

ELECTRONIC PROPERTIES OF DISCLINATIONS IN CARBON NANOSTRUCTURES

Yu.A. Sitenko^{1,2} and N.D. Vlasit^{1,2}

¹*Bogolyubov Institute for Theoretical Physics
National Academy of Sciences, 03680, Kyiv, 143, Ukraine;
e-mail: yusitenko@bitp.kiev.ua;*

²*Physics Department, National Taras Shevchenko University of Kyiv,
03127, Kyiv, 127, Ukraine*

The recent synthesis of strictly twodimensional atomic crystals (monolayers of carbon atoms) is promising a wealth of new phenomena and possible applications in technology and industry. Such materials are characterized by the Dirac-type spectrum of quasiparticle excitations, yielding a unique example of the truly twodimensional “relativistic” electronic system which, in the presence of disclinations, possesses rather unusual properties. We consider the influence of disclinations on densities of states and induced vacuum quantum numbers in graphene.

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1. INTRODUCTION

Carbon nanostructures are intensively studied both experimentally and theoretically, in view of their expected important implications for the development of electronic devices, flat panel displays, nanoswitches, etc. (see, e.g. Ref. [1]). The observation of anomalous transport properties, and, most exciting, the recent discovery of substantial field effect and magnetism at room temperature allows one to envisage graphene (monolayer of graphite) as a reasonable replacement of nanotubes in electronic applications [2, 3].

In the case of isolated graphene, the electronic states near the Fermi level can be described in a simple manner. By symmetry, the lower and upper bands touch at the corners of the hexagonal Brillouin zone. In the vicinity of these points, the dispersion relation is isotropic and linear, and the density of states at the Fermi level is strictly zero, rising linearly in energy. An effective long wavelength description of these electronic states can be written in terms of a continuum model which is based on the massless Dirac equation in 2+1-dimensional space-time [4, 5]. Due to the vanishing density of states at the Fermi level, the long-range Coulomb interaction is marginal, scaling to zero at low energies or long wavelengths. Incidentally, short-range interactions responsible for ferromagnetic effects are irrelevant in this context. On the contrary, peculiarities of electronic states which are due to topological defects are essential and have been observed in different kinds of nanoparticles by scanning tunneling microscopy.

2. TOPOLOGICAL DEFECTS IN GRAPHENE

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 warps the grapheme sheet. More generally, a hexagon can be substituted by an n -sided ring without affecting the threefold coordination of the carbon atoms. Rings with $n < 6$ ($n > 6$) induce locally positive

(negative) curvature, whereas the graphene sheet is flat away from the defect, as is the conical surface away from the apex. In the case of nanocones with $n < 6$, apex angle α is related to n :

$$\sin \frac{\alpha}{2} = \frac{n}{6}. \quad (1)$$

Certainly, defects with $n < 5$ and $n > 7$ are mathematical abstractions, as are cones with a pointlike apex. In reality, the defect are smoothed: 2 pentagons instead of $n = 4, 3$ pentagons instead of $n = 3, 4$ pentagons instead of $n = 2, 5$ pentagons instead of $n = 1$; such nanocones were observed experimentally. Theory predicts an infinite series of the saddle-like nanocones with defects: 1 heptagon ($n = 7$), 2 heptagons (instead of $n = 8$), 3 heptagons (instead of $n = 9$), etc.

In the continuum limit a disclination is presented by a vortex with a fixed flux at the apex of a conical surface with a fixed deficit angle. Electronic excitations are described by four-components spinors which are composed from two-component spinors of two sublattices corresponding to two inequivalent Fermi points. These spinors interact with the background in the form of a vortex and curvature accumulated at the apex of the conical surface.

Apex angle is related to deficit angle

$$\delta = 2\pi \left(1 - \sin \frac{\alpha}{2} \right). \quad (2)$$

Defining $\Phi_K = \delta/2\pi$, and using Eq. (1), one gets

$$\Phi_K = 1 - \frac{n}{6}. \quad (3)$$

Defining $\Phi = \phi/2\pi$, where ϕ is the vortex flux, one gets

$$\Phi = \frac{3}{2} - \frac{n}{4}. \quad (4)$$

Thus, a general disclination with $n > 0$ is characterized by vortex flux $2\pi\Phi$ and deficit angle $2\pi\Phi_K$, where Φ and Φ_K are given by Eqs. (4) and (3), respectively.

In the standard representation of γ -matrices, γ^5 -matrix ($\gamma^5 = -i\gamma^0\gamma^1\gamma^2\gamma^3$) is

$$\gamma^5 = i \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}. \quad (5)$$

When a hexagon is substituted by a pentagon (disclination with $n = 5$), the deficit angle is $\pi/3$, two sublattices are exchanged after completing a rotation around the apex, and a spinor wave function satisfies condition

$$\psi_0(r, \varphi + 2\pi) = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} \psi_0(r, \varphi) = e^{-i\gamma^5 \frac{\pi}{2}} \psi_0(r, \varphi), \quad (6)$$

where $r=0$ corresponds to the location of the apex. Condition (6) is generalized to the case of arbitrary $n > 0$:

$$\psi_0(r, \varphi + 2\pi) = e^{-i\gamma^5 2\pi\Phi} \psi_0(r, \varphi), \quad (7)$$

where Φ is given by Eq. (4). Performing gauge transformation,

$$\psi = e^{i\Omega} \psi_0, \quad \Omega = \gamma^5 \Phi \varphi, \quad (8)$$

one obtains the single-valued spinor wave function

$$\psi(r, \varphi + 2\pi) = \psi(r, \varphi). \quad (9)$$

While the initial spinor obeys free Dirac equation,

$$(i\partial_0 + i\gamma^0 \vec{\gamma} \cdot \vec{\nabla}) \psi_0 = 0, \quad (10)$$

the final spinor obeys Dirac equation in the vortex background

$$\begin{aligned} & \left(i\partial_0 + e^{i\Omega} i\gamma^0 \vec{\gamma} \cdot \vec{\nabla} e^{-i\Omega} \right) \psi \\ & = \left[i\partial_0 + i\gamma^0 \vec{\gamma} \cdot (\vec{\nabla} - i\vec{A}) \right] \psi = 0, \end{aligned} \quad (11)$$

where

$$\vec{A} = \vec{\partial}\Omega: \quad A^r = 0, \quad A^\varphi = \gamma^5 \Phi. \quad (12)$$

3. SOLUTION TO THE DIRAC EQUATION IN GRAPHENE WITH A DISCLINATION

Stationary Dirac equation on a two-dimensional surface which is orthogonal to external magnetic field is

$$H\psi = E\psi, \quad (13)$$

where

$$H = -i\gamma^0 \vec{\gamma}(\vec{x}) \left[\vec{\partial} + \frac{i}{2} \vec{\omega}(\vec{x}) - \vec{A}(\vec{x}) \right], \quad (14)$$

$\vec{\omega}$ is the spin connection and \vec{A} is the bundle connection. In the case of the graphene layer with a disclination, the metric takes form

$$ds^2 = dr^2 + r^2(1 - \Phi_K)^2 d\varphi^2, \quad \Phi_K = 1 - \frac{n}{6}. \quad (15)$$

In the chiral representation with the diagonal γ^5 -matrix,

$$\gamma^5 = \begin{pmatrix} -I & 0 \\ 0 & I \end{pmatrix}, \quad (16)$$

the Dirac Hamiltonian takes form (see Ref. [6])

$$H = \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix}, \quad (17)$$

where

$$H = \begin{pmatrix} 0 & D_\pm^+ \\ D_\pm^- & 0 \end{pmatrix}, \quad (18)$$

$$\begin{aligned} D_\pm^\pm &= e^{i\varphi} \left[-\partial_r + r^{-1}(1 - \Phi_K)^{-1}(-i\partial_\varphi \mp \Phi + \frac{1}{2}\Phi_K) \right] \\ D_\pm^\pm &= e^{-i\varphi} \left[\partial_r + r^{-1}(1 - \Phi_K)^{-1}(-i\partial_\varphi \mp \Phi - \frac{1}{2}\Phi_K) \right] \end{aligned} \quad (19)$$

Solution to Eq. (13) is presented as

$$\begin{aligned} \psi(\vec{x}, t) &= \sum_{n \in \mathbb{Z}} \int_0^\infty dE E e^{-iEt} \langle \vec{x} | E, n \rangle a_{En} \\ &+ \int_0^{-\infty} dE E e^{-iEt} \langle \vec{x} | E, n \rangle b_{En}^\dagger, \end{aligned} \quad (20)$$

where a_{En}^\dagger and a_{En} (b_{En}^\dagger and b_{En}) are the fermion (antifermion) creation and destruction operators satisfying the anticommutation relations

$$\left[a_{En}, a_{E'n'}^\dagger \right]_+ = \left[b_{En}, b_{E'n'}^\dagger \right]_+ = \frac{\delta(E - E')}{\sqrt{|EE'|}} \delta_{nn'},$$

and

$$\langle \vec{x} | E, n \rangle = \begin{pmatrix} f_n^+(r, E) e^{in\varphi} \\ g_n^+(r, E) e^{i(n+1)\varphi} \\ f_n^-(r, E) e^{in\varphi} \\ g_n^-(r, E) e^{i(n+1)\varphi} \end{pmatrix}. \quad (21)$$

Let us restrict ourselves to the range of the most accessible experimentally disclinations: $-1 < \Phi_K < 1$ ($1 \leq n \leq 12$). An irregular mode appears in the spectrum of the Dirac Hamiltonian if

$$\begin{aligned} \frac{1}{2}\Phi_K < \llbracket \Phi \rrbracket < 1 - \frac{1}{2}\Phi_K \quad (0 < \Phi_K < 1), \\ -\frac{1}{2}\Phi_K < \llbracket \Phi \rrbracket < 1 + \frac{1}{2}\Phi_K \quad (-1 < \Phi_K < 0), \end{aligned} \quad (22)$$

where $\Phi = \llbracket \Phi \rrbracket + \{\Phi\}$, $\llbracket u \rrbracket$ is the integer part of u and $\{\!| u \}\!$ is the fractional part of u , $0 \leq \{\!| u \}\! < 1$. Namely, the upper components are:

$$\begin{aligned} \begin{pmatrix} f_n^+ \\ g_n^+ \end{pmatrix} &= \frac{1}{2\sqrt{(1 - \Phi_K)\pi}} \begin{pmatrix} J_{\frac{l}{1 - \Phi_K} - F}(kr) \\ \text{sgn}(E) J_{\frac{l}{1 - \Phi_K} + 1 - F}(kr) \end{pmatrix}, \\ l &= n - \llbracket \Phi \rrbracket > 0, \end{aligned} \quad (23)$$

$$\begin{pmatrix} f_n^+ \\ g_n^+ \end{pmatrix} = \frac{1}{2\sqrt{(1-\Phi_K)\pi}} \begin{pmatrix} J_{l'+F}(kr) \\ -\text{sgn}(E)J_{l'-1+F}(kr) \end{pmatrix}, \quad (24)$$

$$l' = \llbracket \Phi \rrbracket - n > 0,$$

which are regular, and the following one

$$\begin{pmatrix} f_{\llbracket \Phi \rrbracket}^+ \\ g_{\llbracket \Phi \rrbracket}^+ \end{pmatrix} = \frac{1}{2\sqrt{(1-\Phi_K)\pi[1+\sin(2\nu_E)\cos(F\pi)]}} \times \begin{pmatrix} \sin(\nu_E)[J_{-F}(kr) + \cos(\nu_E)J_F(kr)] \\ \text{sgn}(E)[\sin(\nu_E)J_{1-F}(kr) - \cos(\nu_E)J_{-1+F}(kr)] \end{pmatrix}, \quad (25)$$

which is irregular; here $k = |E|$, $J_\rho(u)$ is the Bessel function of order ρ , and

$$F = \frac{\llbracket \Phi \rrbracket - \frac{1}{2}}{1 - \Phi_K} + \frac{1}{2}; \quad (26)$$

note that $0 < F < 1$ due to conditions in Eq. (22). The lower components $\begin{pmatrix} f_n^- \\ g_n^- \end{pmatrix}$ are obtained from $\begin{pmatrix} f_n^+ \\ g_n^+ \end{pmatrix}$ by substitution $F \rightarrow 1 - F$.

To determine parameter ν_E , one has to implement self-adjoint extension of the partial Hamiltonian with $n = \llbracket \Phi \rrbracket$, see Refs. [7-9]. The family of self-adjoint extensions is parameterized by one real continuous variable Θ , thus yielding

$$\tan \nu_E = \text{sgn}(E) \left(\frac{k}{M} \right)^{1-2F} \tan \left(\frac{\Theta}{2} + \frac{\pi}{4} \right), \quad (27)$$

and the boundary condition for the irregular mode:

$$\tau_5(E) = \frac{2(1-2F)\sin(F\pi) \left[\left(\frac{|E|}{M} \right)^{2F-1} \tan \left(\frac{\Theta}{2} + \frac{\pi}{4} \right) + \left(\frac{|E|}{M} \right)^{1-2F} \cot \left(\frac{\Theta}{2} + \frac{\pi}{4} \right) \right]}{\pi E \left[\left(\frac{|E|}{M} \right)^{2(2F-1)} \tan^2 \left(\frac{\Theta}{2} + \frac{\pi}{4} \right) + \left(\frac{|E|}{M} \right)^{2(1-2F)} \cot^2 \left(\frac{\Theta}{2} + \frac{\pi}{4} \right) - 2\cos(2F\pi) \right]}. \quad (32)$$

Near the Fermi level, the axial density of states diverges, unless $F = \frac{1}{2}$:

$$\tau_5(E) \underset{E \rightarrow 0}{=} \begin{cases} \frac{2}{\pi}(1-2F)\text{sgn}(E) \left(\frac{M}{|E|} \right)^{2F} M \cot \left(\frac{\Theta}{2} + \frac{\pi}{4} \right), & 0 < F < \frac{1}{2} \\ \frac{2}{\pi}(1-2F)\text{sgn}(E) \left(\frac{M}{|E|} \right)^{2(1-F)} M \tan \left(\frac{\Theta}{2} + \frac{\pi}{4} \right), & \frac{1}{2} < F < 1 \end{cases}. \quad (33)$$

Using Eq. (26), we get $F = \frac{1}{5}$ for the pentagon defect and $F = \frac{5}{7}$ for the heptagon defect. Consequently, we get

$$\left. \begin{aligned} \lim_{r \rightarrow 0} (Mr)^F f_{\llbracket \Phi \rrbracket}^+ &= -2^{2F-1} \frac{\Gamma(F)}{\Gamma(1-F)} \tan \left(\frac{\Theta}{2} + \frac{\pi}{4} \right) \\ \lim_{r \rightarrow 0} (Mr)^{1-F} g_{\llbracket \Phi \rrbracket}^+ & \\ \lim_{r \rightarrow 0} (Mr)^{1-F} f_{\llbracket \Phi \rrbracket}^- &= -2^{1-2F} \frac{\Gamma(1-F)}{\Gamma(F)} \cot \left(\frac{\Theta}{2} + \frac{\pi}{4} \right) \\ \lim_{r \rightarrow 0} (Mr)^F g_{\llbracket \Phi \rrbracket}^- & \end{aligned} \right\}, \quad (28)$$

where M is the parameter with dimension of inverse length.

4. DENSITIES OF STATES

What is the influence of disclinations in graphene on the density of states? The conventional density of states is defined as

$$\tau(E) = \text{Tr} \delta(H - E), \quad (29)$$

where Tr is the trace of an integro-differential operator in the functional space: $\text{Tr} U = \int d^2x \text{tr} \langle \vec{x} | U | \vec{x} \rangle$; tr denotes the trace over spinor indices only. In the absence of disclinations, the density of states is proportional to the size of the sample:

$$\tau(E) = \frac{V_2}{2\pi} |E|, \quad (30)$$

where V_2 is the twodimensional volume (area) of the graphene layer; since Eq. (30) is even in energy, the total charge of the sample,

$$Q = \frac{1}{2} \int_{-\infty}^{\infty} dE \tau(E) \text{sgn}(E),$$

is zero. Disclinations do not change this result, due to the presence of γ^5 in potential \vec{A} . However, disclinations lead to the nontrivial axial density of states,

$$\tau_5(E) = \text{Tr} \gamma^5 \delta(H - E), \quad (31)$$

which is due to the appearance of the irregular mode, see Eq. (25),

$$\tau_5(E) \underset{E \rightarrow 0}{=} \frac{6}{5\pi} \text{sgn}(E) \left(\frac{M}{|E|} \right)^{\frac{2}{5}} M \cot \left(\frac{\Theta}{2} + \frac{\pi}{4} \right) \quad (34)$$

for the pentagon defect, and

$$\tau_5(E) = -\frac{6}{7\pi} \text{sgn}(E) \left(\frac{M}{|E|} \right)^{\frac{2}{7}} M \tan\left(\frac{\Theta}{2} + \frac{\pi}{4}\right) \quad (35)$$

for the heptagon defect.

Let us consider the spin density of states,

$$\tau_\Sigma(E) = \text{Tr} \Sigma \delta(H - E) \quad (36)$$

and the orbital angular momentum density of states

$$\tau_\Lambda(E) = \text{Tr} \Lambda \delta(H - E), \quad (37)$$

where

$$\Sigma = \frac{i}{2} \gamma^1 \gamma^2, \quad (38)$$

and

$$\Lambda = -i(x^1 \partial_2 - x^2 \partial_1) - \gamma^5 \Phi \quad (39)$$

are the spin and the orbital angular momentum directed orthogonally to the graphene sheet. Defining total angular momentum,

$$J = \Lambda + \Sigma, \quad (40)$$

one gets the appropriate density of states

$$\tau_J(E) = \tau_\Sigma(E) + \tau_\Lambda(E). \quad (41)$$

In the presence of disclination we get

$$\tau_\Sigma(E) = \frac{1}{2(1-2F)} \tau_5(E), \quad (42)$$

$$\tau_\Lambda(E) = -\frac{1-2F(1-F)}{1-2F} \tau_5(E) \quad (43)$$

and

$$\tau_J(E) = -\frac{1}{2}(1-2F)\tau_5(E). \quad (44)$$

In the case of disclinations with $n=4$ (2 pentagons) and $n=8$ (2 heptagons) we get $F = \frac{1}{2}$, and, consequently,

$$\tau_J(E) = \tau_5(E) = 0 \quad (45)$$

and

$$\tau_\Sigma(E) = -\tau_\Lambda(E) = \frac{\cos \Theta}{2\pi E}. \quad (46)$$

5. VACUUM QUANTUM NUMBERS INDUCED IN GRAPHENE BY A DISCLINATION

Spectral asymmetries determine the appropriate quantum numbers

$$Q_Y = -\frac{1}{2} \int_{-\infty}^{\infty} dE \tau_Y(E) \text{sgn}(E). \quad (47)$$

Thus we get: axial charge

$$Q_5 = -\text{sgn}_0[(1-2F)\cos \Theta], \quad (48)$$

spin

$$Q_\Sigma = -\frac{1}{2} \frac{\text{sgn}_0(\cos \Theta)}{|1-2F|}, \quad (49)$$

orbital angular momentum

$$Q_\Lambda = \frac{1-2F(1-F)}{|1-2F|} \text{sgn}_0(\cos \Theta); \quad (50)$$

and total angular momentum

$$Q_J = \frac{1}{2} |1-2F| \text{sgn}_0(\cos \Theta). \quad (51)$$

One can conclude that axial charge and total angular momentum vanish in the case of disclinations corresponding to either 2 pentagons or 2 heptagons (spin and orbital angular momentum diverge in this case). In the case of disclinations corresponding to single pentagon and single heptagon, we get the following predictions. Ground state quantum numbers are not induced if

$$\Theta = \frac{\pi}{2} \text{ mod } 2\pi. \text{ Otherwise, the values of axial charge}$$

are of the opposite sign:

$$Q_5^{(5)} = -Q_5^{(7)} = -\text{sgn}_0(\cos \Theta); \quad (52)$$

the values of spin are negative:

$$Q_\Sigma^{(5)} = -\frac{5}{6} \text{sgn}_0(\cos \Theta), \quad Q_\Sigma^{(7)} = -\frac{7}{6} \text{sgn}_0(\cos \Theta); \quad (53)$$

the values of orbital angular momentum are positive exceeding 1:

$$Q_\Lambda^{(5)} = \frac{17}{15} \text{sgn}_0(\cos \Theta), \quad Q_\Lambda^{(7)} = \frac{29}{21} \text{sgn}_0(\cos \Theta); \quad (54)$$

the values of total angular momentum are positive and less than 1:

$$Q_J^{(5)} = \frac{3}{10} \text{sgn}_0(\cos \Theta), \quad Q_J^{(7)} = \frac{3}{14} \text{sgn}_0(\cos \Theta). \quad (55)$$

The possibilities of experimental verification of our predictions for the ground state quantum numbers in graphene are under study.

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ЭЛЕКТРОННЫЕ СВОЙСТВА ДИСКЛИНАЦИЙ В УГЛЕРОДНЫХ НАНОСТРУКТУРАХ

Ю.А. Ситенко, Н.Д. Власий

Недавний синтез строго двумерных атомных кристаллов углерода обещает изобилие новых явлений и возможные приложения в технологии и промышленности. Такие материалы характеризуются спектром квазичастичных возбуждений дираковского типа, что дает уникальный пример истинно двумерных «релятивистских» электронных систем, которые при наличии дисклинаций обладают достаточно необычными свойствами. Рассматривается влияние дисклинаций на плотности состояний и индуцированные вакуумные квантовые числа графена.

ЕЛЕКТРОННІ ВЛАСТИВОСТІ ДИСКЛІНАЦІЙ У ВУГЛЕЦЕВИХ НАНОСТРУКТУРАХ

Ю.О. Ситенко, Н.Д. Власій

Нещодавній синтез строго двовимірних атомних кристалів вуглецю обіцяє багато нових явищ та можливі застосування в технології і промисловості. Такі матеріали характеризуються спектром квазічастинкових збуджень діраківського типу, що дає унікальний приклад справді двовимірних «релятивістських» електронних систем, котрі при наявності дисклінацій мають досить незвичні властивості. Розглядається вплив дисклінацій на густини станів та індуковані вакуумні квантові числа графена.