delta(E-\tilde{E})}{\sqrt{E\tilde{E}}}\delta_{n\tilde{n}}, \tag{26}$$

where $g = \det g_{jj'} = (1-\eta)^2 r^2$, and a factor of 2 in the right hand side of the last relation is due to the existence of two inequivalent Fermi points (valleys).

As it was shown in Ref. 3, the fermion field on a graphitic nanocone obeys the Möbius–strip–type condition:

$$\Psi(vt, r, \varphi + 2\pi) = -\exp(-i3\pi\eta R)\Psi(vt, r, \varphi), \tag{27}$$

where η is given by Eq. (19). Condition (27) in the case of odd N_d involves the exchange of sublattices, as well as valleys. Note that since $R^2 = I$, the exchange is eliminated after double rotation

$$\Psi(vt, r, \varphi + 4\pi) = \cos(N_d\pi)\Psi(vt, r, \varphi); \tag{28}$$

that is why the mention of the Möbius strip seems to be relevant.

By performing a singular gauge transformation (see Ref. 3 for more details), one gets the fermion field obeying usual condition

$$\Psi'(vt, r, \varphi + 2\pi) = -\Psi'(vt, r, \varphi), \tag{29}$$

in the meantime, Hamiltonian (21) is transformed to

$$H' = -i\hbar v\left\{\alpha^1_{(0)}\partial_r + \alpha^2_{(0)} r^{-1}\left[(1-\eta)^{-1}(\partial_\varphi - i\frac{3}{2}\eta R) - i\Sigma\right]\right\}. \tag{30}$$

Thus, a topological defect in graphene is represented by a pseudomagnetic vortex with flux $N_d\pi/2$ through the apex of a cone with deficit angle $N_d\pi/3$. Note that, due to commutation relations

$$[P,R]_- = [P,\Sigma]_- = [T,R]_+ = [T,\Sigma]_+ = 0, \tag{31}$$

discrete symmetries of spatial inversion and time reversal are maintained:

$$PH' = -H'P, \quad T(H')^* = H'T. \tag{32}$$

3. Solution to the Dirac–Weyl equation

Vacuum expectation values are independent of the matrix representation used, therefore a choice of representation is a matter of convenience. As it was already noted, the $\alpha^1_{(0)}$ -and $\alpha^2_{(0)}$-matrices (and, consequently, Σ) are of the block-diagonal form. Since the R-matrix satisfies relation (8), it can be unitarily transformed to the block-diagonal form also:

$$URU^{-1} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad U\boldsymbol{\alpha}_{(0)}U^{-1} = \boldsymbol{\alpha}_{(0)}. \tag{33}$$

Thus Hamiltonian attains the block-diagonal form after this unitary transformation:

$$H'' = UH'U^{-1} = \begin{pmatrix} H_1 & 0 \\ 0 & H_{-1} \end{pmatrix}. \qquad (34)$$

To be more precise, let us assign the definite sublattice and valley indices to components of the initial fermion field in the following way [18]:

$$\Psi = (\Psi_{A+}, \Psi_{B+}, \Psi_{A-}, \Psi_{B-})^T, \qquad (35)$$

where subscripts A and B correspond to two sublattices and subscripts « + » and « − » correspond to two valleys. After performing the singular gauge transformation and the unitary one, we get Ψ'' with components mixing up different sublattices and valleys. The appropriate solution to the Dirac–Weyl equation takes form

$$\psi''_{En} = (\psi_{En,1}, \psi_{En,-1})^T, \qquad (36)$$

where the two-component functions satisfy equations

$$H_s \psi_{En,s} = E\psi_{En,s}, \quad s = \pm 1. \qquad (37)$$

Corresponding to Eq. (35), the $\alpha^1_{(0)}$- and $\alpha^2_{(0)}$-matrices can be chosen in the form

$$\alpha^1_{(0)} = -\begin{pmatrix} \sigma^2 & 0 \\ 0 & \sigma^2 \end{pmatrix}, \quad \alpha^2_{(0)} = \begin{pmatrix} \sigma^1 & 0 \\ 0 & -\sigma^1 \end{pmatrix}, \qquad (38)$$

where σ^1 and σ^2 are the off-diagonal Pauli matrices. Then the matrices of spatial inversion and time reversal in the initial representation take form

$$P = \begin{pmatrix} 0 & \sigma^1 \\ \sigma^1 & 0 \end{pmatrix}, \quad T = i\begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}. \qquad (39)$$

Separating the radial and angular variables in the solution to Eq. (37),

$$\psi_{En,s}(r,\varphi) = \begin{pmatrix} f_{En,s}(r) & \exp[i(n+s/2)\varphi] \\ g_{En,s}(r) & \exp[i(n+s/2)\varphi] \end{pmatrix}, \qquad (40)$$

we get that the radial components satisfy equations

$$\begin{pmatrix} 0 & D^+_{n,s} \\ D_{n,s} & 0 \end{pmatrix}\begin{pmatrix} f_{En,s}(r) \\ g_{En,s}(r) \end{pmatrix} = E\begin{pmatrix} f_{En,s}(r) \\ g_{En,s}(r) \end{pmatrix}, \qquad (41)$$

where

$$\begin{aligned} D_{n,s} &= \hbar v[-\partial_r + r^{-1}(1-\eta)^{-1}(sn-\eta)], \\ D^+_{n,s} &= \hbar v[\partial_r + r^{-1}(1-\eta)^{-1}(sn+1-2\eta)]. \end{aligned} \qquad (42)$$

Let us consider graphitic nanocones with $1 > \eta \geq -1/2$ and $\eta = -1$, and define quantity

$$F = \begin{cases} \left[\frac{1}{2} - \frac{1}{2}\,\mathrm{sgn}(\eta) + \eta\right](1-\eta)^{-1}, & 1 > \eta \geq -\frac{1}{2}\ (\eta \neq 0), \\ \frac{1}{2} & \eta = -1. \end{cases} \qquad (43)$$

A pair of linearly independent solutions to Eq. (41) is written in terms of the cylinder functions. In the case of $1 > \eta > 1/2$ ($N_d = 5, 4, 3$), the condition of regularity at the origin is equivalent to the condition of square integrability at this point, and this selects a physically reasonable solution. Thus, in view of the orthonormality condition (26), the complete set is given by regular modes with $sn > 0$

$$\begin{pmatrix} f_{En,s}(r) \\ g_{En,s}(r) \end{pmatrix} = \frac{1}{2\sqrt{\pi(1-\eta)}}\begin{pmatrix} J_{l(1-\eta)^{-1}-F}(kr) \\ \mathrm{sgn}(E)J_{l(1-\eta)^{-1}+1-F}(kr) \end{pmatrix},$$
$$l = sn, \qquad (44)$$

and regular modes with $sn \leq 0$

$$\begin{pmatrix} f_{En,s}(r) \\ g_{En,s}(r) \end{pmatrix} = \frac{1}{2\sqrt{\pi(1-\eta)}}\begin{pmatrix} J_{l'(1-\eta)^{-1}+F}(kr) \\ -\mathrm{sgn}(E)J_{l'(1-\eta)^{-1}+1-F}(kr) \end{pmatrix},$$
$$l' = -sn, \qquad (45)$$

where $k = |E|(\hbar v)^{-1}$, and $J_\mu(u)$ is the Bessel function of order μ; note that F is integer belonging to range $5 \geq F \geq 1$ in this case.

In the case of $1/2 > \eta > 0$ ($N_d = 2, 1$), $0 > \eta \geq -1/2$ ($N_d = -1, -2, -3$) and $\eta = -1$ ($N_d = -6$), there is a mode, for which the condition of regularity at the origin is not equivalent to the condition of square integrability at this point: both linearly independent solutions for this mode are at once irregular and square integrable at the origin. To be more precise, let us define in this case

$$n_c = \begin{cases} \frac{s}{2}[\mathrm{sgn}(\eta) - 1], & \frac{1}{2} > \eta \geq -\frac{1}{2}\ (\eta \neq 0), \\ -2s & \eta = -1. \end{cases} \qquad (46)$$

Then the complete set of solutions to Eq. (41) is chosen in the following form: regular modes with $sn > sn_c$

$$\begin{pmatrix} f_{En,s}(r) \\ g_{En,s}(r) \end{pmatrix} = \frac{1}{2\sqrt{\pi(1-\eta)}}\begin{pmatrix} J_{l(1-\eta)^{-1}-F}(kr) \\ \mathrm{sgn}(E)J_{l(1-\eta)^{-1}+1-F}(kr) \end{pmatrix},$$
$$l = s(n - n_c), \qquad (47)$$

regular modes with $sn < sn_c$

$$\begin{pmatrix} f_{En,s}(r) \\ g_{En,s}(r) \end{pmatrix} = \frac{1}{2\sqrt{\pi(1-\eta)}}\begin{pmatrix} J_{l'(1-\eta)^{-1}+F}(kr) \\ -\mathrm{sgn}(E)J_{l'(1-\eta)^{-1}-1+F}(kr) \end{pmatrix},$$
$$l' = s(n_c - n), \qquad (48)$$

and an irregular mode

$$\begin{pmatrix} f_{En_c,s}(r) \\ g_{En_c,s}(r) \end{pmatrix} = \frac{1}{2\sqrt{\pi(1-\eta)[1+\sin(2\nu_E)\cos(F\pi)]}} \times$$

$$\times \begin{pmatrix} \sin(\nu_E)J_{-F}(kr) + \cos(\nu_E)J_F(kr) \\ \mathrm{sgn}(E)[\sin(\nu_E)J_{1-F}(kr) - \cos(\nu_E)J_{-1+F}(kr)] \end{pmatrix}, \quad (49)$$

note that F belongs to range $0 < F < 1$ in this case. Thus, the requirement of regularity for all modes is in contradiction with the requirement of completeness for these modes. The problem is to find a condition allowing for irregular at $r \to 0$ behavior of the mode with $n = n_c$, i.e. to fix ν_E in Eq. (49). To solve this problem, first of all one has to recall the result of Ref. 19, stating that for the partial Dirac Hamiltonian to be essentially self-adjoint, it is necessary and sufficient that a non-square-integrable (at $r \to 0$) solution exist. Since such a solution does not exist in the case of $n = n_c$, the appropriate partial Hamiltonian is not essentially self-adjoint. The Weyl-von Neumann theory of self-adjoint operators (see, e.g., Ref. 20) is to be employed in order to consider a possibility of the self-adjoint extension for this operator. It can be shown (see Ref. 3) that the self-adjoint extension exists indeed, and the partial Hamiltonian at $n = n_c$ is defined on the domain of functions obeying condition

$$\frac{\lim\limits_{r\to 0}(rMv/\hbar)^F f_{n_c,s}(r)}{\lim\limits_{r\to 0}(rMv/\hbar)^{1-F} g_{n_c,s}(r)} = -2^{2F-1}\frac{\Gamma(F)}{\Gamma(1-F)}\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right), \quad (50)$$

where $\Gamma(u)$ is the Euler gamma function, M is the parameter of the dimension of mass, and Θ is the self-adjoint extension parameter. Substituting the asymptotics of Eq. (49) at $r \to 0$ into Eq. (50), one gets the relation fixing parameter ν_E,

$$\tan(\nu_E) = \mathrm{sgn}(E)\left(\frac{\hbar k}{Mv}\right)^{2F-1}\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right). \quad (51)$$

In the case of graphitic nanocones with $-1/2 > \eta > -1$ ($N_d = -4, -5$) and $\eta < -1$ ($N_d < -6$), there are more than one irregular modes; this case will be considered elsewhere.

4. Condensate

It is instructive to rewrite Eq. (16) as

$$\rho(\mathbf{x}) = \boldsymbol{\nabla}\cdot\mathbf{i}(\mathbf{x}), \quad (52)$$

where

$$\mathbf{i}(\mathbf{x}) = -\frac{i}{4}\hbar v\,\mathrm{tr}\langle\mathbf{x}|\boldsymbol{\alpha}P|H|^{-1}|\mathbf{x}\rangle. \quad (53)$$

Although the trace of $\boldsymbol{\alpha}P$ is formally zero, it may appear that current $\mathbf{i}$ is nonvanishing; then its nonconservation results in the emergence of condensate ρ.

The contribution of regular modes is canceled upon summation over the sign of energy; thus, current (53) is vanishing in the case of $1 > \eta \geq 1/2$, and we are left with the cases of $1/2 > \eta > 0$, $0 > \eta \geq -1/2$, and $\eta = -1$, when an irregular mode appears. Summing over $s = \pm 1$ corresponds to summing contributions of the inequivalent irreducible representations. These contributions are canceled for angular component $i^{\varphi}(\mathbf{x}) = -(i/4)\hbar v\,\mathrm{tr}\,\langle\mathbf{x}|\alpha^{\varphi}P|H|^{-1}|\mathbf{x}\rangle$ and doubled for radial component $i^{r}(\mathbf{x}) = -(i/4)\hbar v\,\mathrm{tr}\,\langle\mathbf{x}|\alpha^{r}P|H|^{-1}|\mathbf{x}\rangle$. Consequently, we get

$$i^r(\mathbf{x}) = -\frac{1}{4\pi(1-\eta)}\int_0^\infty dk\left\{\left(\frac{\hbar k}{Mv}\right)^{2F-1}\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)[L_{(+)}+L_{(-)}]J_{-F}(kr)J_{1-F}(kr) + \right.$$
$$\left. + [L_{(+)}-L_{(-)}][J_F(kr)J_{1-F}(kr) - J_{-F}(kr)J_{-1+F}(kr)] - \left(\frac{\hbar k}{Mv}\right)^{1-2F}\cot\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)[L_{(+)}+L_{(-)}]J_F(kr)J_{-1+F}(kr)\right\}, \quad (54)$$

where

$$L_{(\pm)} = \left[\pm\left(\frac{\hbar k}{Mv}\right)^{2F-1}\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right) + 2\cos(F\pi) \pm \left(\frac{\hbar k}{Mv}\right)^{1-2F}\cot\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)\right]^{-1}. \quad (55)$$

Extending the integrand in Eq. (54) to the complex k-plane, using the Cauchy theorem to deform the contour of integration (for more details see Ref. 2), and introducing the dimensionless integration variable, we recast Eq. (54) into the form

$$i^r(\mathbf{x}) = \frac{\sin(F\pi)}{\pi^3(1-\eta)r^2}\int_0^\infty dw \frac{K_F(w)K_{1-F}(w)}{\cosh\left[(2F-1)\ln\left(\frac{\hbar w}{rMv}\right)+\ln\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)\right]}, \tag{56}$$

where $K_\mu(u)$ is the Macdonald function of order μ. Since in our case $\nabla\cdot\mathbf{i} = r^{-1}\partial_r r i^r$, by differentiating Eq. (56) we get the following expression for the vacuum condensate:

$$\rho(\mathbf{x}) = -\frac{\sin(F\pi)}{\pi^3(1-\eta)r^2}\int_0^\infty dw\, w \frac{K_F^2(w)+K_{1-F}^2(w)}{\cosh\left[(2F-1)\ln\left(\frac{\hbar w}{rMv}\right)+\ln\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)\right]}. \tag{57}$$

Evidently, Eq. (57) vanishes at $\cos\Theta = 0$, while at $F = 1/2$ it is simplified,

$$\rho(\mathbf{x})\big|_{F=\frac{1}{2}} = -\frac{\cos\Theta}{2\pi^2(1-\eta)r^2}. \tag{58}$$

If $\cos\Theta \neq 0$ and $F \neq 1/2$, then at large distances from the defect we get

$$\rho(\mathbf{x})_{r\to\infty} = -\frac{\sin(F\pi)}{\pi^2(1-\eta)r^2}\begin{cases}\left(\frac{rMv}{\hbar}\right)^{2F-1}\frac{\Gamma\left(\frac{3}{2}-F\right)\Gamma\left(\frac{3}{2}-2F\right)}{\Gamma(1-F)}\cot\left(\frac{\Theta}{2}+\frac{\pi}{4}\right), & 0<F<\frac{1}{2},\\[2ex] \left(\frac{rMv}{\hbar}\right)^{1-2F}\frac{\Gamma\left(F+\frac{1}{2}\right)\Gamma\left(2F-\frac{1}{2}\right)}{\Gamma(F)}\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right), & \frac{1}{2}<F<1,\end{cases} \tag{59}$$

5. Current

It is straightforward to conclude that the radial component, $j^r(\mathbf{x}) = -(1/2)\mathrm{tr}\,\langle\mathbf{x}|\alpha^r R\,\mathrm{sgn}(H)|\,\mathbf{x}\rangle$, is vanishing, so it remains to consider the angular component, $j^\varphi(\mathbf{x}) = -(1/2)\mathrm{tr}\langle\mathbf{x}|\alpha^\varphi R\,\mathrm{sgn}(H)|\,\mathbf{x}\rangle$. The contribution of irregular mode (49) to this quantity is

$$\sqrt{g}\, j^\varphi_{\mathrm{irreg}}(\mathbf{x}) = -\frac{1}{4\pi(1-\eta)}\int_0^\infty dk k\left\{\left(\frac{\hbar k}{Mv}\right)^{2F-1}\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)[L_{(+)}-L_{(-)}]J_{-F}(kr)J_{1-F}(kr)+[L_{(+)}+L_{(-)}]\times\right.$$
$$\left.[J_F(kr)J_{1-F}(kr)-J_{-F}(kr)J_{-1+F}(kr)]-\left(\frac{\hbar k}{Mv}\right)^{1-2F}\cot\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)[L_{(+)}-L_{(-)}]J_F(kr)J_{-1+F}(kr)\right\}, \tag{60}$$

where $L_{(\pm)}$ is given by Eq. (55). Similarly as in the previous section, we get

$$\sqrt{g} j^\varphi_{\mathrm{irreg}}(\mathbf{x}) = -\frac{1}{\pi^2(1-\eta)r^2}\int_0^\infty dw\, w\left\{I_F(w)K_{1-F}(w) - I_{1-F}(w)K_F(w) + \right.$$
$$\left.+\frac{2\sin(F\pi)}{\pi}K_F(w)K_{1-F}(w)\tanh\left[(2F-1)\ln\left(\frac{\hbar w}{rMv}\right)+\ln\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)\right]\right\}, \tag{61}$$

where $I_\mu(u)$ is the modified Bessel function of order μ. The contribution of regular modes (47) and (48) is

$$\sqrt{g} j^\varphi_{\mathrm{reg}}(\mathbf{x}) = -\frac{1}{\pi(1-\eta)}\int_0^\infty dk\, k\left[\sum_{l=1}^\infty J_{l(1-\eta)^{-1}-F}(kr)J_{l(1-\eta)^{-1}+1-F}(kr) - \sum_{l'=1}^\infty J_{l'(1-\eta)^{-1}+F}(kr)J_{l'(1-\eta)^{-1}-1+F}(kr)\right]. \tag{62}$$

Performing the summation (details will be published elsewhere), we get

$$\sqrt{g}\, j^{\varphi}_{\rm reg}(\mathbf{x}) = \frac{1}{\pi(1-\eta)r^2}\left\{G(\eta,F) + \frac{1}{2}\left(F-\frac{1}{2}\right)\tan(F\pi) + \frac{1}{\pi}\int_0^\infty dw\, w\,[I_F(w)K_{1-F}(w) - I_{1-F}(w)K_F(w)]\right\}, \tag{63}$$

where

$$G(\eta,F) = \frac{1}{4\pi}\int_0^\infty du\, \frac{\sin(F\pi)\cosh\left[\left(\frac{1}{1-\eta}+\frac{1}{2}-F\right)u\right] + \sin\left[\left(\frac{1}{1-\eta}-F\right)\pi\right]\cosh\left[\left(F-\frac{1}{2}\right)u\right]}{\cosh^2\left(\frac{u}{2}\right)\left[\cosh\left(\frac{u}{1-\eta}\right) - \left(\cos\frac{\pi}{1-\eta}\right)\right]}. \tag{64}$$

Thus we get the following expression for the vacuum current:

$$\sqrt{g}\, j^{\varphi}(\mathbf{x}) = \frac{1}{\pi(1-\eta)r^2}\left\{G(\eta,F) + \frac{1}{2}\left(F-\frac{1}{2}\right)\tan(F\pi) - \frac{2\sin(F\pi)}{\pi^2}\right.$$

$$\left.\times\int_0^\infty dw\, wK_F(w)K_{1-F}(w)\tanh\left[(2F-1)\ln\left(\frac{\hbar w}{rMv}\right) + \ln\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)\right]\right\}. \tag{65}$$

At $\cos\Theta = 0$ we get

$$\sqrt{g}\, j^{\varphi}(\mathbf{x}) = \frac{1}{\pi(1-\eta)r^2}\left[G(\eta,F) + \frac{1}{2}(1\pm 1)\left(F-\frac{1}{2}\right)\tan(F\pi)\right],\quad \Theta = \pm\frac{\pi}{2}(\mathrm{mod}\,2\pi). \tag{66}$$

Also Eq. (65) at $F = \frac{1}{2}$ is simplified,

$$\sqrt{g}\, j^{\varphi}(\mathbf{x})\Big|_{F=\frac{1}{2}} = -\frac{\sin\Theta}{2\pi^2(1-\eta)r^2}. \tag{67}$$

If $\cos\Theta \neq 0$ and $F \neq 1/2$, then at large distances from the defect we get

$$\sqrt{g}\, j^{\varphi}(\mathbf{x})_{r\to\infty} = \frac{1}{\pi(1-\eta)r^2}\left[G(\eta,F) + \frac{1}{2}\left(F-\frac{1}{2}-\left|F-\frac{1}{2}\right|\right)\tan(F\pi)\right]. \tag{68}$$

In the case of $1 > \eta \geq 1/2$ ($N_d = 5, 4, 3$), the vacuum current takes form

$$\sqrt{g}\, j^{\varphi}(\mathbf{x}) = -\frac{1}{\pi(1-\eta)}\int_0^\infty dk\, k\left[\sum_{l=1}^{\infty} J_{l(1-\eta)^{-1}-F}(kr)J_{l(1-\eta)^{-1}+1-F}(kr) - \sum_{l'=0}^{\infty} J_{l'(1-\eta)^{-1}+F}(kr)J_{l'(1-\eta)^{-1}-1+F}(kr)\right]. \tag{69}$$

In the cases of $N_d = 3$ and $N_d = 4$, the sums in Eq. (69) are canceled term by term; thus the current is vanishing. In the case of $N_d = 5$, the current can be presented in the following form

$$\sqrt{g}\, j^{\varphi}(\mathbf{x}) = -\frac{6}{\pi^2 r^2}\int_0^\infty dw\, w\sum_{l=0}^{\infty}(-1)^l[I_{3l+1}(w)K_{3l+2}(w) - I_{3l+2}(w)K_{3l+1}(w)],\quad N_d = 5. \tag{70}$$

Using the Schläfli contour integral representation for $I_\mu(u)$ and $K_{\mu'}(u)$, one can show (details will be published elsewhere) that the current is vanishing in this case also.

6. Summary

In the present paper we study the ground state polarization in graphene with a disclination, i.e. $6-N_d$-gonal ($N_d \neq 0$) defect inserted in the otherwise perfect twodimensional honeycomb lattice. The variation of the bond length and the mixing of π- with σ-orbitals caused by extrinsic curvature of the lattice surface are neglected, and our consideration, focusing on global aspects of coordination of carbon atoms, is based on the long-wavelength continuum model originating in the tight-binding approximation for the nearest neighbour interactions. Our general conclusion is that the ground state is polarized in cases when the Dirac—Weyl equation possesses a solution which is irregular, although square integrable, at the location of the defect; thus the ground state polarization is depending on the boundary parameter at this point, which exhibits itself as the self-adjoint extension parameter. The conclusion is consistent with the previously obtained result for the induced ground state charge in graphene with a disclination [3,4].

It is straightforward to demonstrate that the usual ground state current, $\langle \mathrm{vac}|\Psi^{+}\boldsymbol{\alpha}\Psi|\mathrm{vac}\rangle$, and the ground state pseudospin-condensate, $\langle \mathrm{vac}|\Psi^{+}\Sigma\Psi|\mathrm{vac}\rangle$, are zero. In the present paper we consider other ground state characteristics: the P-condensate (9) and the R-current (10), which in terms of the sublattice and valley field components (see Eq. (35)) are explicitly written as

$$\rho(x) = \langle \mathrm{vac}|[\Psi^{+}_{A+}(x)\Psi_{B-}(x) + \Psi^{+}_{B+}(x)\Psi_{A-}(x) + \\ + \Psi^{+}_{A-}(x)\Psi_{B+}(x) + \Psi^{+}_{B-}(x)\Psi_{A+}(x)]|\mathrm{vac}\rangle \qquad (71)$$

and

$$\sqrt{g}\, j^{\varphi}(x) = \langle \mathrm{vac}|[-\Psi^{+}_{A+}(x)\Psi_{A-}(x) + \Psi^{+}_{B+}(x)\Psi_{B-}(x) - \\ - \Psi^{+}_{A-}(x)\Psi_{A+}(x) + \Psi^{+}_{B-}(x)\Psi_{B+}(x)]|\mathrm{vac}\rangle \qquad (72)$$

(the radial current is vanishing). Whereas the current is invariant under time reversal, the condensate is invariant under time reversal and spatial inversion as well. In particular, in the chiral representation of the Dirac matrices (with diagonal γ^{5}-matrix) one gets $P = \gamma^{0}$ and the condensate corresponds to the conventional chiral symmetry breaking condensate, $\langle \mathrm{vac}|\overline{\Psi}\Psi|\mathrm{vac}\rangle$.

In the cases of the one-pentagon ($N_d = 1$), one-heptagon ($N_d = -1$) and three-heptagon ($N_d = -3$) defects, our results take form

$$\rho(\mathbf{x}) = -\frac{6\sin(\pi/5)}{5\pi^{3}r^{2}}\int_{0}^{\infty} dw\, w \frac{K^{2}_{1/5}(w) + K^{2}_{4/5}(w)}{\cosh\left[\frac{3}{5}\ln\left(\frac{\hbar w}{rMv}\right) - \ln\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)\right]}, \quad N_d = 1, \qquad (73)$$

$$\sqrt{g}\, j^{\varphi}(\mathbf{x}) = \frac{6}{5\pi r^{2}}\left\{G\left(\frac{1}{6},\frac{1}{5}\right) - \frac{3}{20}\tan\left(\frac{\pi}{5}\right) + \right. ,$$

$$\left. + \frac{2\sin(\pi/5)}{\pi^{2}}\int_{0}^{\infty} dw\, wK_{1/5}(w)K_{4/5}(w)\tanh\left[\frac{3}{5}\ln\left(\frac{\hbar w}{rMv}\right) - \ln\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)\right]\right\}, \quad N_d = 1, \qquad (74)$$

$$\rho(\mathbf{x}) = -\frac{6\sin(2\pi/7)}{7\pi^{3}r^{2}}\int_{0}^{\infty} dw\, w \frac{K^{2}_{2/7}(w) + K^{2}_{5/7}(w)}{\cosh\left[\frac{3}{7}\ln\left(\frac{\hbar w}{rMv}\right) + \ln\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)\right]}, \quad N_d = -1, \qquad (75)$$

$$\sqrt{g}\, j^{\varphi}(\mathbf{x}) = \frac{6}{7\pi r^{2}}\left\{G\left(-\frac{1}{6},\frac{5}{7}\right) - \frac{3}{28}\tan(2\pi/7) - \right.$$

$$\left. - \frac{2\sin(2\pi/7)}{\pi^{2}}\int_{0}^{\infty} dw\, wK_{2/7}(w)K_{5/7}(w)\tanh\left[\frac{3}{7}\ln\left(\frac{\hbar w}{rMv}\right) + \ln\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)\right]\right\}, \quad N_d = -1 \qquad (76)$$

$$\rho(\mathbf{x}) = -\frac{1}{\sqrt{3}\pi^{3}r^{2}}\int_{0}^{\infty} dw\, w \frac{K^{2}_{1/3}(w) + K^{2}_{2/3}(w)}{\cosh\left[\frac{1}{3}\ln\left(\frac{\hbar w}{rMv}\right) - \ln\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)\right]}, \quad N_d = -3, \qquad (77)$$

$$\sqrt{g}\, j^{\varphi}(\mathbf{x}) = \frac{2}{3\pi r^{2}}\left\{G\left(-\frac{1}{2},\frac{1}{3}\right) - \frac{1}{4\sqrt{3}} + \right.$$

$$\left. + \frac{\sqrt{3}}{\pi^{2}}\int_{0}^{\infty} dw\, wK_{1/3}(w)K_{2/3}(w)\tanh\left[\frac{1}{3}\ln\left(\frac{\hbar w}{rMv}\right) - \ln\tan\left(\frac{\Theta}{2}+\frac{\pi}{4}\right)\right]\right\}, \quad N_d = -3, \qquad (78)$$

At large distances from the defect, the current decreases as r^{-2}, see Eq. (68), whereas the condensate decreases faster, see Eq. (59), with the same power law as for the decrease of the charge density [3].

In the cases of the two-pentagon ($N_d = 2$), two-heptagon ($N_d = -2$) and six-heptagon ($N_d = -6$) defects, the expressions for the condensate and the current are simplified and are given by Eqs.(58) and (67), respectively. Note that in these cases the charge is zero [3].

One can see that the ground state polarization effects cannot be eliminated at all by the choice of the value of the boundary parameter (Θ). Even in the case of $\cos\Theta = 0$, when the condensate and the charge are vanishing, the current is nonvanishing, see Eq. (66). The question of which of the values of Θ is realized in nature has to be answered by future experimental measurements, probably with the use of scanning tunnel and transmission electron microscopy.

Acknowledgements

We would like to thank V.P. Gusynin for stimulating discussions. The work of Yu.A. S. was supported by grant No. 10/07-N «Nanostructure systems, nanomaterials, nanotechnologies» of the National Academy of Sciences of Ukraine and grant No. 05-1000008-7865 of the INTAS. We acknowledge the partial support of the Department of Physics and Astronomy of the National Academy of Sciences of Ukraine under Special program «Fundamental properties of physical systems in extremal conditions» and the Swiss National Science Foundation under the SCOPES project No. IB7320-110848.

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