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# On the possible induced charge on a graphitic nanocone at finite temperature

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## Abstract

Electronic excitations in a graphitic monolayer (graphene) in the long-wavelength approximation are characterized by the linear dispersion law, representing a unique example of the really two-dimensional ‘ultrarelativistic’ fermionic system which in the presence of topological defects possesses rather unusual properties. A disclination that rolls up a graphitic sheet into a nanocone is described by a pointlike pseudomagnetic vortex at the apex of the cone, and the flux of the vortex is related to the deficit angle of the conical surface. A general theory of planar relativistic fermionic systems in the singular vortex background is employed, and we derive the analytical expression for the charge which is induced at finite temperature on some graphitic nanocones.

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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. [1]). The recent synthesis of strictly two-dimensional atomic crystals of carbon (monolayers of graphite–graphene) [2, 3] is promising a wealth of new phenomena and applications in technology. The observation of anomalous transport properties, and, most exciting, the discovery of substantial field effect and magnetism at room temperature allow one to envisage graphene as a reasonable replacement of nanotubes in electronic applications [4, 5].

In the case of isolated graphene, the electronic states near the Fermi level can be described in a simple manner [6]. 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. 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 massless electrons in 2 + 1-dimensional spacetime with the role of speed of light  $c$  played by the Fermi velocity  $v \approx c/300$  [7, 8]. The one-particle Hamiltonian operator of the model takes the form

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

where the  $4 \times 4$  matrices can be chosen in the form [9]

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

$\sigma^j$  ( $j = 1, 2, 3$ ) are the Pauli matrices. The one-particle electronic wavefunction possesses four components:

$$\psi = (\psi_{A+}, \psi_{B+}, \psi_{A-}, \psi_{B-})^T, \quad (3)$$

where subscripts  $A$  and  $B$  correspond to two sublattices of the honeycomb lattice and subscripts  $+$  and  $-$  correspond to two inequivalent Fermi points. The linear dispersion law,  $E = \pm\hbar v|\mathbf{k}|$ , results in the density of states

$$\tau(E) = \frac{S|E|}{\pi\hbar^2 v^2}, \quad (4)$$

which is the density of states of two-dimensional ultrarelativistic Fermi gas (here  $S$  is the area of the graphene sample). Consequently, the thermal average charge of electronic excitations in graphene,

$$Q(T) = -\frac{e}{2} \int_{-\infty}^{\infty} dE \tau(E) \tanh\left(\frac{1}{2}\beta E\right), \quad \beta = (k_B T)^{-1}, \quad (5)$$

is evidently zero, because equation (4) is even in energy ( $k_B$  is the Boltzmann constant).

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 a 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  $N_d$  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 graphene 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; such nanocones were observed experimentally [10]. 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 cones serve as an element which is necessary for joining parts of carbon nanotubes of differing radii and for creating schwarzite [11], a structure appearing in many forms of carbon nanofoam [12]. As it was shown by using molecular-dynamics simulations [13], in the case of  $N_d \leq -4$ , 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  $N_d \rightarrow -\infty$  limit of a  $6 - N_d$ -gonal defect.

In the present paper we consider the influence of topological defects in graphene on its electronic properties at finite temperature<sup>3</sup>. The effects of the variation of the bond length or the mixing of  $\pi$ - with  $\sigma$ -orbitals caused by the 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. We employ a general theory of planar relativistic fermionic systems in the singular vortex background [19, 20]; its version for the case of massless fermions was elaborated in [21–23].

## 2. Hamiltonian, resolvent and density of states on a graphitic nanocone

The Dirac–Weyl Hamiltonian for electronic excitations on a graphitic nanocone with a pointlike apex takes the form

$$H = -i\hbar v \left\{ \alpha^1 \partial_r + \alpha^2 r^{-1} \left[ (1 - \eta)^{-1} \partial_\varphi - i\Sigma \right] \right\}, \quad (6)$$

where

$$\Sigma = \frac{1}{2i} \alpha^1 \alpha^2 = \frac{1}{2} \begin{pmatrix} \sigma^3 & 0 \\ 0 & -\sigma^3 \end{pmatrix} \quad (7)$$

is the pseudospin and  $r$  and  $\varphi$  are the polar coordinates centred at the apex of the cone with metric

$$g_{rr} = 1, \quad g_{\varphi\varphi} = (1 - \eta)^2 r^2, \quad (8)$$

and

$$\eta = N_d/6. \quad (9)$$

The electronic wavefunction on a graphitic nanocone obeys the Möbius-strip-type condition [9]:

$$\psi(r, \varphi + 2\pi) = -\exp\left(-i\frac{\pi}{2} N_d R\right) \psi(r, \varphi), \quad (10)$$

where

$$R = i \begin{pmatrix} 0 & \sigma^2 \\ -\sigma^2 & 0 \end{pmatrix} \quad (11)$$

is the operator exchanging sublattices, as well as inequivalent Fermi points, and commuting with the Hamiltonian (6).

By performing the singular gauge transformation

$$\psi' = e^{i\Omega} \psi, \quad \Omega = \varphi \frac{N_d}{4} R, \quad (12)$$

one gets the wavefunction obeying usual condition

$$\psi'(r, \varphi + 2\pi) = -\psi'(r, \varphi), \quad (13)$$

in the meantime, Hamiltonian (6) is transformed to

$$H' = e^{i\Omega} H e^{-i\Omega} = -i\hbar v \left\{ \alpha^1 \partial_r + \alpha^2 r^{-1} \left[ (1 - \eta)^{-1} \left( \partial_\varphi - i\frac{3}{2} \eta R \right) - i\Sigma \right] \right\}, \quad (14)$$

where relation (9) is recalled. Thus, a topological defect in graphene is presented by a pseudomagnetic vortex with flux  $N_d\pi/2$  through the apex of a cone with the deficit angle  $N_d\pi/3$ .

<sup>3</sup> The case of zero temperature was discussed earlier in works [9, 14–18].

By performing a unitary transformation which diagonalizes  $R$ , one gets Hamiltonian in the block-diagonal form

$$H'' = \begin{pmatrix} H_1 & 0 \\ 0 & H_{-1} \end{pmatrix}, \quad (15)$$

where

$$H_s = \hbar v \left\{ i\sigma^2 \partial_r - \sigma^1 r^{-1} \left[ (1 - \eta)^{-1} \left( is \partial_\varphi + \frac{3}{2} \eta \right) + \frac{1}{2} \sigma^3 \right] \right\}, \quad s = \pm 1. \quad (16)$$

Let us consider the kernel of resolvent (Green's function) of Hamiltonian (16)

$$\langle r, \varphi | (H_s - \omega)^{-1} | r', \varphi' \rangle = \frac{1}{2\pi} \sum_{n \in \mathbb{Z}} e^{i(n+\frac{s}{2})(\varphi-\varphi')} \begin{pmatrix} a_{11}^{(n)}(r, r') & a_{21}^{(n)}(r, r') \\ a_{12}^{(n)}(r, r') & a_{22}^{(n)}(r, r') \end{pmatrix}, \quad (17)$$

where  $\mathbb{Z}$  is the set of integer numbers and  $\omega$  is a complex parameter with dimension of energy. Off-diagonal radial components are expressed through the diagonal ones, while the latter satisfy the second-order differential equations. All radial components behave asymptotically at large distances as outgoing waves, i.e. as  $e^{ikr} (2\pi\sqrt{r})^{-1}$  at  $r \rightarrow \infty$  and as  $e^{ikr'} (2\pi\sqrt{r'})^{-1}$  at  $r' \rightarrow \infty$ , where  $k = \sqrt{\omega^2 - (\hbar v)^{-2}}$  and a physical sheet for the square root is chosen as  $0 < \text{Arg } k < \pi$  ( $\text{Im } k > 0$ ). In the cases of  $N_d = 3, 4, 5$  all radial components are regular at small distances, i.e. at  $r \rightarrow 0$  and at  $r' \rightarrow 0$ . In all other cases there are radial components that are irregular at  $r = 0$  and  $r' = 0$  for some values of  $n$ . This is related to the fact that in these cases Hamiltonian (16) is not essentially self-adjoint and is characterized by the nonzero deficiency index. According to the Weyl-von Neumann theory of self-adjoint operators (see, e.g. [24]), a procedure of the self-adjoint extension is implemented yielding the condition for the irregular radial components, which depends on the set of self-adjoint extension parameters. It should be emphasized that only irregular radial components can produce a piece in the density of states, which is odd in energy. Thus, if charge (5) is nonvanishing, then it depends on the set of self-adjoint extension parameters.

Let us consider the possibility of charge generation in the cases of  $N_d = 2, 1, -1, -2, -3, -6$ , when Hamiltonian (16) is characterized by the deficiency index  $(1, 1)$ , and there is only one self-adjoint extension parameter  $-\Theta$ . The irregular diagonal radial components are given by expressions

$$a_{11}^{(n_c)}(r; r') = \frac{i\pi}{2(1-\eta)} \frac{\omega}{(\sin v_\omega + \cos v_\omega e^{iF\pi})} \times \left\{ \theta(r-r') H_{-F}^{(1)}(kr) [\sin v_\omega J_{-F}(kr') + \cos v_\omega J_F(kr')] + \theta(r'-r) [\sin v_\omega J_{-F}(kr) + \cos v_\omega J_F(kr)] H_{-F}^{(1)}(kr') \right\}, \quad (18)$$

$$a_{22}^{(n_c)}(r; r') = \frac{i\pi}{2(1-\eta)} \frac{\omega}{(\sin v_\omega + \cos v_\omega e^{iF\pi})} \times \left\{ \theta(r-r') H_{1-F}^{(1)}(kr) [\sin v_\omega J_{1-F}(kr') - \cos v_\omega J_{-1+F}(kr')] + \theta(r'-r) [\sin v_\omega J_{1-F}(kr) - \cos v_\omega J_{-1+F}(kr)] H_{1-F}^{(1)}(kr') \right\}, \quad (19)$$

where

$$n_c = \begin{cases} \frac{s}{2} [\text{sgn}(N_d) - 1] & N_d = 2, 1, -1, -2, -3, \\ -2s, & N_d = -6, \end{cases} \quad (20)$$

$$F = \begin{cases} [3 - 3\text{sgn}(N_d) + N_d](6 - N_d)^{-1}, & N_d = 2, 1, -1, -2, -3, \\ 1/2, & N_d = -6, \end{cases} \quad (21)$$

$J_\mu(u)$  is the Bessel function of order  $\mu$ ,  $H_\mu^{(1)}(u)$  is the first-kind Hankel function of the order  $\mu$ ,

$$\theta(u) = \begin{cases} 1, & u > 0 \\ 0, & u < 0 \end{cases}, \quad \text{sgn}(u) = \theta(u) - \theta(-u),$$

parameter  $\nu_\omega$  is related to  $\Theta$  in the following way

$$\tan \nu_\omega = \frac{\hbar v k^{2F}}{\omega} \left( \frac{Mv}{\hbar} \right)^{1-2F} \tan \left( \frac{\Theta}{2} + \frac{\pi}{4} \right), \quad (22)$$

$M$  is the scale-invariance-breaking parameter of the dimension of mass. The diagonal radial components for  $n \neq n_c$  are regular.

Computing the contribution of the irregular radial components to the functional trace of the resolvent, we get

$$[\text{Tr}(H_s - \omega)^{-1}]_{\text{irreg}} = (1 - \eta) \int_0^\infty dr r [a_{11}^{(n_c)}(r, r) + a_{22}^{(n_c)}(r, r)] = \frac{2F - 1}{\omega(e^{-iF\pi} \tan \nu_\omega + 1)}, \quad (23)$$

where  $\text{Tr} \dots = \int d^2x \sqrt{g} \text{tr} \langle \mathbf{x} | \dots | \mathbf{x} \rangle$  and  $\text{tr}$  denotes the trace over pseudospinor indices only. Using the relation between the resolvent trace and the density of states,

$$\tau(E) = \frac{1}{2\pi i} [\text{Tr}(H - E - i0)^{-1} - \text{Tr}(H - E + i0)^{-1}], \quad (24)$$

we get the expression for the piece of the density of states, which is odd in energy:

$$\begin{aligned} \tau_{\text{odd}}(E) &= \frac{2(2F - 1) \sin(F\pi)}{\pi E} \\ &\times \frac{\left(\frac{|E|}{Mv^2}\right)^{2F-1} \tan\left(\frac{\Theta}{2} + \frac{\pi}{4}\right) + \left(\frac{|E|}{Mv^2}\right)^{1-2F} \cot\left(\frac{\Theta}{2} + \frac{\pi}{4}\right)}{\left(\frac{|E|}{Mv^2}\right)^{2(2F-1)} \tan^2\left(\frac{\Theta}{2} + \frac{\pi}{4}\right) - 2 \cos(2F\pi) + \left(\frac{|E|}{Mv^2}\right)^{2(1-2F)} \cot^2\left(\frac{\Theta}{2} + \frac{\pi}{4}\right)}, \end{aligned} \quad (25)$$

where the summation over  $s = \pm 1$  is performed. Although quantity (25) is negligible as compared to the ideal gas contribution (4), lacking the factor of the sample area, it provides the generation of nonzero charge on some graphitic nanocones.

### 3. Induced charge

Substituting (25) into (5), we get the thermal average of charge,

$$\begin{aligned} Q(T) &= 2e(1 - 2F) \frac{\sin(F\pi)}{\pi} \int_0^\infty \frac{du}{u} \tanh\left(\frac{1}{2}u\beta Mv^2\right) \\ &\times \frac{u^{2F-1} \tan\left(\frac{\Theta}{2} + \frac{\pi}{4}\right) + u^{1-2F} \cot\left(\frac{\Theta}{2} + \frac{\pi}{4}\right)}{u^{2(2F-1)} \tan^2\left(\frac{\Theta}{2} + \frac{\pi}{4}\right) - 2 \cos(2F\pi) + u^{2(1-2F)} \cot^2\left(\frac{\Theta}{2} + \frac{\pi}{4}\right)}. \end{aligned} \quad (26)$$

Taking into account relation (24), one can present thermal average (5) in the form

$$Q(T) = -\frac{e}{2} \int_C \frac{d\omega}{2\pi i} \text{Tr}(H - \omega)^{-1} \tanh\left(\frac{1}{2}\beta\omega\right), \quad (27)$$

where  $C$  is the contour consisting of two collinear straight lines,  $(-\infty + i0, +\infty + i0)$  and  $(+\infty - i0, -\infty - i0)$ , in the complex  $\omega$ -plane. By deforming the contour  $C$  to encircle poles of the hyperbolic tangential function on the imaginary axis, one gets

$$Q(T) = -\frac{e}{\beta} \sum_{m \in \mathbb{Z}} \text{Tr}(H - i\omega_m)^{-1}, \quad (28)$$

where  $\omega_m = (2m + 1)\pi/\beta$ . Using (23) and summing over  $s = \pm 1$ , we get

$$Q(T) = \frac{4e}{\beta M v^2} (1 - 2F) \times \sum_{\substack{m \in \mathbb{Z} \\ m \geq 0}} \left\{ \left[ \frac{(2m + 1)\pi}{\beta M v^2} \right]^{2F} \tan\left(\frac{\Theta}{2} + \frac{\pi}{4}\right) + \left[ \frac{(2m + 1)\pi}{\beta M v^2} \right]^{2(1-F)} \cot\left(\frac{\Theta}{2} + \frac{\pi}{4}\right) \right\}^{-1} \quad (29)$$

Representation (26) can be regarded as the Sommerfeld–Watson transform of the infinite sum representation (29).

Thus, the charge is zero for graphitic nanocones with  $N_d = 2, -2, -6$ , since in these cases one has  $F = 1/2$ , see (21). Note that one has  $F = 1/5$  for  $N_d = 1$ ,  $F = 5/7$  for  $N_d = -1$  and  $F = 1/3$  for  $N_d = -3$ . Therefore the charge, if any, for the one-pentagon ( $N_d = 1$ ) defect is of opposite sign to that for the one-heptagon ( $N_d = -1$ ) defect and is of the same sign to that for the three-heptagon ( $N_d = -3$ ) defect.

In the high-temperature limit ( $\beta \rightarrow 0$ ), the charge tends to zero as the inverse power of temperature:

$$Q(T \rightarrow \infty) = \frac{4e}{\pi} (1 - 2F) \times \begin{cases} (1 - 2^{-2+2F}) \zeta(2 - 2F) \tan\left(\frac{\Theta}{2} + \frac{\pi}{4}\right) \left(\frac{\beta M v^2}{\pi}\right)^{1-2F}, & 0 < F < \frac{1}{2} \\ (1 - 2^{-2F}) \zeta(2F) \cot\left(\frac{\Theta}{2} + \frac{\pi}{4}\right) \left(\frac{\beta M v^2}{\pi}\right)^{2F-1}, & \frac{1}{2} < F < 1, \end{cases} \quad (30)$$

where  $\zeta(u)$  is the Riemann zeta function (see, e.g. [25]). In the zero-temperature limit the charge tends to a finite value [9]:

$$Q(0) = e \operatorname{sgn}_0[(1 - 2F) \cos \Theta], \quad (31)$$

where

$$\operatorname{sgn}_0(u) = \begin{cases} \operatorname{sgn}(u), & u \neq 0 \\ 0, & u = 0 \end{cases}.$$

Thus, there is a remarkable equation relating the ground state charges which are induced by the one-pentagon, one-heptagon and three-heptagon defects:

$$Q(0)|_{N_d=1} = -Q(0)|_{N_d=-1} = Q(0)|_{N_d=-3}. \quad (32)$$

As it is shown in [9], the induced ground state charge is accumulated around a defect. This suggests that the same happens for the temperature-induced charge as well, and the local density of states is modified in an essential way in the vicinity of a defect.

We conclude that the theory predicts the dependence of the induced charge on the self-adjoint extension parameter in the cases of graphitic nanocones with one pentagon, one heptagon and three heptagons at the apex. This is due to the fact that the density of electronic states attains an additional piece which is odd in energy, see (25). Actually, there are three possibilities:  $\cos \Theta > 0$ ,  $\cos \Theta < 0$  and  $\cos \Theta = 0$ . The question of which of the possibilities is realized has to be answered by future experimental measurements.

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