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Dirac fermions on graphite cones

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The electronic structure of graphitic cones is investigated within the self-consistent field-theory model. The local and total density of states near the apex is found for cones of different opening angles. For extended electronic states, total density of states is found to vanish at the Fermi level at any opening angles more than 60°. In turn, for power-law localized states, normalized zero-energy modes are shown to emerge.

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The recently achieved atomic resolution of scanning tunneling microscope (STM) provides a further progress in experimental study of graphitic nanoparticles giving important information about electronic states of sample surfaces. Of special interest are graphitic cones where peculiar electronic states (due to topological defects in their apexes) were theoretically predicted [1, 2]. In particular, an analysis within the effective-mass theory shows that specific superstructures induced by pentagon defects can appear with the wave functions decaying as $r^{-1/5}$ [1]. An important conclusion made in [1] is that these superstructures are not the interference pattern of extended Bloch waves. On the other hand, the continuum model suggested in [2] predicts apical enhancement of density of states density of states at the Fermi energy (E_F)in the vicinity of the apex for cones with 120° disclinations. The states contributing to the nonzero density of states at E_F are found to be the extended states. This result looks rather unexpected (as is known the only cone with 60° opening angle is distinctive from the geometrical point of view) thus provoking our interest to reconsider the problem within a recently formulated self-consistent gauge model of disclinations on fluctuating elastic surfaces [3]. This model was also adapted for description of electronic states of a fullerene molecule in [4], where the normalized zero-energy states (at E_F) were found. Notice that specific electronic states at the Fermi level due to disclinations are similar to the fermion zero modes in topologically nontrivial manifolds which have been of current interest both in the field theory and condensed matter physics (see, e.g., [5 – 7]).

Before proceeding, it is necessary to make two important remarks. First, conical morphologies have been observed not only for graphite but also for other layered materials like boron nitride and aluminosilicates. It is intriguing that a departure from a flat surface can be solely determined by the topological defect located at the apex of a cone. In other words, a cone structure is formed when a pentagon is introduced into a graphite sheet. To gain a better understanding, one can imagine a cut-and-glue procedure in which the pentagon in the hexagonal network is constructed by cutting out a 60° sector from a graphene (a single layer of graphite) sheet. In this context, pentagonal defects in cones can be considered as apical disclinations and the opening angle is directly connected to the Frank index of a disclination (see below).

Second, the field-theory models for Dirac fermions on hexatic surfaces were formulated earlier to describe electronic structure of variously shaped carbon materials: fullerenes [8, 4], nanotubes [9], and cones [2]. The basic element for all these models is the self-consistent effective-mass theory for a description of electron dynamics in the vicinity of impurity in graphite intercalation compounds [10]. The most important fact found in [10] is that the electronic spectrum of a single graphite plane linearized around the corners of the hexagonal Brillouin zone coincides with that of the Dirac equation in (2+1) dimensions. In our approach, both electrons and disclinations are considered in the curved two-dimensional background. Thus, we formulate the Dirac equation on a cone with the flux due to pentagonal apical disclination represented by abelian gauge field.

To start let us briefly discuss a relevant geometrical background. In the polar coordinates $(r,\varphi) \in R^2$ a cone can be regarded as an embedding

$$(r,\varphi) \to (ar\cos\varphi,\, ar\sin\varphi,\, cr),\ 0 < r < 1,\ 0 \le \varphi < 2\pi,$$

with a and c being the cone parameters. From this the components of the induced metric can be easily read off:

$$g_{rr} = a^2 + c^2, \qquad g_{\varphi\varphi} = a^2 r^2, \qquad g_{r\varphi} = g_{\varphi r} = 0. \quad (1)$$

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The opening angle of a cone, θ, is determined by $\sin(\theta/2) = a/\sqrt{a^2+c^2}$. Since the cone itself appears when one or more sectors are removed from a graphene, all the possible disclination angles, ω, are divisible by $60°$. Thus, the Frank index, ν ($\nu = \omega/2\pi$), of the apical disclination can be specified by $\nu = 1 - \sin(\theta/2)$. At $\nu = 0$ one gets a flat graphene sheet ($\theta = 180°$). For $\nu = 1/6$ ($60°$ disclination), $\nu = 1/3$ ($120°$ disclination) and $\nu = 1/2$ ($180°$ disclination) one obtains $\theta = 112.9°, 83.6°, 60°$, respectively. For convenience, we introduce a parameter $\chi = 1 + c^2/a^2$, so that $\sin(\theta/2) = 1/\sqrt{\chi} = 1 - \nu$.

The basic field equation for the $U(1)$ gauge field in a curved background reads

$$D_\mu F^{\mu k} = 0, \quad F^{\mu k} = \partial^\mu W^k - \partial^k W^\mu \tag{2}$$

where covariant derivative $D_\mu := \partial_\mu + \Gamma_\mu$ includes the Levi-Civita (torsion-free, metric compatible) connection

$$\Gamma^k_{\mu\lambda} := (\Gamma_\mu)^k_\lambda = \frac{1}{2} g^{kl}\left(\frac{\partial g_{l\lambda}}{\partial x^\mu} + \frac{\partial g_{\mu l}}{\partial x^\lambda} - \frac{\partial g_{\mu\lambda}}{\partial x^l}\right),$$

$g_{\mu k}$ being the metric tensor on a Riemannian surface Σ with local coordinates (x^1, x^2). For a single disclination on arbitrary elastic surface a singular solution to (2) is found to be [3]

$$W^k = -\nu\varepsilon^{k\lambda} D_\lambda G(x^1, x^2), \tag{3}$$

where

$$D_\mu D^\mu G(x^1, x^2) = 2\pi\delta^2(x^1, x^2)/\sqrt{g}, \tag{4}$$

with $\varepsilon_{\mu k} = \sqrt{g}\epsilon_{\mu k}$ being the fully antisymmetric tensor on Σ, $\epsilon_{12} = -\epsilon_{21} = 1$. It should be mentioned that eqs. (2) and (4) self-consistently describe a defect located on an arbitrary surface [3].

From eqs. (3) and (4) the following solution can be obtained

$$W^r = 0, \qquad W^\varphi = -\nu\varepsilon^{\varphi r}\partial_r G, \qquad G = \sqrt{\chi}\log r. \tag{5}$$

As a result, $W^\varphi = (\nu/r)\sqrt{\chi/g}$ and $W_\varphi = \nu$.

To incorporate fermions we need a set of orthonormal frames $\{e_\alpha\}$ which yield the same metric, g, each of which is related to the other by the local $SO(2)$ rotation,

$$e_\alpha \to e'_\alpha = \Lambda^\beta_\alpha\, e_\beta, \quad \Lambda^\beta_\alpha \in SO(2).$$

It then follows that $g_{\mu\nu} = e^\alpha{}_\mu e^\beta{}_\nu \delta_{\alpha\beta}$ where $e_\alpha{}^\mu$ is the zweibein, with the orthonormal frame indices being $\alpha, \beta = \{1, 2\}$, and coordinate indices – $\mu, \nu = \{r, \varphi\}$. Explicitly, one may choose the only nonzero components to be $e^1{}_r = \sqrt{a^2+c^2}$ and $e^2{}_\varphi = ar$. Notice that $e_\alpha{}^\mu$ is the inverse of $e^\alpha{}_\mu$.

The Dirac equation on a cone takes the form (E_F is chosen to be zero)

$$H\psi := i\gamma^\alpha e_\alpha{}^\mu(\nabla_\mu + iW_\mu)\psi = E\psi, \tag{6}$$

where $\nabla_\mu = \partial_\mu + \Omega_\mu$ with

$$\Omega_\mu = -\frac{1}{8}\Gamma^\alpha{}_\mu{}^\beta[\gamma_\alpha, \gamma_\beta]$$

being the spin connection term which, as is known, does not contribute to the Dirac equation if $\dim\Sigma = 2$ [11].

In 2D the Dirac matrices can be chosen to be the Pauli matrices: $\gamma^1 = -\sigma^2, \gamma^2 = \sigma^1$. For massless fermions σ^3 serves as a conjugation matrix, and the energy eigenmodes are symmetric about $E = 0$ ($\sigma^3\psi_E = \psi_{-E}$). Generator of the local Lorentz transformations Λ takes the form $-i\partial_\varphi$, whereas the generator of the Dirac spinor transformations $\rho(\Lambda)$ is

$$\Sigma_{12} = \frac{i}{4}[\gamma_1, \gamma_2] = \frac{1}{2}\sigma^3.$$

Total angular momentum of a 2D Dirac system is, therefore

$$L_z = -i\partial_\varphi + \frac{1}{2}\sigma^3,$$

which commutes with the hamiltonian (6). Consequently, the eigenfunctions are classified with respect to the eigenvalues of $J_z = j + 1/2$, $j = 0, \pm1, \pm2, ...$, and are to be taken in the form

$$\psi = \begin{pmatrix} u(r)e^{i\varphi j} \\ v(r)e^{i\varphi(j+1)} \end{pmatrix}. \tag{7}$$

In this case (6) reduces to the pair

$$\begin{aligned} \partial_r u - \frac{\sqrt{\chi}(j+\nu)}{r}u &= \tilde{E}v, \\ -\partial_r v - \frac{\sqrt{\chi}(j+1+\nu)}{r}v &= \tilde{E}u, \end{aligned} \tag{8}$$

where $\tilde{E} = \sqrt{\chi}aE$. The most distinctive feature of (8) in comparison with the alternative model given in [2] is the appearance of the factor χ which characterizes geometry of a cone (cf. Eq.(5) from that paper). This plays a decisive role in the following consideration and finally leads to the remarkably different results. A general solution to (8) is found to be

$$\begin{pmatrix} u \\ v \end{pmatrix} = Ar^\xi \begin{pmatrix} J_\eta(\tilde{E}r) \\ \pm J_{\bar{\eta}}(\tilde{E}r) \end{pmatrix} \tag{9}$$

with $\xi = (1-\sqrt{\chi})/2$, $\eta = \pm(\sqrt{\chi}(j+\nu+1/2) - 1/2)$, and $\bar{\eta} = \pm(\sqrt{\chi}(j+\nu+1/2) + 1/2)$. A is a normalization factor. Thus, there are two independent solutions with $\eta(\bar{\eta}) > 0$ and $\eta(\bar{\eta}) < 0$. Notice also that signs $\pm$ in (9) correspond to states with $E > 0$ and $E < 0$, respectively. Due to the above-mentioned symmetry properties one can consider either case, for instance $E > 0$.

The important restrictions come from the normalization condition

$$\int (|u|^2 + |v|^2)\sqrt{g}dx^1 dx^2 = 1 \qquad (10)$$

which in view of (9) takes the form

$$2\pi\sqrt{\mu}a^2 A^2 \int_0^1 r^{2\xi+1}(J_\eta^2(\tilde{E}r) + J_{\bar{\eta}}^2(\tilde{E}r))dr = 1. \qquad (11)$$

The normalization factor can be deduced from the asymptotic formula for Bessel functions at large arguments. Indeed, in our case, $\bar{\eta} - \eta = 1$ so that $J_\eta^2 + J_{\bar{\eta}}^2 \to 2/\pi\tilde{E}r$ for $\tilde{E}r \gg 1$. Substituting this in (11) yields $A^2 = (2\xi + 1)E/4a$. Additionally, a restriction in the form $2\xi > -1$ (i.e., $\nu < 1/2$) serves to avoid divergence in (11). This means that the solution (9) is appropriate only for cones with opening angles more than $60°$. At the same time, (11) must be nonsingular at small r. This imposes a restriction on possible values of j. Namely, for $\eta, \bar{\eta} > 0$ one gets $j > -1$ (i.e., $j = 0, 1, 2...$) while for $\eta, \bar{\eta} < 0$ one has $j < -2\nu$ ($j = -1, -2, ...$). As is seen, possible values of j are not overlapped at any ν.

We are interested in the electron states near the apex of a cone. As it follows directly from (9), for small r the wave functions behave as

$$\begin{pmatrix} u \\ v \end{pmatrix} \sim \begin{pmatrix} E^{1/2+\eta} r^{\xi+\eta}, \\ E^{1/2+\bar{\eta}} r^{\xi+\bar{\eta}} \end{pmatrix}, \quad \eta, \bar{\eta} > 0,$$

$$\begin{pmatrix} u \\ v \end{pmatrix} \sim \begin{pmatrix} E^{1/2-\eta} r^{\xi-\eta}, \\ E^{1/2-\bar{\eta}} r^{\xi-\bar{\eta}} \end{pmatrix}, \quad \eta, \bar{\eta} < 0. \qquad (12)$$

To the leading order one obtains

$$\Psi \sim E^{(1-2\nu)/2(1-\nu)} r^{-\nu/(1-\nu)}.$$

In particular, for $\nu = 0,\ 1/6,\ 1/3$ we get $\Psi \sim \sqrt{E}$, $\Psi \sim E^{2/5} r^{-1/5}$, and $\Psi \sim E^{1/4} r^{-1/2}$, respectively.

Since the local density of states diverges as $r \to 0$ it is more relevant to consider the total density of states on a patch $0 < r \le \delta$ for small δ. To this end, one has to integrate the electron density over a small disk and to divide the result by $\Delta k = \pi/a$ which is the spacing of k values. The result is

$$D(E,\delta) \propto \begin{cases} E^{(1+2\nu)/(1-\nu)}\delta^{2/(1-\nu)}, & \eta, \bar{\eta} > 0; \\ E^{(1-2\nu)/(1-\nu)}\delta^{2(1-2\nu)/(1-\nu)}, & \eta, \bar{\eta} < 0. \end{cases} \qquad (13)$$

It should be stressed that according to (13) a specific behavior of $D(E,\delta)$ takes place only for $\nu = 1/2$ where $D \sim E^0\delta^0$. Thus, this prediction of our model agrees well with earlier remark that it is the $60°$ opening angle ($180°$ sector is removed from the flat graphene sheet) which is distinctive from the geometrical point of view. What is also important, in accordance with (13) there are no extended states with the nonzero density of states at E_F (recall that the case $\nu = 1/2$ is beyond the scope of our consideration). This conclusion markedly disagrees with the results obtained in [2]. As we show below, only power-law localized zero-energy states can exist. In the leading order one obtains from (13)

$$D(E,\delta) \propto \begin{cases} E\delta^2, & \nu = 0; \\ E^{4/5}\delta^{8/5}, & \nu = 1/6; \\ E^{1/2}\delta, & \nu = 1/3. \end{cases} \qquad (14)$$

It is interesting that the model [2] predicts the same δ-dependence while the E-dependence is completely different.

To study the electron states at the Fermi energy, one has to return to (8) and put $E = 0$. The solution reads

$$u_0 = Ar^\alpha, \qquad v_0 = Br^{-(\alpha+\sqrt{\chi})}. \qquad (15)$$

Here A and B are the normalization factors. A simple analysis shows that either u_0 or v_0 are normalizable on the cone of finite size. Thus, one can construct self-conjugate solutions $\binom{u_0}{0}$ and $\binom{0}{v_0}$. The first solution is nonsingular and, in the leading order, the electron density behaves as $|u_0|^2 \sim r^\beta/a^2$ with $\beta = 2\nu/(1-\nu)$. The second solution is singular, $|v_0|^2 \sim r^{-\beta}/a^2$. As before, in this case one can consider the total density of states for comparison to experiments. For our purposes, we dwell on the analysis of the case $\nu = 1/6$. As is seen, for $\nu = 1/6$ one gets $v_0 \sim r^{-1/5}$ and, accordingly, $D \sim \delta^{8/5}$. This is in a good agreement with the results obtained in [1]. Thus, our study confirms the results of [1, 12] that the states contributing to the nonzero density of states at the Fermi energy are power-law localized. Notice also that in monolayer graphite ($\nu = 0$) of infinite length ($a \to \infty$) there are no localized zero-energy electronic states on disclinations. It should be emphasized that this conclusion agrees with the results of numerical calculations [12] where the local density of states at the Fermi level was found to be zero for the case of five-membered rings (pentagons).

In conclusion, we have formulated a self-consistent field-theory model to describe electronic states on a graphitic cone. The topological nature of the apical defect is found to markedly modify the low-energy electronic structure. In particular, the total density of extended states has a rather specific dependence on both energy and a distance from the apex of a cone. In contrast to [2] we predict that there are no extended states with the nonzero density of states at the Fermi level for any disclinations with $\nu < 1/2$. At the same time, we found that power-like localized states can exist at the Fermi level in accordance with [1, 12]. It would be interesting to verify our conclusions in scanning tunneling microscope experiments with the graphitic cones.

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