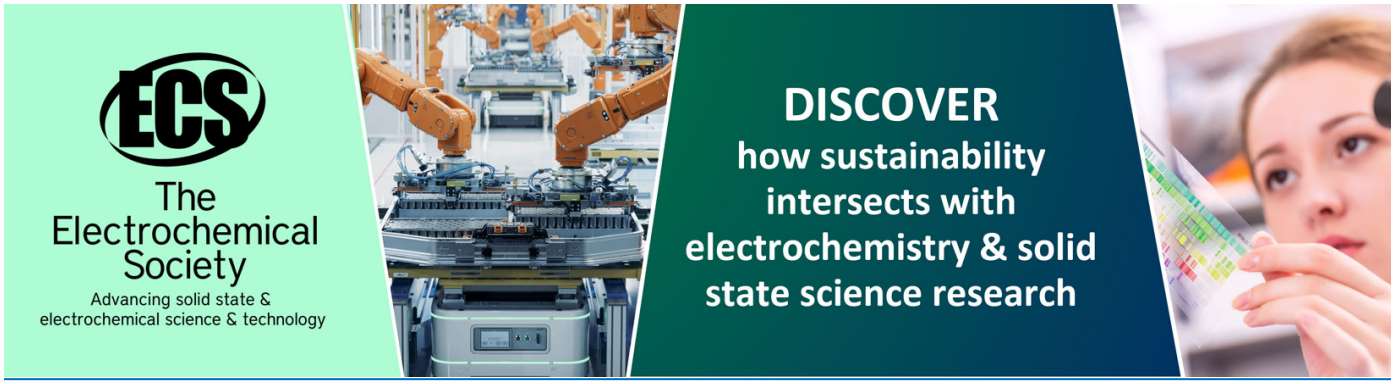
Topology, cosmic strings and quantum dynamics – a case study with graphene



Topology, cosmic strings and quantum dynamics - a case study with graphene

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Abstract. We explore the possibility to study the quantum dynamics of Dirac fermions in presence of a cosmic string by introducing a conical topological defect in gapped graphene in the presence of a Coulomb charge. When the Coulomb charge exceeds a certain critical strength, quantum instability sets in. Below the critical regime and for certain values of the system parameters, the allowed boundary conditions in gapped graphene cone can be classified in terms of a single real quantity. Observables such as local density of states, scattering phase shifts and the bound state spectra are dependent on the value of this real parameter, which has to be determined empirically. For a supercritical Coulomb charge, we analyze the system with a regularized potential as well as with a zigzag boundary condition and find the effect of the sample topology on the observable features of the system.

1. Introduction

The study of the topological properties of lower dimensional quantum systems show remarkable properties in various physical systems [1, 2, 3]. In the presence of a topological defect such as a cosmic string, whose exterior space-time has a topology, the dynamics of Dirac fermions exhibit novel nonperturbative quantum features such as inequivalent quantizations [2]. Though these features are theoretically interesting, it is difficult to devise an experiment with cosmic strings which will exhibit such quantum effects. In 2004 the experimental fabrication of monolayer graphene [4, 5, 6] offered a chance to observe the effects of topological defects [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26] in the laboratory. The low energy excitations in pristine graphene obey a 2D massless Dirac equation[27, 28, 29, 30, 31, 32, 33]. However violation of sublattice symmetry in graphene due to various impurities or short distance effects can lead to a mass gap in the system [34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51]. When a conical topological defect is introduced in such a system, some nontrivial holonomies [9, 10, 16] arise. The boundary conditions associated with the holonomies can be realized by introducing a suitable flux tube, analogous to a cosmic string, passing through the origin [2, 52, 53, 54, 55, 56, 57]. In our analysis, such a flux tube shall be used to model the conical topological defect on the 2D graphene sheet. Thus the gapped graphene cone in presence of an external Coulomb impurity offers a possibility to study the inequivalent quantization of massive Dirac fermions in the presence of cosmic strings.

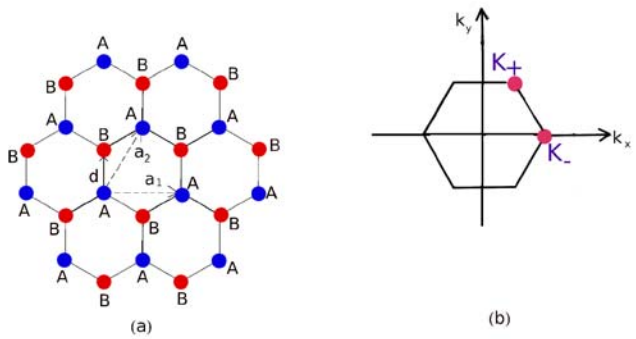

Figure 1. Hexagonal lattice structure of graphene and the Brillouin zone

The external Coulomb charge in a gapped graphene system can either be sub or supercritical. Here the critical charge refers to that value of Coulomb potential strength when the system dives into the negative energy continuum [58, 59, 60] indicating the quantum instability. The two different regimes of Coulomb potential are characterized by markedly different behaviour of the local density of states (LDOS) [58].

For a subcritical Coulomb charge impurity in the presence of the flux tube, we shall show that the quantization of the gapped graphene system is not unique and an additional parameter is required to fully characterize the boundary conditions at the origin, analogous to what was obtained for Dirac fermions in 2+1 dimensional gravity with a topological defect [2, 52].We shall also show that the experimental observables such as the LDOS, phase shifts and the bound state energies depend explicitly on that new parameter.

In the supercritical region the external Coulomb charge in gapped graphene cone can produce strong nonperturbative electric field effect [37, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72], at a relatively small value $Ze \sim 1$, due to the Fermi velocity $v_F \approx 10^6 m/s$ in graphene, which is 300 times smaller than the velocity of light. For supercritical charge, we study the system with a regularized Coulomb potential[58, 59] and also with a zigzag edge boundary condition. We shall show that the critical charge in gapped graphene cone is renormalized to a value higher than that of the gapless case and the value depends on the gap, the cut off parameter, the topology of the system and also on the boundary conditions used to obtain the quasibound state spectra in the supercritical region. It will be shown that with the increase in gap or cut off parameter the critical charge in presence of zigzag edge boundary condition increases more rapidly than in presence of a regularized Coulomb potential.

2. Low energy excitations in graphene cone with a Coulomb charge

Graphene has a hexagonal honeycomb lattice structure which is formed by two inter penetrating triangular sublattices [5, 6, 27, 29, 30] A and B. The low energy gapped excitations of planer graphene have minimum energy eigenvalues at the six vertices of the hexagonal first Brillouin zone of graphene and these vertices are known as the Dirac points. Among the six Dirac points, two are inequivalent [5, 6, 27, 29, 30]. We consider them to be situated at the opposite corners of the Brillouin zone and we denote their wave vectors by $\mathbf{K}_+$ and $\mathbf{K}_-$. The low-energy properties of the quasiparticle states in graphene near the Dirac point having valley index K_+, can be described by the Dirac equation

$$H\Psi = \left[-i(\sigma_1\partial_x + \sigma_2\partial_y) + m\sigma_3\right]\Psi = E\Psi, \tag{1}$$

where m denotes the Dirac mass generated due to sublattice symmetry breaking, E is the energy eigenvalue and we have set $\hbar = v_F = 1$. The Hamiltonian acts on the array of the slowly varying envelope functions $\Psi = \begin{pmatrix} \Psi_{K_+,A} \\ \Psi_{K_+,B} \end{pmatrix}$ and the Pauli matrices $\sigma_{1,2,3}$ act on the pseudospin indices A, B.

To study the effect of topology on this system, we consider to introduce local defects in the hexagonal lattice structure of graphene[9, 10] to form a cone.

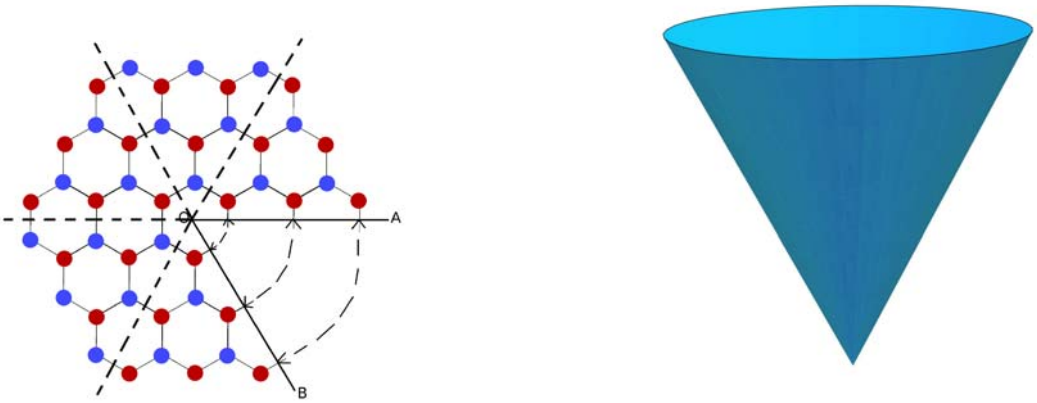

Figure 2. Formation of a cone from plane graphene sheet by cut and paste procedure.

The conical topology gives rise to nontrivial holonomies for the pseudoparticle wavefunctions in graphene. When a cone with angle of deficit $\frac{2n\pi}{6}$ is formed, where n can take only discrete values $1, 2, 3, 4, 5$, the angular boundary condition obeyed by the Dirac spinor as it goes around a closed path is given by

$$\Psi(r, \theta = 2\pi) = e^{i2\pi(1-\frac{n}{6})\frac{\sigma_3}{2}}\Psi(r, \theta = 0). \tag{2}$$

Here (r, θ) denotes the polar coordinate of the lattice points.

When the cone is formed by removing odd number of wedges of angle $\frac{2\pi}{6}$ an additional phase shift appears affecting the valley indices of the wave function in the boundary condition[9, 10, 11, 18]. The states with valley index K_- will be affected in the same manner as the states with valley index K_+ but there will be a relative phase difference of 180° between them (for details see [73]). Therefore this boundary condition can be described by involving a τ_2 matrix in it where the matrix τ_2 operate on the valley indices[9, 10, 74]. When n is even, this off diagonal matrix does not play any role and the exponential factor appearing in the boundary condition just gives ± 1 depending on the value of n. We diagonalize the matrix τ_2 for all allowed odd values of n. As a result the valley indices of the electronic states become mixtures of K_+ and K_-. Then the angular boundary condition satisfied for all values of n, by a branch of electronic states having a fixed Fermi index, is given by [9, 10]

$$\Psi(r, \theta = 2\pi) = e^{i2\pi[\pm\frac{n}{4}\sigma_0 + (1-\frac{n}{6})\frac{\sigma_3}{2}]}\Psi(r, \theta = 0). \tag{3}$$

Here σ_0 is an identity matrix which acts on the pseudospin indices A, B. $\Psi = \begin{pmatrix} \Psi_{A,K'} \\ \Psi_{B,K'} \end{pmatrix}$ where K' is a mixture of K_+ and K_-.

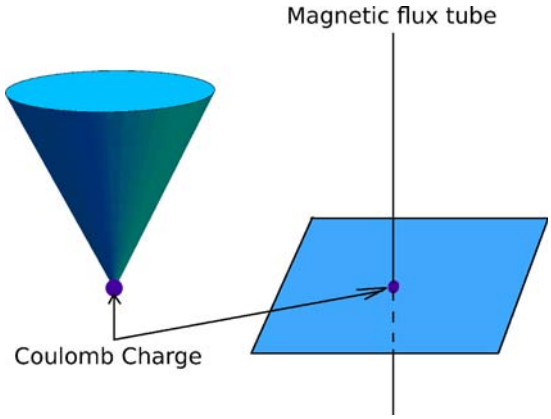

Figure 3. Graphene cone = planar graphene + flux tube

The effect of these holonomies can be modelled by introducing a fictitious magnetic flux tube [13] passing through the apex of the cone. The magnetic vector potential modifies the boundary condition on a Dirac spinor as

$$\Psi(r,\theta=2\pi) = e^{ie\oint \vec{A}\cdot\vec{ds}}\Psi(r,\theta=0). \tag{4}$$

Here $\vec{ds}$ is a line element on the circumference of the cone at a distance r from the apex, i.e.

$$\vec{ds} = \hat{e}_\theta \; r(1-\frac{n}{6})d\theta. \tag{5}$$

Substituting (5) in (4) and assuming that the component A_θ of the magnetic vector potential is independent of the angle θ, we have from Equation(3)

$$A_\theta = \frac{1}{er}[\pm\frac{\frac{n}{4}\sigma_0}{(1-\frac{n}{6})} + \frac{\sigma_3}{2}]. \tag{6}$$

Thus an external Coulomb charge localized at the apex of the gapped graphene cone can be equivalently described by a suitable combination of electric charge and magnetic flux tube [74]. Replacing the ordinary derivatives in the Hamiltonian by the corresponding covariant derivatives, the Dirac equation for the low energy excitations of gapped graphene cone in presence of a Coulomb charge at its apex is given by

$$H\Psi(r,\theta) = \begin{pmatrix} m-\frac{\alpha}{r} & \partial_r - \frac{i}{r(1-\frac{n}{6})}\partial_\theta \pm \frac{\frac{n}{4}}{r(1-\frac{n}{6})} + \frac{1}{2r} \\ -\partial_r - \frac{i}{r(1-\frac{n}{6})}\partial_\theta \pm \frac{\frac{n}{4}}{r(1-\frac{n}{6})} - \frac{1}{2r} & -m-\frac{\alpha}{r} \end{pmatrix} \begin{pmatrix} \Psi_A(r,\theta) \\ \Psi_B(r,\theta) \end{pmatrix}$$

$$= E \begin{pmatrix} \Psi_A(r,\theta) \\ \Psi_B(r,\theta) \end{pmatrix}. \tag{7}$$

Let

$$\Psi(r,\theta) = \sum_j \begin{pmatrix} \Psi_A^{(j)}(r) \\ \Psi_B^{(j)}(r) \end{pmatrix} e^{ij\theta}, \tag{8}$$

where j is half-integer. Substituting (8) in (2), we obtain that the leading short distance behavior of the wavefunction is given by

$$\Psi^{(j)}_{A,B}(r) \sim r^{\beta-\frac{1}{2}} \quad \text{where} \quad \beta = \sqrt{\gamma^2-\alpha^2} \quad \text{and} \quad \gamma = \frac{(j \pm \frac{n}{4})}{(1-\frac{n}{6})}. \tag{9}$$

From (9) we can see that when $|\alpha|$ exceeds $|\gamma|$, β becomes imaginary. Therefore, the eigenstates $\Psi^{(j)}_A(r)$ and $\Psi^{(j)}_B(r)$ becomes wildly oscillatory and have no well defined limit as $r \to 0$. For massive excitations the critical coupling α_c corresponds to that value of α for which $E = -m$. When $m = 0$, the value of α_c is equal to the minimum allowed value of γ and depending on the magnitude of Dirac mass and boundary conditions α_c increases gradually from γ. It will be shown that the critical coupling for the gapped graphene cone explicitly depends on the angle of the cone and also on the product of gap and cutoff parameter.

Depending on the strength of the external Coulomb charge compared to that of the critical charge of a gapped graphene cone with a particular opening angle, the effect of the charge impurity on the cone can be analyzed in two separate regions: subcritical and supercritical.

3. Inequivalent quantizations for graphene cone in the presence of a subcritical Coulomb charge

In this Section we discuss the bound and scattering state solutions of the Dirac fermions in a gapped graphene cone in the presence of a subcritical Coulomb charge impurity. To get the solutions following [37], we consider the ansatz

$$\Psi^j_A(\rho) = \sqrt{m+E}e^{-\frac{\rho}{2}}\rho^{\beta-\frac{1}{2}}[F(\rho)+G(\rho)] \tag{10}$$

and

$$\Psi^j_B(\rho) = \sqrt{m-E}e^{-\frac{\rho}{2}}\rho^{\beta-\frac{1}{2}}[F(\rho)-G(\rho)], \tag{11}$$

where $\rho = 2\kappa r$, $\kappa = \sqrt{m^2-E^2}$, $\beta = \sqrt{\gamma^2-\alpha^2}$, $\gamma = \frac{(j\pm\frac{n}{4})}{(1-\frac{n}{6})}$ and total angular momentum j takes all half integer values. Bound states occur when the wavefunctions reduce to polynomials i.e. when

$$\beta - \frac{\alpha E}{\kappa} = -N, \tag{12}$$

where

$$N = \begin{cases} 0,1,2,..., \text{ when } \gamma > 0, \\ 1,2,3...., \text{ when } \gamma < 0. \end{cases} \tag{13}$$

The corresponding bound state spectra is obtained as

$$E_p = \frac{m\ \mathrm{sgn}(\alpha)}{\sqrt{1+\frac{\alpha^2}{(p+\beta)^2}}}. \tag{14}$$

Here the energy should be of the same sign (positive or negative) as α because otherwise the value of N will become negative and in our range of interest, it is not allowed (for details see [73]).

In the scattering state sector the parameter $\kappa = \sqrt{m^2-E^2}$ is purely imaginary, i.e. $\kappa = -ik$ [37], where k is defined as $k = \sqrt{E^2-m^2}$. Consequently, the variable ρ also becomes purely imaginary, $\rho = -2ikr$. Using the $r \to \infty$ limit of the scattering states the scattering matrix is obtained as

$$S(k) = (2ik)^{\frac{2i\alpha E}{k}} \frac{(\gamma + i\frac{m\alpha}{k})}{\left(\beta - i\frac{E\alpha}{k}\right)} \frac{\Gamma\left(1+\beta-i\frac{\alpha E}{k}\right)}{\Gamma\left(1+\beta+i\frac{E\alpha}{k}\right)} e^{i\pi\left(\beta+i\frac{\alpha E}{k}\right)}. \tag{15}$$

From Equation(15) it can be seen that the poles of the S matrix determined by $\left(1+\beta-i\frac{\alpha E}{k}\right)=1-N$, where N is a nonzero positive integer and $\left(\beta-i\frac{E\alpha}{k}\right)=0$ when $\gamma>0$, gives back the corresponding bound states as expected.

The Dirac equation discussed in the previous section is valid only for low energy excitations. Therefore the short range interactions produced by the conical defect as well as the Coulomb charge impurity, cannot be incorporated as dynamical terms in the Dirac equation. However, a suitable choice of boundary conditions can take into account the combined effect of those short range interactions. In systems with unitary time evolution those allowed boundary conditions can be determined using the well defined prescription due to von Neumann[75, 76, 77, 78]. Below we recall the salient features of this idea.

A symmetric operator T with domain $D(T)\subset\mathcal{H}$ is self-adjoint if and only if

$$T=T^{*} \text{ and } D(T)=D(T^{*}).$$

where T^{*} denote the operator adjoint to T and $\mathcal{H}$ is the Hilbert space. To check whether T is self-adjoint or not we consider the equations

$$T^{*}\phi_{+}=+i\phi_{+}$$

$$T^{*}\phi_{-}=-i\phi_{-}.$$

Let $n_{\pm}$ denote the number of linearly independent square integrable solutions of the above two equations respectively. The pair (n_{+},n_{-}) are called the deficiency indices for the operator T. The operator T can be classified in terms of the deficiency indices as follows:

1. T is essentially self-adjoint iff $(n_{+},n_{-})=(0,0)$.
2. T is not self-adjoint but has self-adjoint extensions iff $n_{+}=n_{-}=n\neq 0$.
3. If $n_{+}\neq n_{-}$,then T has no self-adjoint extensions.

If T admits self-adjoint extension, von Neumann's prescription tells us that its domain of self adjointness is given by

$$\begin{aligned} D_{U}(T) &= \Big\{\phi+\phi_{+}+U\phi_{-}\Big|\phi\in D(T) \\ &\qquad \text{and } U \text{ is a } n\times n \text{ unitary matrix}\Big\}. \end{aligned} \tag{16}$$

We can see from Equation(2) that the angular part of Dirac operator H operates on a domain $Y(\theta)$ which is spanned by the antiperiodic functions $e^{ij\theta}$ where j is a half integer and the corresponding boundary condition is kept unchanged. The radial Dirac operator H_{ρ}, given by

$$H_{\rho}=\begin{pmatrix} \rho\frac{d}{d\rho}+\left(\beta-\frac{\alpha E}{\kappa}\right) & -\left(\gamma+\frac{m\alpha}{\kappa}\right) \\ \left(-\gamma+\frac{m\alpha}{\kappa}\right) & \rho\frac{d}{d\rho}+\left(\beta-\rho+\frac{\alpha E}{\kappa}\right) \end{pmatrix},$$

is symmetric in the domain $\mathcal{D}_{0}=C_{0}^{\infty}(R^{+})$ which consists of infinitely differentiable functions of compact support in the real half line R^{+} and its adjoint operator $H_{\rho}^{\dagger}$ has the same expression as H_{ρ} but its domain can be different. Now to determine the domain of self-adjointness of the Dirac operator H, consider the equations

$$H^{\dagger}\Psi_{\pm}=\pm\frac{i}{l}\Psi_{\pm}, \tag{17}$$

where l has the dimension of length. The total number of square integrable, linearly independent solutions of Equation(17) gives the deficiency indices for H and they are denoted by $n_{\pm}$.

To find the deficiency indices $n_{\pm}$ let us first consider the following.

$$\Psi^{j}_{A\pm}(\rho) = \sqrt{m \pm \frac{i}{l}} e^{-\frac{\rho}{2}} \rho^{\beta-\frac{1}{2}} [F_{\pm}(\rho) + G_{\pm}(\rho)] \tag{18}$$

and

$$\Psi^{j}_{B\pm}(\rho) = \sqrt{m \mp \frac{i}{l}} e^{-\frac{\rho}{2}} \rho^{\beta-\frac{1}{2}} [F_{\pm}(\rho) - G_{\pm}(\rho)], \tag{19}$$

where $\rho = 2\kappa_1 r$, $\kappa_1 = \sqrt{m^2 + \frac{1}{l^2}}$, $\beta = \sqrt{\gamma^2 - \alpha^2}$ and $\gamma = \frac{(j \pm \frac{n}{4})}{(1-\frac{n}{6})}$.

Using these expressions and proceeding as prescribed by von Neumann it can be shown that $\psi_{A\pm}$ and $\psi_{B\pm}$ are square integrable everywhere provided $0 < \beta < \frac{1}{2}$ and for this parameter range $n_{\pm} = 1$ (for details see [73]).

Thus we have a one parameter family of self-adjoint extensions, labeled by a real parameter $z \in R \bmod (2\pi)$ which enters the low energy dynamics of the Dirac fermions of gapped graphene cone through boundary conditions to ensure the unitary time evolution of the system. All the physically interesting quantities such as bound state energies, scattering phase shifts and LDOS depend on the choice of this self-adjoint extension parameter z. The parameter z cannot be determined theoretically, but instead must be obtained empirically. It would be interesting to see if there is any corresponding effect in the full tight-binding description of graphene. In terms of the system parameters and the self-adjoint extension parameter z the spectrum is determined by the equation

$$f(E) \equiv \left(\frac{\kappa^2}{1+m^2}\right)^{\beta} \frac{\left(1-\beta-\frac{\alpha E}{\kappa}\right)\Gamma\left(1+\beta-\frac{\alpha E}{\kappa}\right)\Gamma\left(1-2\beta\right)}{\left(1+\beta-\frac{\alpha E}{\kappa}\right)\Gamma\left(1-\beta-\frac{\alpha E}{\kappa}\right)\Gamma\left(1+2\beta\right)}$$

$$= \frac{\xi_1 \cos\left(\phi_1 + \frac{z}{2}\right)}{\xi_2 \cos\left(\phi_2 + \frac{z}{2}\right)}.$$

where

$$\sqrt{m + \frac{i}{l}}(P_+ + R_+) = \xi_1 e^{i\phi_1}$$

$$\text{and} \quad \sqrt{m + \frac{i}{l}}(Q_+ + S_+) = \xi_2 e^{i\phi_2}.$$

and P_+, Q_+, R_+ and S_+ are system parameter dependent constants (for detailed calculation see [73]). Though the equation cannot be solved analytically, from a typical plot of $f(E)$ it can be obtained numerically.

We have used the following expression given in Equation(20) for LDOS during the plotting.

$$\mu(E, r) = \frac{4}{\pi \hbar v_F} \sum_j |\Psi^{(j)}(k, r)|^2. \tag{20}$$

We have plotted the energy dependence of LDOS at a distance close to the charge impurity ($r = 1.2$). From these Figures we can observe that LDOS depend on the values of self-adjoint extension parameter z and also on the topology of the system. Therefore measurement of LDOS is a major experimental activity in graphene physics which should yield information about the self-adjoint extension parameter and the topology of the system.

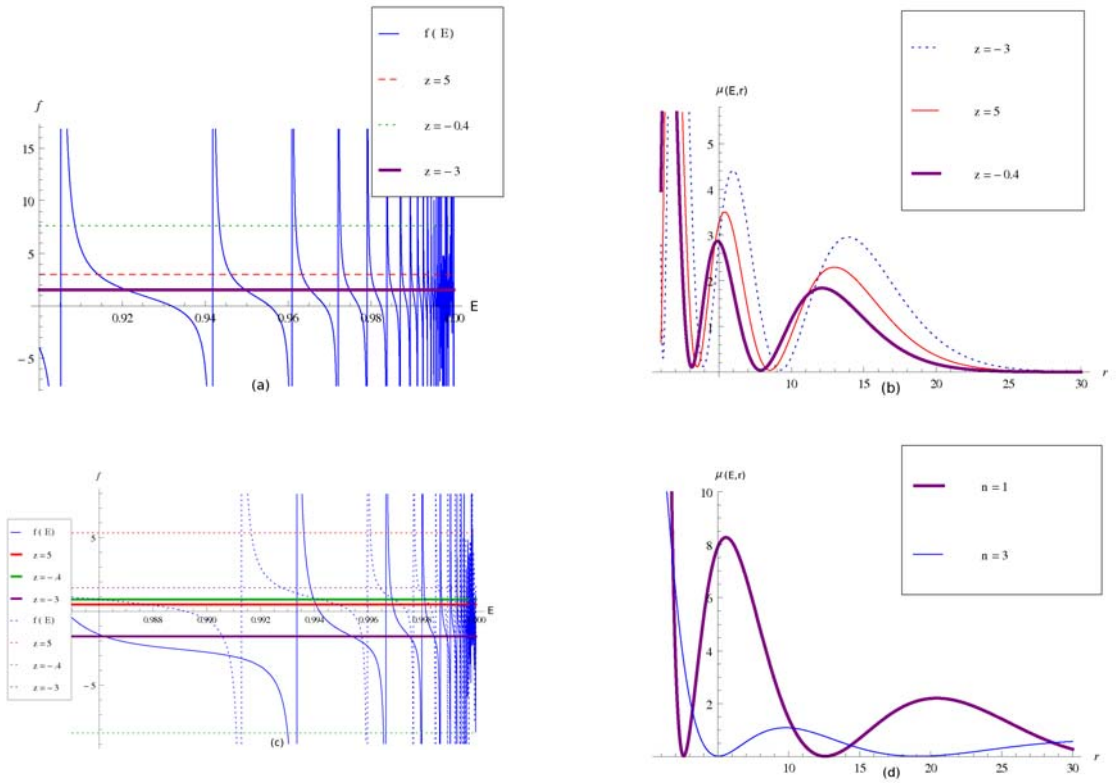

Figure 4. (a)Plot of $f(E)$ is shown for system parameters $j = \frac{3}{2},\ n = 1,\ \alpha = 1.49$ and $m = 1$. The three horizontal line corresponds to the three different values of the self-adjoint extension parameter $z = 5, -0.4, -3$. (b) Dependence of LDOS in the bound state sector of the gapped graphene cone on the distance r from the external charge impurity is shown for three different values of bound state energy corresponding to three different values of self-adjoint extension parameter. Here the contribution from angular momentum channel $j = \frac{3}{2}$ is shown and the system parameters are $n = 1,\ \alpha = 1.49$ and $m = 1$. We have assumed $l = 1$. (c) Plot of $f(E)$ is shown for two different values of n (1 and 3) with system parameters $j = \frac{1}{2}$, $\alpha = 0.28$ and $m = 1$. The three horizontal line corresponds to the three different values of the self-adjoint extension parameter $z = 5, -0.4, -3$. The solid lines correspond to $n = 3$ and the dotted lines correspond to $n = 1$. (d) Dependence of LDOS on the distance r from the external charge impurity is shown for two different values of bound state energy corresponding to two different values of n with the self-adjoint extension parameter $z = -0.4$. Here the contribution from angular momentum channel $j = \frac{1}{2}$ is shown and the system parameters are $\alpha = 0.28$ and $m = 1$.

The scattering matrix $\mathbf{S}(k)$ for gapped graphene cone for the parameter range $0 < \beta < \frac{1}{2}$ is given as

$$\mathbf{S}(k) = (2ik)^{2i\frac{\alpha E}{k}} \frac{-\frac{\xi_1\cos(\phi_1+\frac{z}{2})}{\xi_2\cos(\phi_2+\frac{z}{2})}(2\kappa_1)^{2\beta}(2\kappa)^{-2\beta}\frac{1+f_2}{1+f_1}f_1\frac{\Gamma(1+2\beta)}{\Gamma(1+\beta+i\frac{\alpha E}{k})} + f_2\frac{\Gamma(1-2\beta)}{\Gamma(1-\beta+i\frac{\alpha E}{k})}}{-\frac{\xi_1\cos(\phi_1+\frac{z}{2})}{\xi_2\cos(\phi_2+\frac{z}{2})}(2\kappa_1)^{2\beta}(2\kappa)^{-2\beta}\frac{1+f_2}{1+f_1}\frac{\Gamma(1+2\beta)}{\Gamma(1+\beta-i\frac{\alpha E}{k})}e^{-i\pi(\beta+i\frac{\alpha E}{k})} + \frac{\Gamma(1-2\beta)}{\Gamma(1-\beta-i\frac{\alpha E}{k})}e^{-i\pi(-\beta+i\frac{\alpha E}{k})}},$$

where

$$f_1 \equiv \frac{\beta + \frac{i\alpha E}{k}}{\gamma - \frac{im\alpha}{k}}, \quad f_2 \equiv \frac{-\beta + \frac{i\alpha E}{k}}{\gamma - \frac{im\alpha}{k}}. \tag{21}$$

Thus we can see scattering phase shifts also depend explicitly on the self-adjoint extension

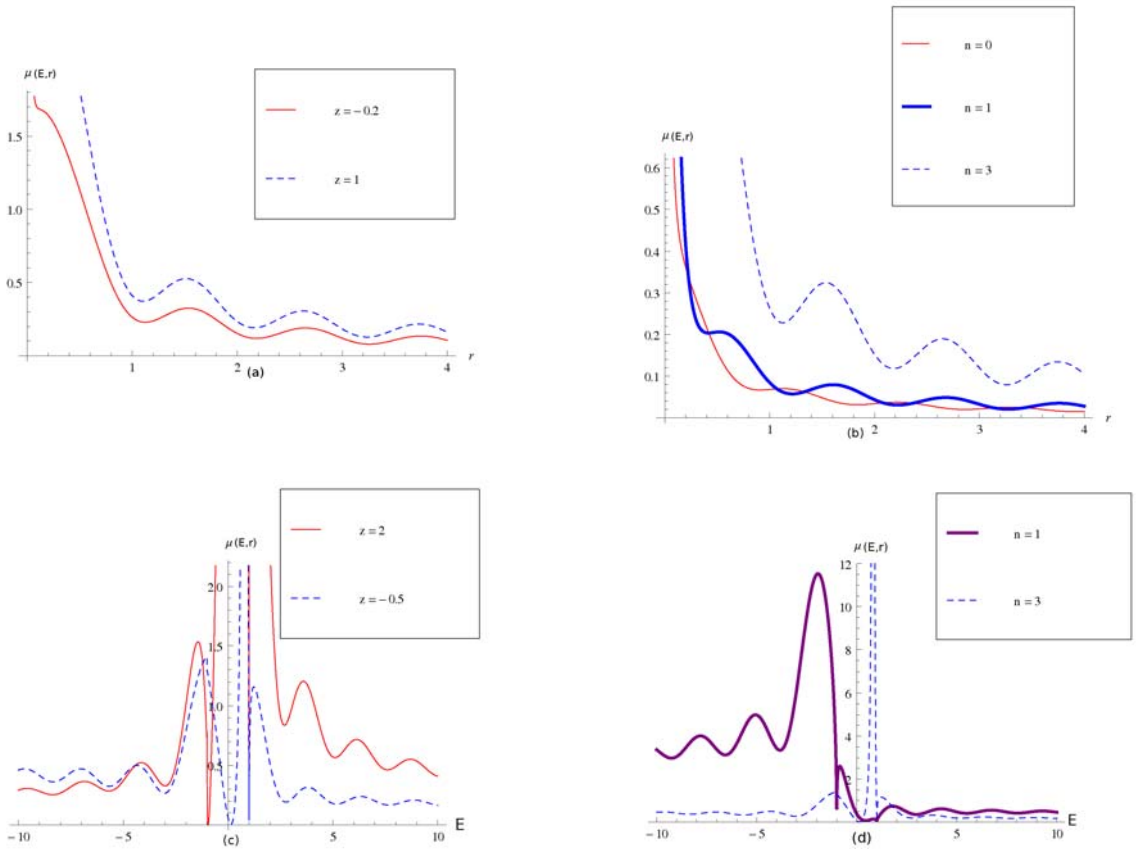

Figure 5. (a)Dependence of LDOS on the distance r from the Coulomb impurity is shown for two different values of self-adjoint extension parameter $z = -0.2, 1$ and a particular value of $E = 3$ and with $j = \frac{1}{2}$, $n = 3$, $\alpha = 0.28$ and $m = 1$. (b) Effect of topology on r dependence of LDOS is shown for self-adjoint extension parameter $z = -0.2$, $E = 3$ and system parameters $\alpha = 0.28$, $n = 0, 1, 3$ and $m = 1$ considering contribution coming from the angular momentum channel $j = \frac{1}{2}$. (c)Energy dependence of LDOS is shown for two different values of self-adjoint extension parameter $z = 5, -0.8$ at a distance $r = 1.2$ from the external Coulomb impurity. The system parameters used for the plot are $\alpha = 0.28$ and $m = 1$ and contribution coming from the angular momentum channel $j = \frac{1}{2}$ is considered. (d) Effect of topology on the energy dependence of LDOS is shown for self-adjoint extension parameter $z = -0.8$, angular momentum channel $j = \frac{1}{2}$ and system parameters $\alpha = -0.28$, $n = 1, 3$ and $m = 1$

parameter z and the topology of the system. For each value of z (mod 2π), we have an inequivalent set of the scattering data.

4. Effects of topological defects in the supercritical regime of gapped graphene

In the supercritical region β is always imaginary as the Coulomb potential strength α exceeds the value of γ. We denote $\beta = i\eta = \sqrt{\alpha^2 - \gamma^2}$. This region is marked by the quantum instability in the system. Therefore we need to regularize the Coulomb potential to study the effect of an external supercritical Coulomb charge on the gapped graphene cone. We shall also consider the zigzag edge boundary condition in our analysis.

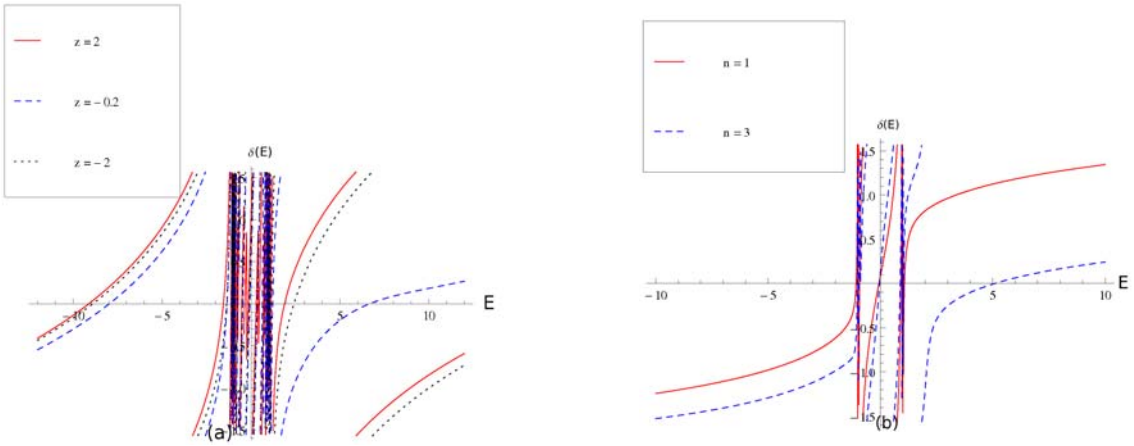

Figure 6. (a)Phase shifts in the gapped graphene cone is shown for three different values of the self-adjoint extension parameter $z = 2, -0.2, -2$ where the system parameters are $n = 1, j = \frac{3}{2}, \alpha = 1.46$, and $m = 1$. (b) Scattering phase shifts are shown for different angles of the gapped graphene cone with the self-adjoint extension parameter $z = -0.2$ and system parameters $j = \frac{1}{2}, \alpha = 0.28$ and $m = 1$.

4.1. Regularized Coulomb potential

In presence of a regularized Coulomb potential the bound states can be extended until the negative continuum $E = -m$ is reached[58, 59]. The regularization of the Coulomb potential is given by

$$V(r) = \begin{cases} -\alpha/r, & r > a, \\ -\alpha/a, & r \leq a. \end{cases} \tag{22}$$

Here a is the minimum distance of the Dirac electron from the apex where the Coulomb charge is placed and it is of the order of the lattice parameter. The Dirac equation for gapped graphene cone is solved for the two different regions $r > a$ and $r \leq a$ separately. Then we use the continuity condition of the wave function at $r = a$ to determine the quasibound state energy spectrum which is given by

$$f(E) \equiv f_r(E) = \mathrm{Arg}[\Gamma(1 + 2i\eta)] \tag{23}$$

where

$$f_r(E) = \mathrm{Arg}\left[\Gamma\left(1 + i\eta - \frac{E\alpha}{\kappa}\right)\right] + \mathrm{Arg}\left[\gamma - \frac{\alpha}{\kappa}(m - E) + i\eta\right] + \eta \ln(2\kappa a) + \mathrm{Arg}\left[\gamma - \alpha \frac{J_{|\gamma+\frac{1}{2}|}(\alpha)}{J_{|\gamma-\frac{1}{2}|}(\alpha)} - i\eta\right] + p\pi$$

and p is a positive integer (for details see [73]).

As the regularized potential allows the bound states to dive into negative energies and the critical charge of a gapped graphene cone refers to that value of a Coulomb potential for which $E = -m$, we have

$$\alpha_c = \gamma + \frac{\pi^2}{2\gamma \log^2[2m\gamma Ca]} \tag{24}$$

where

$$C = \exp\left[-2\psi(1) - \frac{J_{|\gamma-\frac{1}{2}|}(\gamma)}{\gamma(J_{|\gamma-\frac{1}{2}|}(\gamma) - J_{|\gamma+\frac{1}{2}|}(\gamma))}\right] \tag{25}$$

for the region near the critical potential. From Equation (24) we can see when $ma \to 0, \alpha_c \approx \gamma$ which agrees with the result obtained for massless case [74]. Also for $n = 0, \gamma = j$ and for $j = \frac{1}{2}$, the dependence of the critical charge on the gap and the cutoff parameter agrees with that obtained in [59].

4.2. Zigzag edge boundary condition

To find out the energies of the quasistationary states formed in the supercritical region now we use the zigzag edge boundary condition $\Psi^j_B(a) = 0$, where a is a distance from the apex, of the order of the lattice scale in graphene. The quasibound state energy spectrum is given by

$$f(E) \equiv f_z(E) = \mathrm{Arg}[\Gamma(1 + 2i\eta)] \tag{26}$$

where

$$f_z(E) = \mathrm{Arg}\left[\Gamma\left(i\eta - \frac{E\alpha}{\kappa}\right)\right] + \mathrm{Arg}\left[\gamma + \frac{\alpha}{\kappa}(m + E) - i\eta\right] + \eta \ln(2\kappa a) + p\pi$$

and p is a positive integer (for detailed calculation see [73]). This quasibound state energy

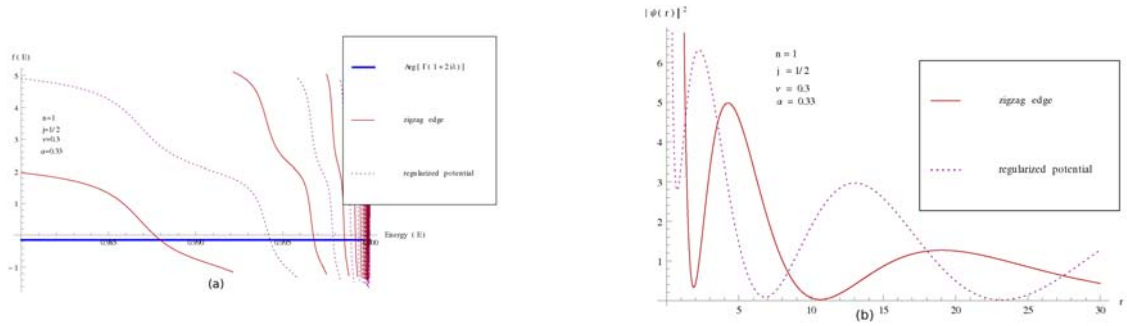

Figure 7. (a)Quasibound state energy spectrum with zigzag edge boundary condition and regularized Coulomb potential. Here the blue line represents $\mathrm{Arg}[\Gamma(1 + 2i\eta)]$ and the dashed and the solid line represents $f_z(E)$ and $f_r(E)$ respectively. (b)Dependence of $|\Psi(r)|^2$ on the distance r from the charge impurity placed at the apex of the gapped graphene cone is shown for both the zigzag edge boundary condition and regularized Coulomb potential. The values of energy are obtained from the quasibound state energy spectrum.

spectrum for zigzag edge boundary can be compared with the spectrum obtained for the regularized potential and the effect of the two different boundary conditions on the spectrum can be observed from Fig.(7).

Proceeding in the same manner as for regularized potential, we can see with zigzag edge boundary the critical charge of the system is given by

$$\alpha_c = \gamma + \frac{\pi^2}{2\gamma \log^2[2m\gamma a \exp(-2\psi(1))]}. \tag{27}$$

Here also from Equation (27) we can see when $ma \to 0, \alpha_c \approx \gamma$ which agrees with the result obtained for massless case [74]. The critical charge has been shown to depend on the nonzero mass, cutoff parameter and the different opening angles of the gapped graphene cone. The dependence of the critical charge on ma is compared for two different boundary conditions.

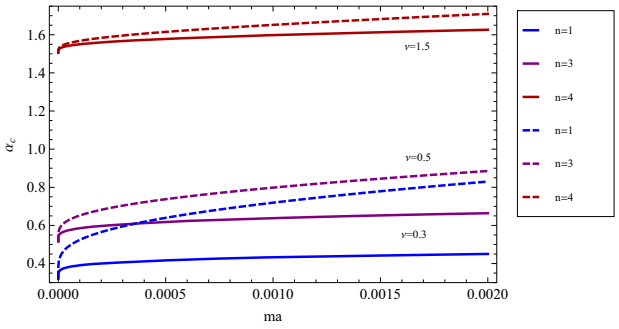

Figure 8. Dependence of critical charge on the nonzero mass and cutoff parameter are shown for both zigzag edge boundary condition and regularized Coulomb potential for different opening angles of the gapped graphene cone. The dotted lines show the dependence for zigzag edge boundary condition and the solid lines show the dependence for regularized Coulomb potential.

5. Conclusion

Inequivalent quantization arising from self-adjoint extensions is one of the earliest predictions of quantum mechanics. To experimentally realize that prediction, here in our analysis we have considered the opportunity provided by the massive Dirac fermions in gapped graphene in the presence of a conical defect and an external Coulomb impurity. The combination of this conical defect as well as the Coulomb impurity results in short distance interactions in the system. For a subcritical charge impurity, the effect of these short range interactions can be modelled through appropriate choice of boundary conditions which are labelled by a single real parameter and satisfies the requirement of a unitary time evolution. We have shown that the observables such as LDOS, scattering phase shifts and bound state energies depend explicitly on this parameter. This feature of gapped graphene cone agrees well with the prediction made for Dirac fermions in a plane in the presence of a cosmic string and thus the study of the gapped graphene cone considered here have established its importance for being more amenable to empirical analysis.

The supercritical regime of the Coulomb impurity have been analyzed with a regularized Coulomb potential as well as with a zigzag boundary condition. Quantum instability characterizes this regime and we have shown that the quasibound state spectra and the probability amplitude depend explicitly on the number of sectors removed from a planar graphene to form the cone. In addition, the dependence of the critical charge on the product of the Dirac mass m and the cutoff parameter a has been obtained. Though the nature of the dependence is similar for both the regularized Coulomb potential and the zigzag boundary condition but in the latter case the critical charge increases more rapidly with ma than the former case.

Thus the quantum dynamics of massive Dirac fermions of a graphene sample have been studied in presence of a conical topology and an external Coulomb charge and the study has offered a possibility to experimentally observe the inequivalent quantization of Dirac fermions in the presence of a string defect and many other interesting supercritical phenomena. More details of the analysis presented here can be found in [73].

References

[1] Jackiw R and Rebbi C 1976 *Phys. Rev.* D **13** 3398
[2] de Sousa Gerbert P 1989 *Phys. Rev.* D **40** 1346-49
[3] Hindmarsh M B and Kibble T W B 1995 *Rep. Prog. Phys* **58** 477
[4] Novoselov K S, Geim A K, Morozov S V, Jiang D, Katsnelson M I, Grigorieva I V and Firsov A A 2004 *Science* **306** 666
[5] Novoselov K S, Geim A K, Morozov S V, Jiang D, Katsnelson M I, Grigorieva I V, Dubonos S V and Firsov A A 2005 *Nature* **438** 197
[6] Zhang Y, Tan Y-W, Stormer H L and Kim P 2005 *Nature* **438** 201
[7] Gonzalez J, Guinea F and Vozmediano M A H 1992 *Phys. Rev. Lett.* **69** 172
[8] Gonzalez J, Guinea F and Vozmediano M A H 1993 *Nucl. Phys.* B **406** 771

[9] Lammert P E, Crespi V H 2000 *Phys. Rev. Lett.* **85** 5190
[10] Lammert P E, Crespi V H 2004 *Phys. Rev.* B **69** 035406
[11] Kolesnikov D V and Osipov V A 2006 *Eur. Phys. J.* B **49** 465
[12] Sitenko Y A and Vlasii N D 2007 *Nucl. Phys.* B **787** 241
[13] Cortijo A and Vozmediano M A H 2007 *Nucl. Phys.* B **763** 293
[14] de Juan F, Cortijo A and Vozmediano M A H 2007 *Phys. Rev.* B **76** 165409
[15] Hou C Y, Chamon C and Mudry C 2007 *Phys. Rev. Lett.* **98** 186809
[16] Pachos J K, Stone M and Temme K 2008 *Phys. Rev. Lett.* **100** 156806
[17] Furtado C, Moraes F, Carvalho A M de M 2008 *Phys. Lett.* A **372** 5368
[18] Roy A and Stone M 2010 *J. Phys.* A **43** 015203
[19] Vozmediano M A H, Katsnelson M I and Guinea F 2010 *Phys. Reports* **496** 109-148
[20] Gonzalez J and Herrero J 2010 *Nucl. Phys.* B **825** 426-443
[21] Yazyev O V and Louie S G 2010 *Phys. Rev.* B **81** 195420
[22] Fonseca J M, Moura-Melo W A and Pereira A R 2010 *Phys. Lett.* A **374** 4359
[23] de Juan F, Cortijo A, Vozmediano M A H and Cano A 2011 *Nature Physics* **7** 810
[24] Abedpour N, Asgari R and Guinea F 2011 *Phys. Rev.* B **84** 115437
[25] Bakke K, Petrov A Y and Furtado C 2011 Kaluza-Klein description of geometric phases in graphene *Preprint* arXiv:1111.0836 [cond-mat.mes-hall]
[26] Cortijo A, Guinea F and Vozmediano M A H 2012 *J. Phys.* A **45** 383001
[27] Wallace P R 1947 The band theory of graphite. *Phys. Rev.* **71** 622
[28] DiVincenzo D P and Mele E J 1984 *Phys. Rev.* B **29** 1685
[29] Semenoff G W 1984 *Phys. Rev. Lett.* **53** 2449
[30] Geim A K and Novoselov K S 2007 *Nature Materials* **6** 183
[31] Castro Neto A H, Guinea F, Peres N M R, Novoselov K S and Geim A K 2009 *Rev. Mod. Phys.* **81** 109
[32] Peres N M R 2010 *Rev. Mod. Phys.* **82** 2673
[33] Das Sarma S, Adam S, Hwang E H and Rossi E 2011 *Rev. Mod. Phys.* **83** 407
[34] Gorbar E V, Gusynin V P, Miransky V A and Shovkovy I A 2002 *Phys. Rev.* B **66** 045108
[35] Khveshchenko D V and Leal H 2004 *Nucl. Phys.* B **687** 323
[36] Kane C L and Mele E J 2005 *Phys. Rev. Lett.* **95** 226801
[37] Novikov D S 2007 *Phys. Rev.* B **76** 245435
[38] Gusynin V P, Miransky V A, Sharapov S G and Shovkovy I A 2008 *Phys. Rev.* B **77** 205409
[39] Khveshchenko D V 2009 *J. Phys.: Condens. Matter* **21** 075303
[40] Gamayun O V, Gorbar E V and Gusynin V P 2010 *Phys. Rev.* B **81** 075429
[41] Li W, Liu G-Z 2010 *Phys. Lett.* A **374** 2957
[42] Araki Y and Hatsuda T 2010 *Phys. Rev.* B **82** 121403 (R)
[43] Araki Y 2011 *J. Phys.: Conf. Series* **302** 012022
[44] Zhu J L, Sun S and Yang N 2012 *Phys. Rev.* B **85** 035429
[45] Han M Y, Ozyilmaz B, Zhang Y and Kim P 2007 *Phys. Rev. Lett.* **98** 206805
[46] Zhou S Y *et al* 2007 *Nat. Mater.* **6** 770
[47] Zhou S Y *et al* 2008 *Nat. Mater.* **7** 259
[48] Haberer D *et al* 2010 *Nano Letters*, **10** 3360
[49] Cooper D R *et al* 2012 *ISRN Condensed Matter Physics* Vol. **2012** 501686
[50] Andrei E Y *et al* 2012 *Rep. Prog. Phys.* **75** 056501
[51] Ki D-K, Morpurgo A F 2012 *Phys. Rev. Lett.* **108** 266601
[52] de Sousa Gerbert P and Jackiw R 1989 *Commun. Math. Phys.* **124** 229-260
[53] Yamagishi H 1983 *Phys. Rev.* D **27** 2383
[54] Jackiw R and Pi S Y 2007, *Phys. Rev. Lett.* **98** 266402
[55] Chamon C, Hou C Y, Jackiw R, Mudry C, Pi S Y and Semenoff G 2008 *Phys.Rev.* B **77** 235431
[56] Jackiw R and Pi S Y 2008 *Phys. Rev.* B **78** 132104
[57] Jackiw R, Milstein A I, Pi S Y and Terekhov I S 2009 *Phys. Rev.* B **80** 033413
[58] Pereira V M, Kotov V N and Castro Neto A H 2008 *Phys. Rev.* B **78** 085101
[59] Gamayun O V, Gorbar E V and Gusynin V P 2009 *Phys. Rev.* B **80** 165429
[60] Gamayun O V, Gorbar E V and Gusynin V P 2011 *Phys. Rev.* B **83** 235104
[61] Reinhardt J and Greiner W 1977 *Rep. Prog. Phys.* **40** 219
[62] Greiner W, Müller B and Rafelski J 1985 *Quantum Electrodynamics of Strong Fields* (Berlin: Springer-Verlag)
[63] Katsnelson M I, Novoselov K S and Geim A K 2006 *Nature Physics* **2** 620
[64] Katsnelson M I and Novoselov K S 2007 *Solid State Communications* **143** 3
[65] Pereira V M, Nilsson J and Castro Neto A H 2007 *Phys. Rev. Lett.* **99** 166802
[66] Shytov A V, Katsnelson M I and Levitov L S 2007 *Phys. Rev. Lett.* **99** 236801

[67] Shytov A V, Katsnelson M I and Levitov L S 2007 *Phys. Rev. Lett.* **99** 246802
[68] Shytov A, Rudner M, Gu N, Katsnelson M and Levitov L 2009 *Solid State Comm.* **149** 1087
[69] Gupta K S and Sen S 2009 *Mod. Phys. Lett.* A **24** 99
[70] Milstein A I, Terekhov I S 2010 *Phys. Rev.* B **81** 125419
[71] Wang J, Fertig H A and Murthy G 2010 *Phys. Rev. Lett.* **104** 186401
[72] Kotov V N, Uchoa B, Pereira V M, Guinea F and Castro Neto A H 2012 *Rev. Mod. Phys.* **84** 1067
[73] Chakraborty B, Gupta K S and Sen S 2012 *Preprint* arXiv:1207.5705v3 [hep-th], to appear in J. Phys. **A**.
[74] Chakraborty B, Gupta K S and Sen S 2011 *Phys. Rev.* B **83** 115412
[75] Reed M and Simon B 1972 *Methods of Modern Mathematical Physics* Vol. **2** (New York: Academic Press)
[76] Falomir H and Pisani P A G 2001 *J. Phys. A : Math. Gen.* **34** 4143
[77] Gupta K S and Sen S 2008 *Phys. Rev.* B **78** 205429
[78] Gupta K S, Samsarov A and Sen S 2010 *Eur. Phys. J.* B **73** 389