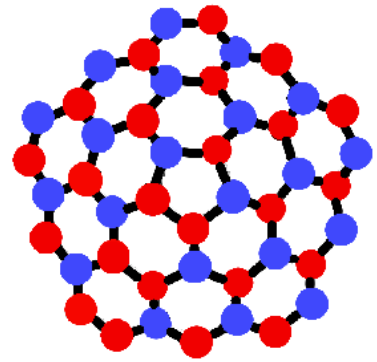
Effect of Topology on Quantum Dynamics in Graphene



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Plan of the Talk:

- Introduction
- Dirac equation obeyed by graphene with a Coulomb charge.
- Definition of critical charge.
- Effect of conical topology on critical charge.
- Effect of conical topology on the supercritical region of gapless graphene.
- Effect of conical topology on the supercritical region of gapped graphene.
- Effect of conical topology on the subcritical region of gapped graphene.
- Discussion on generalized boundary conditions.
- Concluding remarks

Introduction

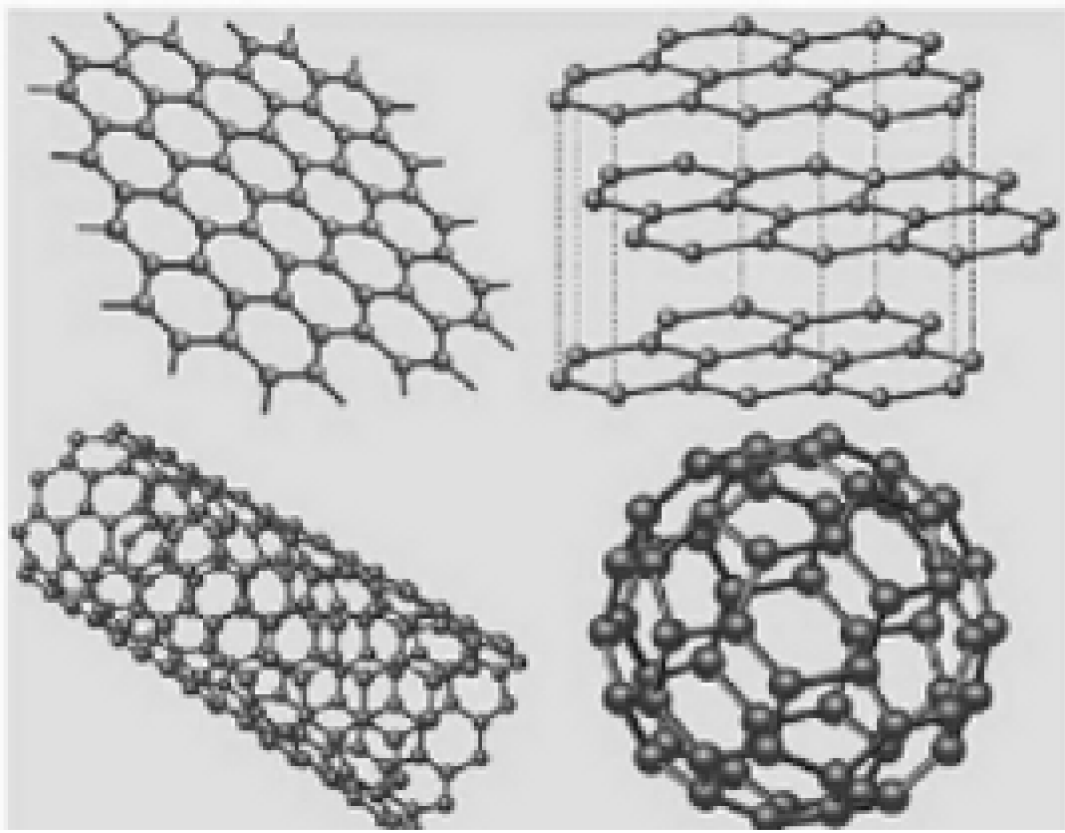


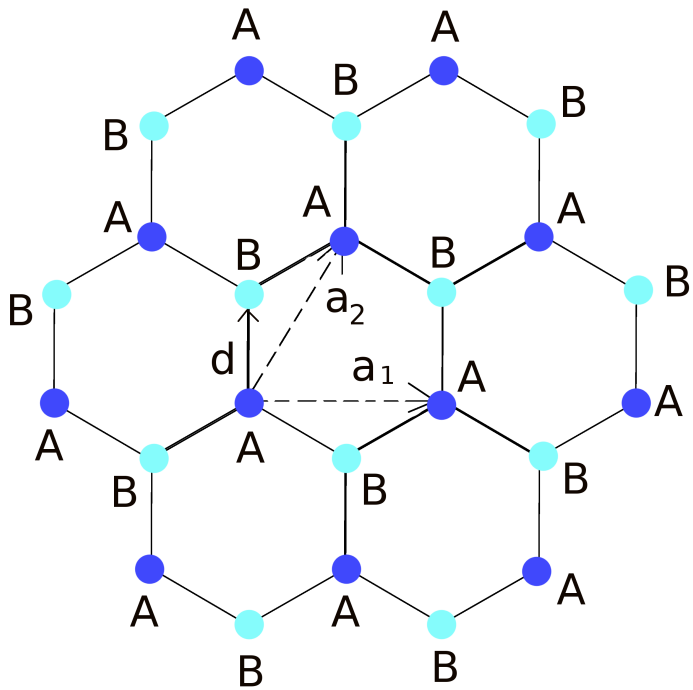
Figure 1: Graphene-Mother of all allotropic forms of carbon.[Source: 'The electronic properties of graphene' by A.H.Castro Neto, F.Guinea, N.M.R.Peres, K.S.Novoselov and A.K.Geim.(Rev. Mod. Phys. 81, 109 (2009))]

Introduction

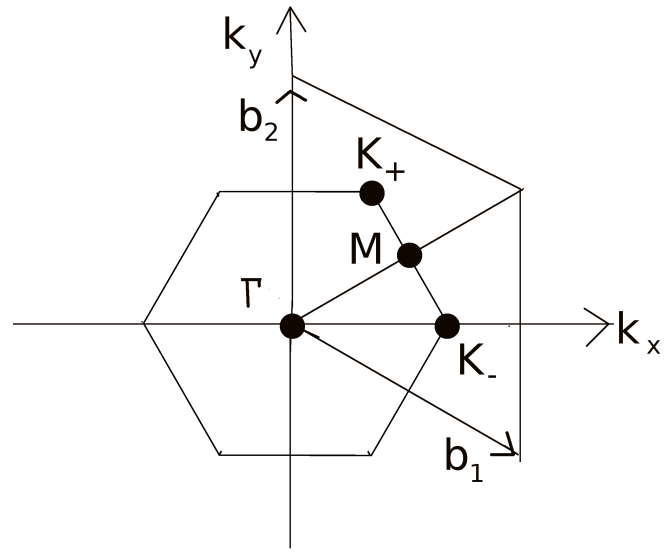
- Graphene is the first example of a truly two dimensional crystal.

- It was experimentally discovered in 2004 when a group of physicists from Manchester University, led by Geim and Novoselov, extracted a single sheet (a monolayer of atoms) of graphene from graphite by the micromechanical cleavage technique.
  [Ref: K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, Science 306, 666 (2004).]

Introduction



(a)



(b)

Figure 2: (a)Lattice structure of graphene and (b)Corresponding Brillouin zone

Introduction

- Graphene has a planer hexagonal honeycomb lattice structure as shown in the figure.
- The hexagonal lattice is made of two triangular sublattices. The lattice sites are denoted by type A and type B.
- The reciprocal lattice is also hexagonal. Among its six vertices only two are inequivalent corresponding to the two sublattices A and B. These two points are known as Dirac points and denoted by K_+ and K_-.

Introduction

- Assuming tight binding approximation in graphene we obtain the Hamiltonian as

$$H = \int_B \frac{d^2k}{(2\pi)^2} \begin{pmatrix} U^\dagger(\vec{k}) & V^\dagger(\vec{k}) \end{pmatrix} \begin{pmatrix} \beta & \gamma \sum_i e^{i\vec{k}\cdot\vec{u_i}} \\ \gamma \sum_i e^{-i\vec{k}\cdot\vec{u_i}} & -\beta \end{pmatrix} \begin{pmatrix} U(\vec{k}) \\ V(\vec{k}) \end{pmatrix}.$$

- Here $U^\dagger$ and U ($V^\dagger$ and V) are the creation and destruction operators for electrons localized on sites A (B) respectively.
- The hopping parameter γ is related to the probability amplitude for electron transfer between neighbouring sites.
- The energy difference between the sublattices A and B are parameterized by β. Semenoff, PRL 53,2449(1984)

Introduction

- The energy eigenvalues can be determined by diagonalizing the matrix given in the expression of tight binding Hamiltonian.

- The separation between the positive and negative energy eigenvalues depends on the parameter β. It is minimum at the Dirac points of the Brillouin zone.

- For gapless graphene $\beta = 0$ and there is no separation between the positive and negative energy eigenvalues at the Dirac points i.e conduction and valence band of graphene touch each other at the six vertices of the Brillouin zone of gapless graphene.

- If an external perturbation breaks the honeycomb lattice symmetry in graphene, a gap can be generated in its electronic spectrum and then $\beta \neq 0$. Consequently the Dirac fermions acquire an effective mass m in gapped graphene.

Introduction

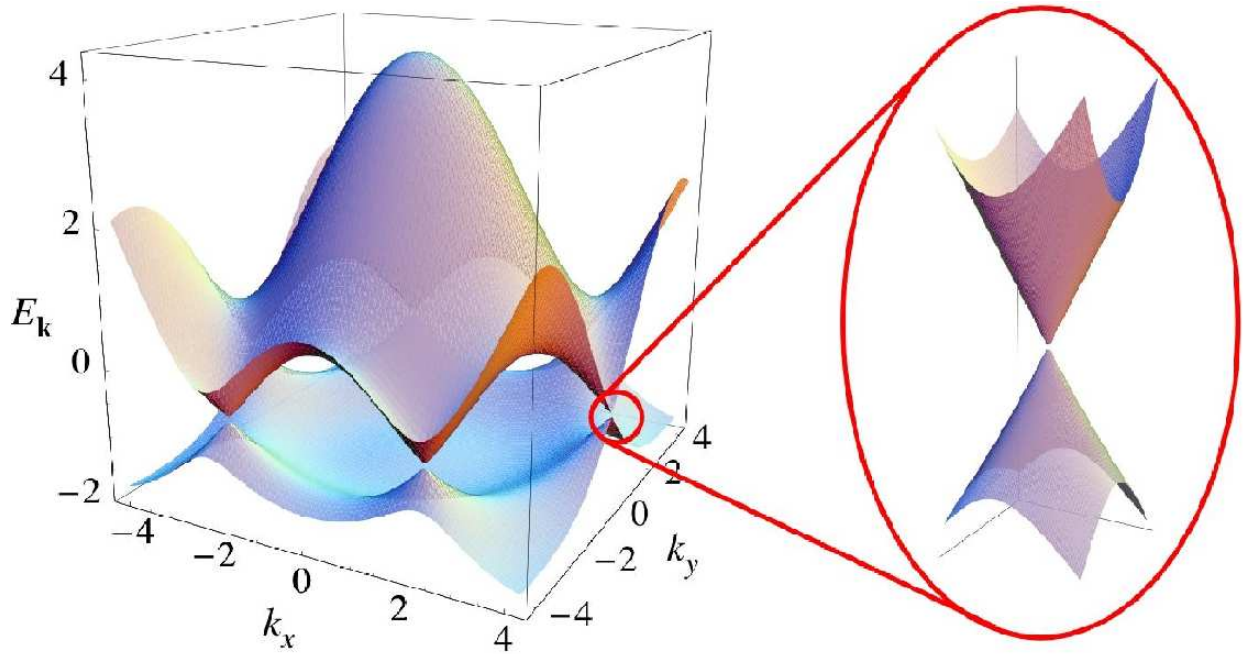


Figure 3: Energy spectrum of planar graphene(Ref:A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, A. K. Geim, Rev. Mod. Phys. 81, 109 (2009))

Introduction

- Low energy excitations of a two dimensional graphene sample behave like Dirac Fermions with the Fermi velocity $v_F \approx 10^6 m/s$.
- Due to a small external charge impurity $Ze \sim 1$, effective Coulomb interaction strength in the sample is given by $\alpha = \frac{Ze^2}{\hbar \kappa v_F} \sim 1$, where the dielectric constant $\kappa \sim 5$.
- When the effective strength of the external charge exceeds a certain critical value α_c, quasi-bound states appear in the spectrum.
- Can nontrivial topology affect α_c and the quantum dynamics ?

The Dirac Equation

- The low energy properties of the quasiparticle states near the Fermi points in graphene can be described by the four component Dirac wave function

$$\Psi = \begin{pmatrix} \Psi_A \\ \Psi_B \end{pmatrix}, \text{ where } \Psi_A = \begin{pmatrix} \Psi_{A_+} \\ \Psi_{A_-} \end{pmatrix} \text{ and } \Psi_B = \begin{pmatrix} \Psi_{B_+} \\ \Psi_{B_-} \end{pmatrix}$$

- The pseudospin indices A and B label the two sublattices of the primitive cell of graphene and the valley indices $+$ and $-$ label the two inequivalent Dirac points $\mathbf{K}_+$ and $\mathbf{K}_-$ respectively.

Dirac equation

- The Dirac equation for the excitations of planar graphene in the presence of a Coulomb charge Ze around the Dirac point K_+ is given by

$$\left[-i\hbar v_F(\sigma_1\partial_x + \sigma_2\partial_y) + \sigma_0\left(\frac{-\alpha}{r}\right) + m\sigma_3\right]\Psi = E\Psi,$$

  where r is the radial coordinate in the two dimensional $x-y$ plane. The Pauli matrices $\sigma_{1,2,3}$ and the identity matrix σ_0 act on the pseudospin indices A, B and m is the Dirac mass generated due to the sublattice symmetry breaking.

- For gapless graphene m=0.

Short Distance Behaviour of Dirac spinor

- The Dirac equation can be separated by assuming the solution of the form

$$\Psi(r,\theta) = \begin{pmatrix} \Psi_A(r) \\ i\Psi_B(r)\, e^{i\theta} \end{pmatrix} \frac{1}{\sqrt{2\pi}} e^{i(j-\frac{1}{2})\theta} e^{-\eta r} r^{\gamma-\frac{1}{2}},$$

  where θ denotes the corresponding polar angle, $\eta = \sqrt{(m^2 - E^2)}$ and j is the half integral azimuthal quantum number.

- The leading short distance behaviour of the wavefunction is given by

$$\Psi^{(j)}_{A,B}(r) \sim r^{\gamma-\frac{1}{2}} \text{ where } \gamma = \sqrt{j^2 - \alpha^2}.$$

Critical Charge in planer graphene

- From the expression of γ it follows that when $|\alpha|$ exceeds $|j|$, γ becomes imaginary and as a result the nature of the wave function becomes oscillatory at the position of the charge impurity.
- The critical value of the coupling is denoted by α_c and it is given by the minimum allowed value of $|j|$ i.e $\frac{1}{2}$.
- For a plane graphene sheet, $\alpha_c = 0.5$.

Formation of Cone from Planar Graphene

- A cone is formed from a two dimensional plane by introducing a topological defect which modifies the angular boundary condition.
- Here we assume that the graphene cone is formed by removing a sector AOB from the plane sheet of graphene and then identifying the edges OA and OB of the sector.
- Due to this identification the frame $\{\hat{e}_x, \hat{e}_y\}$ becomes discontinuous across the joining line. So we choose a new set of frames rotated with respect to the old frame by an angle $\phi = \theta + \frac{\pi}{2}$ in the counter clockwise direction

  Lammert and Crespi, PRL 85, 5190 (2000)

Formation of Cone from Planar Graphene

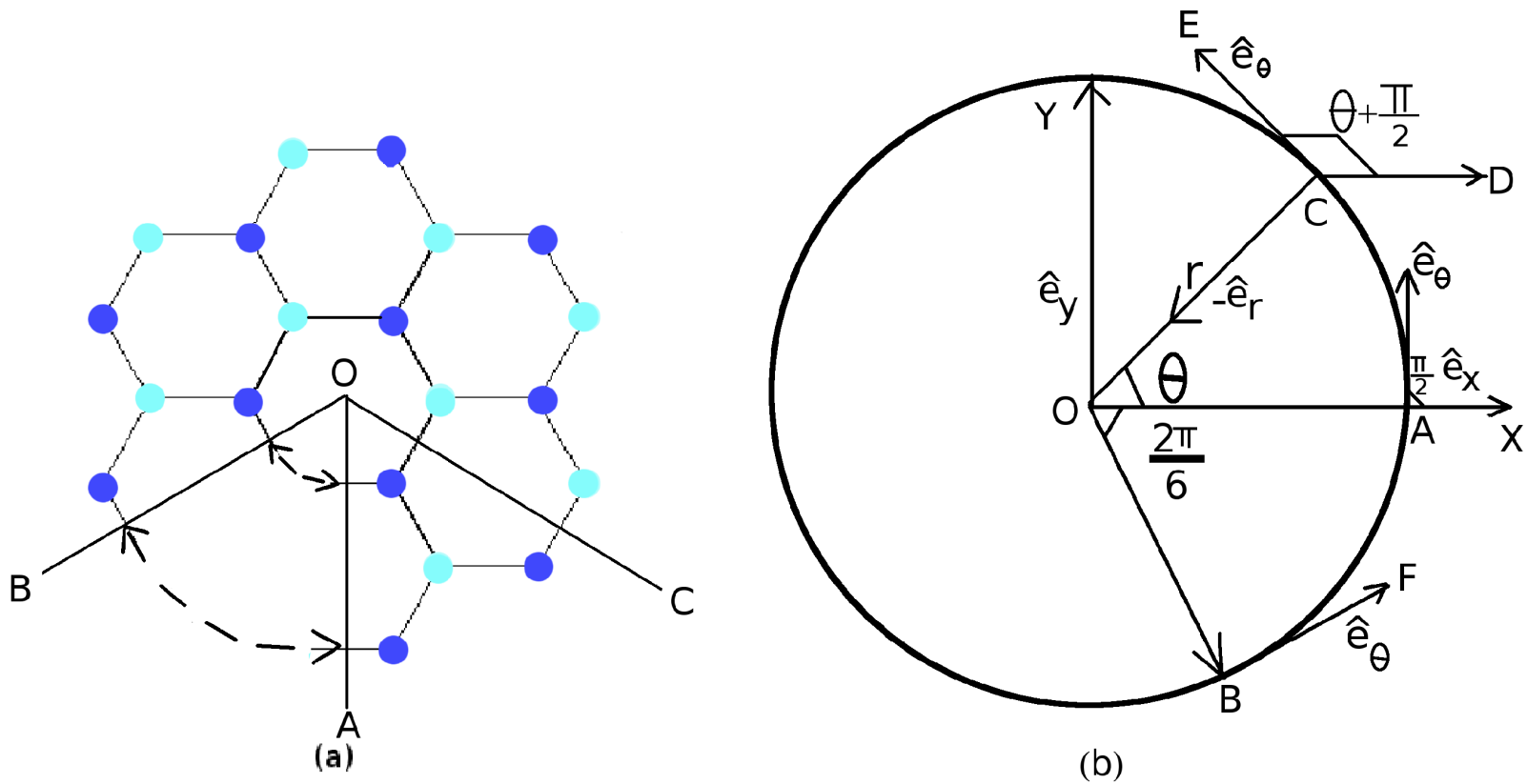


Figure 4: (a)Formation of a cone from plane graphene sheet by cut and paste procedure and (b)Rotation of the coordinate frame due to its new orientation.

Holonomy Modelled Through a Magnetic Flux Tube

- When a cone is formed from a plane graphene sheet by removing n number of sectors, the angular boundary condition obeyed by the Dirac spinor is given by

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

- The effect of the angular boundary condition on the wave function can be equivalently described by introducing a magnetic flux tube passing through the apex of the cone. The presence of a magnetic vector potential modifies the boundary condition on a Dirac spinor as

$$\Psi(\mathbf{r}, \theta = 2\pi) = -e^{ie2\pi r(1-\frac{n}{6})A_\theta}\Psi(\mathbf{r}, \theta = 0).$$

Dirac equation for a graphene cone with a Coulomb charge

- Comparing the two expressions for $\Psi(\mathbf{r}, \theta = 2\pi)$ we get

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

- Thus the Dirac equation can be written as

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

- For gapless graphene m=0.

Gapless Graphene Cone:Short Distance Behaviour

- We use an ansatz for the wavefunction given by

$$\Psi(r,\theta) = \sum_j \begin{pmatrix} \Psi_A^{(j)}(r) \\ i\Psi_B^{(j)}(r) \end{pmatrix} e^{-iEr} r^{\gamma-\frac{1}{2}} e^{ij\theta},$$

  where the total angular momentum j takes all half integer values.

- Substituting this ansatz in the Dirac equation with $m = 0$, we note that the leading short distance behaviour of the wavefunction is given by

$\Psi_{A,B}^{(j)}(r) \sim r^{\gamma-\frac{1}{2}}$ where $\gamma = \sqrt{\nu^2 - \alpha^2}$ and $\nu = \dfrac{(j \pm \frac{n}{4})}{(1-\frac{n}{6})}$.

Critical Charge in graphene cone

- From the expression of γ it follows that when $|\alpha|$ exceeds $|\nu|$, γ becomes imaginary.
- The critical value of the coupling is denoted by α_c and it is given by the minimum allowed value of $|\nu|$.
- The parameter ν depends on j and the number of sectors n removed from a plane to form the graphene cone. Hence we see that the critical coupling α_c explicitly depends on the angle of the graphene cone. Thus a conical topology affects the critical charge of the system.

Dependence of Critical Charge on Conical Topology

Table 1: The values of critical charge α_c i.e the minimum values of $|\nu|$ for different values of opening angle of the graphene cone i.e for different values of n.

value of n	Critical charge (α_c)	Corresponding (j)
0	0.5	$\pm\frac{1}{2}$
1	0.3	$\pm\frac{1}{2}$
2	0	$\pm\frac{1}{2}$
3	0.5	$\pm\frac{1}{2}$
4	1.5	$\pm\frac{1}{2}$
5	1.5	$\pm\frac{3}{2}$

Gapless Graphene Cone:Scattering Matrix

- Using the zigzag edge boundary condition $\Psi_B^{(j)}(a_0) = 0$, where a_0 is a distance from the apex, of the order of the lattice scale in graphene we obtain the scattering matrix S as

$$S = e^{2i\delta_\nu(k)} = \left[\frac{f_{\alpha,\lambda} + e^{2i\zeta(k)}e^{-\pi\lambda}\mu f_{\alpha,-\lambda}}{e^{\pi\lambda}\mu f^*_{\alpha,-\lambda} + e^{2i\zeta(k)} f^*_{\alpha,\lambda}}\right] e^{-2i\alpha \ln(2kr)}$$

where

- $k = -E$, $\lambda = \sqrt{\alpha^2 - \nu^2}$ and $\mu = \sqrt{\frac{\alpha+\lambda}{\alpha-\lambda}}$.
- $f_{\alpha,\lambda} = \frac{\Gamma(1+2i\lambda)}{\Gamma(1+i\lambda-i\alpha)}$ and $e^{2i\zeta(k)} = \frac{i(1+i\mu)}{(1-i\mu)} e^{2i\lambda \ln(2ka_0)}$.

Gapless Graphene Cone:Scattering Phase Shift

- The scattering phase shift is given by

$$\delta_\nu(k) = \arg[e^{-i\zeta(k)} + be^{i\zeta(k)}] - \alpha \ln(2kr) + \arg(f_{\alpha,\lambda})$$

  where $b = e^{-\pi\lambda}\mu\frac{f_{\alpha,-\lambda}}{f_{\alpha,\lambda}}$.

- We plot the scattering phase shift ignoring the Coulomb tail term $-\alpha ln(2kr)$.

- The plot shows that the phase shift depends on the topology through its dependence on n via ν. When the coupling α is deeper in the supercritical region, the phase shift is observed to have more number of kinks, which indicate the bound states.

Plot of Scattering Phase Shift

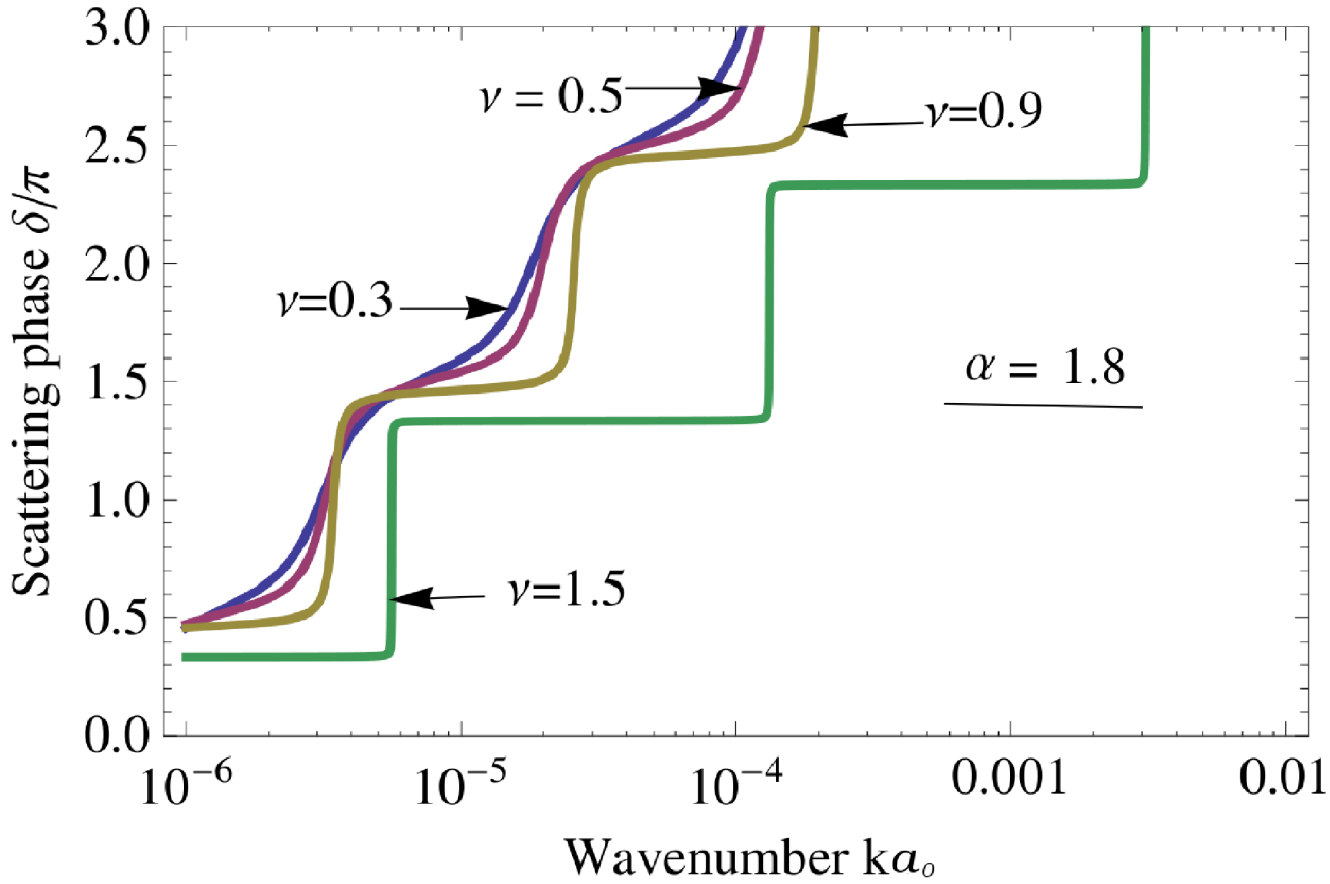


Figure 5: Dependence of scattering phase shift δ on wavenumber ka_0 for $\nu = 0.3, 0.5, 0.9, 1.5$ and $\alpha = 1.8$, ignoring the Coulomb tail term $-\alpha ln(2kr)$. As the value of ν increases, the kinks in the phase shift become sharper, which indicates the dependence of the phase shift on the angle of the graphene cone.

Gapless Graphene Cone:Quasi-bound state Energy

- In gapless graphene we do not expect bound states due to Klein tunneling.
- In the supercritical regime, the system admits quasi-bound states whose spectrum is obtained from the zeroes of the S matrix.
- The quasi-bound state energies are given by

$$E_p = -\frac{1}{2a_0}\exp\left[-\frac{p\pi}{\lambda} + i\left(\frac{1}{2\alpha} - \frac{\pi}{2}\right)\right],$$

where p is a positive integer.

Plot of Quasi-bound state Energy

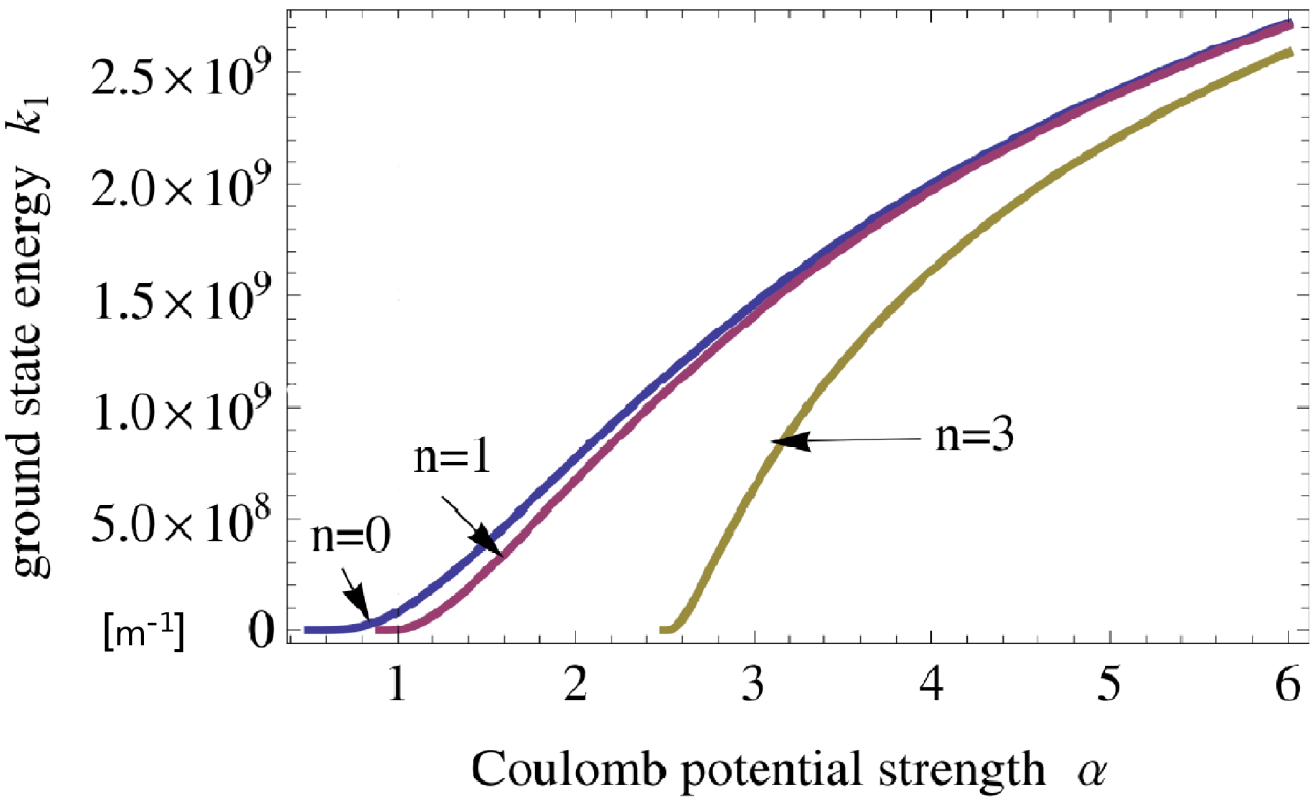


Figure 6: Dependence of ground state energy on the Coulomb potential strength for different angles of the graphene cone. We have considered $\nu = \frac{j+\frac{n}{4}}{1-\frac{n}{6}}$ and $j = \frac{1}{2}$.

Gapless Graphene Cone:LDOS

Another interesting observable in this context is the LDOS. We have plotted the standing wave oscillations in LDOS $\rho(k,r)$ using

$$\rho(k,r) = \frac{4}{\pi\hbar v_F}\sum_j |\Psi^{(j)}(k,r)|^2,$$

where $\Psi^{(j)}(k,r)$ is the radial part of the Dirac spinor, for a given angular momentum channel j.

Plot of Standing Wave Oscillation in LDOS

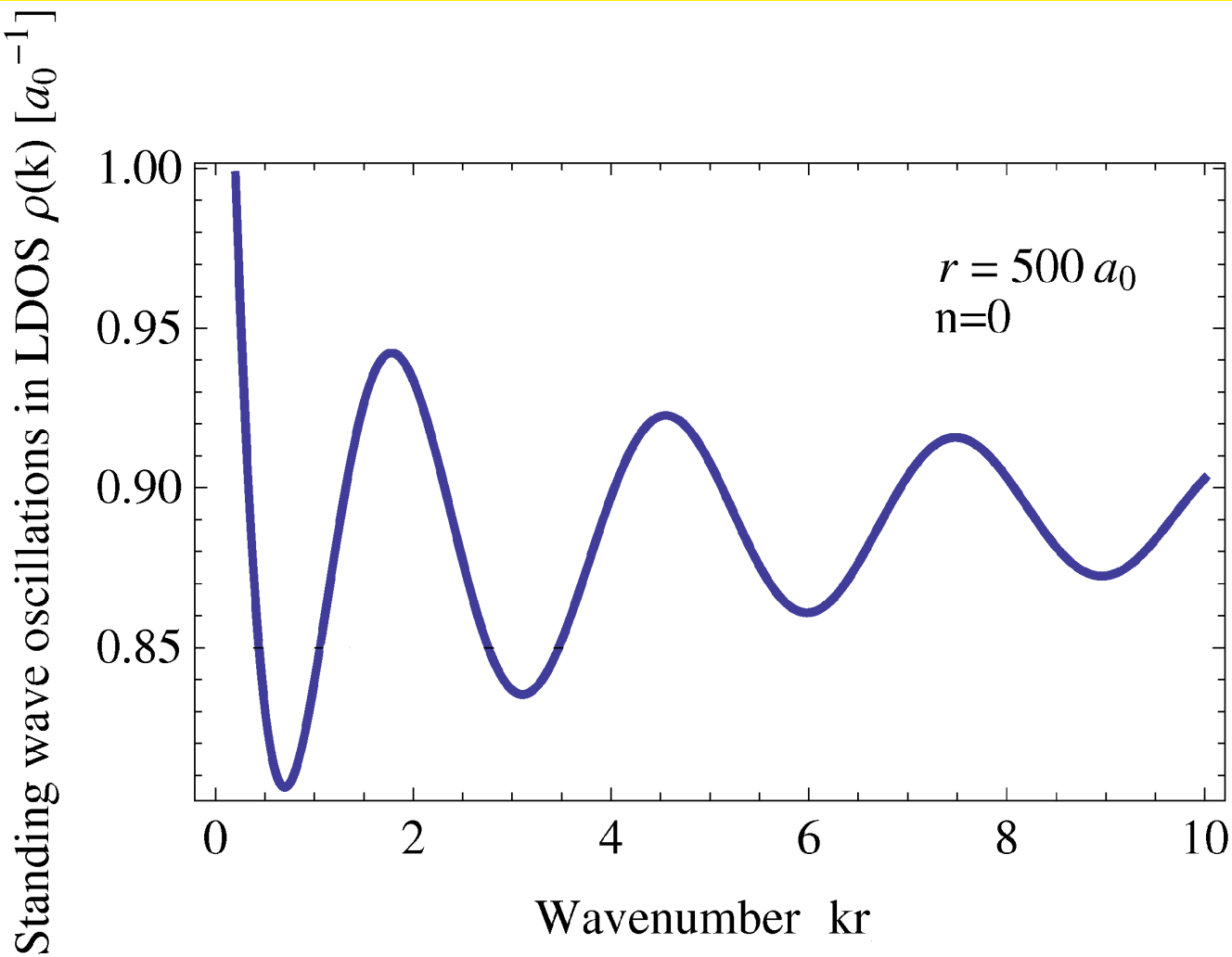


Figure 7: Energy dependence of LDOS in presence of a Coulomb potential for $n = 0$ and a particular value of r and with $j = \frac{1}{2}$ and $\alpha = 0.6$.

Spectrum in graphene cone with a supercritical charge

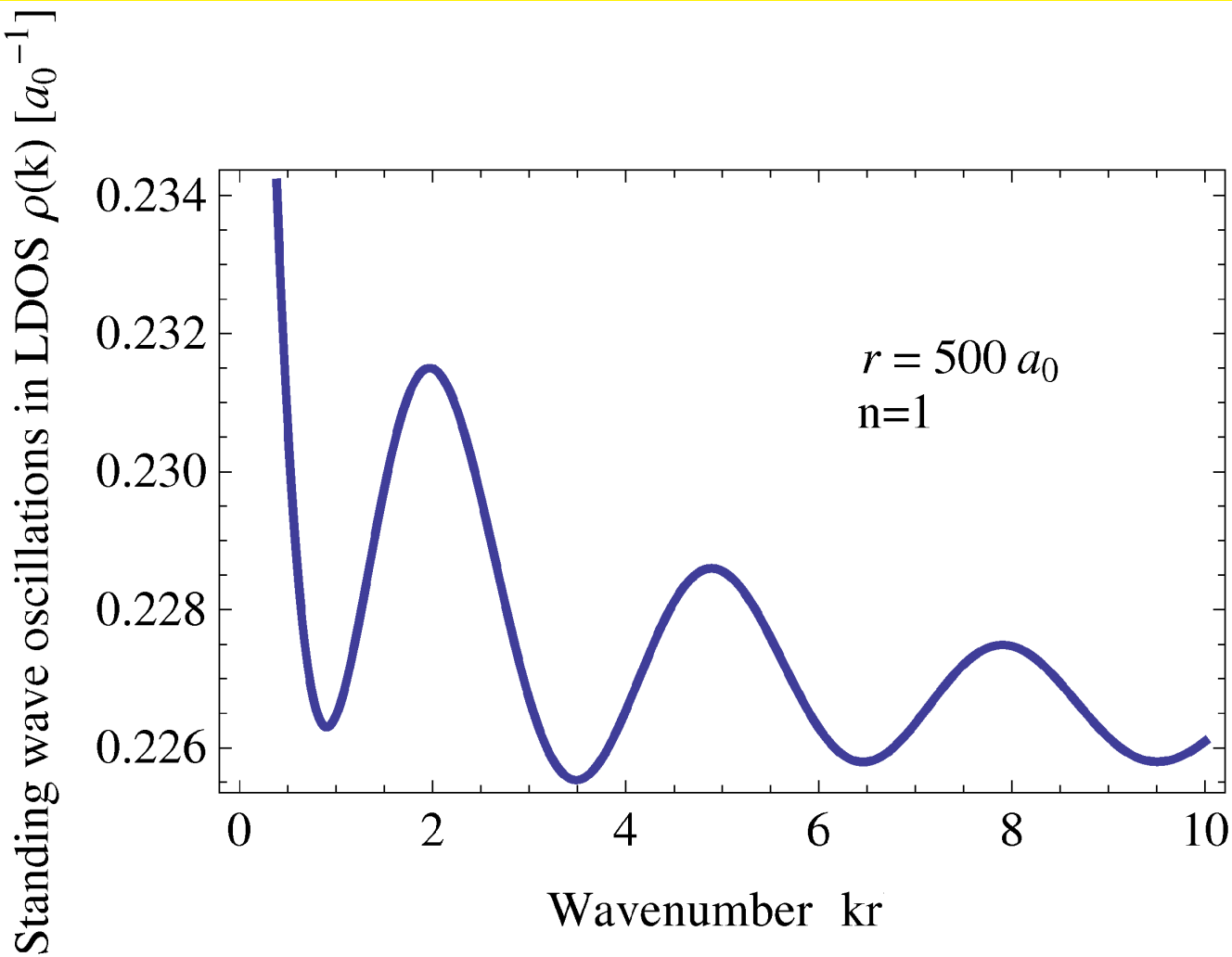


Figure 8: Energy dependence of LDOS in presence of a Coulomb potential for $n = 1$ and a particular value of r and with $j = \frac{1}{2}$ and $\alpha = 0.6$.

RG Flow of Charge Impurity Strength

- The real part of E_p diverges as the cutoff $a_0 \to 0$.
- To study the RG flow, we now promote the coupling constant α as a function of a_0 and demand that as $a_0 \to 0$, the energy for any fixed level p (say $p = 1$) remains independent of the cutoff.
- In the leading order, where α is only slightly above the critical coupling, this prescription gives the β-function as

$$\beta(\lambda) \sim -\lambda^2 + ..$$

- Thus we have an ultraviolet stable fixed point at $\lambda = 0$ or at $\alpha = \nu$. Hence, for any given value of n and j, the coupling α in the supercritical regime is driven to its critical value.

Gapped Graphene Cone:Short Distance Behaviour

- The Dirac equation for a gapped graphene cone can be separated by assuming the solution of the form

$$\Psi(r,\theta) = \sum_j \begin{pmatrix} \Psi_A^{(j)}(r) \\ \Psi_B^{(j)}(r) \end{pmatrix} e^{ij\theta} = \sum_j \begin{pmatrix} \tilde{\Psi}_A^{(j)}(r) \\ \tilde{\Psi}_B^{(j)}(r) \end{pmatrix} e^{-\eta r} r^{\gamma - \frac{1}{2}} e^{ij\theta}.$$

where

- θ denotes the corresponding polar angle,$\eta = \sqrt{m^2 - E^2}$ and j is the half integral azimuthal quantum number.
- Substituting this ansatz in the Dirac equation, we note that the leading short distance behaviour of the wavefunction is given by

$$\Psi_{A,B}^{(j)}(r) \sim r^{\gamma - \frac{1}{2}} \text{ where } \gamma = \sqrt{\nu^2 - \alpha^2}, \nu = \frac{j \pm \frac{n}{4}}{1 - \frac{n}{6}}.$$

Regularized Boundary Condition

- The critical charge α_c is determined by the minimum allowed value of ν.
- To observe the effect of external supercritical Coulomb charge on the gapped graphene cone we shall first consider a regularization of the Coulomb potential given by

$$V(r) = \begin{cases} -\alpha/r, & r > a \\ -\alpha/a, & r \leq a \end{cases}, \tag{1}$$

  where the Coulomb charge is placed at the apex of the gapped graphene cone.
- a is the distance of the Dirac electron from the apex and it is of the order of the lattice parameter.

Quasibound state energy spectrum

- The Dirac equation for gapped graphene cone is solved for the two different regions $r > a$ and $r \leq a$ differently and their solution are matched at $r = a$.
- The continuity condition at $a \longrightarrow 0$ will be satisfied when $f(E) \equiv$ $\mathrm{Arg}[\Gamma(1+i\lambda-\frac{E\alpha}{\eta})]+\mathrm{Arg}[\nu-\frac{\alpha}{\eta}(m-E)+i\lambda]+\lambda\ln(2\eta a)+\mathrm{Arg}[\nu-\alpha\frac{J_{|\nu+\frac{1}{2}|}(\alpha)}{J_{|\nu-\frac{1}{2}|}(\alpha)}-i\lambda]+p\pi$ $= \mathrm{Arg}[\Gamma(1+2i\lambda)]$ where p is a positive integer.
- This condition gives the quasibound state energy spectrum of gapped graphene cone in presence of a regularized Coulomb potential.

Quasibound state energy spectrum

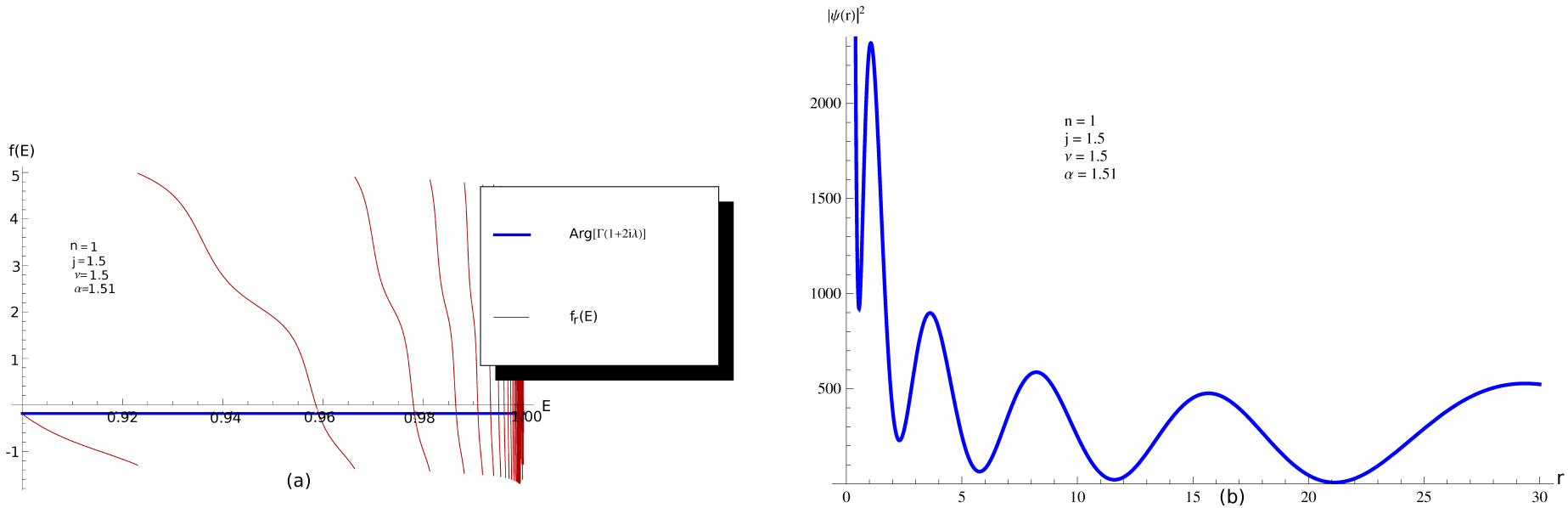


Figure 9: (a)Quasibounstate energy spectrum with regularized potential is shown. (b)Dependence of $|\Psi(r)|^2$ on the distance r from the charge impurity placed at the apex of the gapped graphene cone is shown for a particular energy $E = 0.96m$ obtained from the plot of the quasiboundstate energy spectrum.

Regularized potential : Critical charge

- The mass affects the critical charge of the system.
- Here the critical charge refers to that value of Coulomb potential strength for which $E = -m$.
- For the region near critical potential we have

  $\alpha_c = \nu + \frac{\pi^2}{2\nu \log^2[2m\nu Ca]}$ where

  $C = \exp\left[-2\Psi(1) - \frac{J_{|\nu-\frac{1}{2}|}(\nu)}{\nu(J_{|\nu-\frac{1}{2}|}(\nu) - J_{|\nu+\frac{1}{2}|}(\nu))}\right]$

Plot : Critical charge vs ma

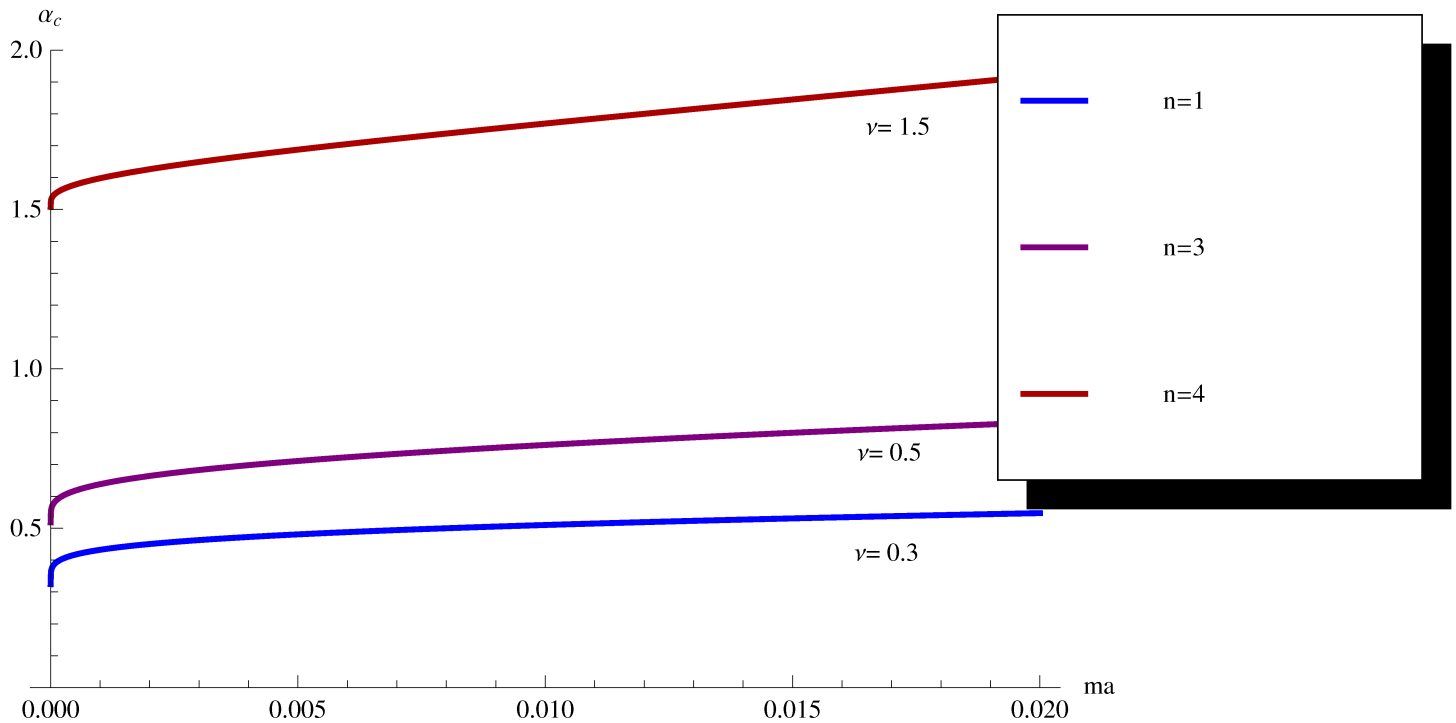


Figure 10: Dependence of critical charge on the nonzero mass and cutoff parameter are shown for zigzag edge boundary condition for different opening angles of the gapped graphene cone.

Zigzag edge boundary condition

- The zigzag edge boundary condition is given by $\Psi^j_B(a) = 0$, where a is a distance from the apex, of the order of the lattice scale in graphene.
- The square integrability condition of the wave function indicates that as $r \longrightarrow \infty$ the diverging part of the wave function must vanish.
- This gives the condition

  $f(E) \equiv \mathrm{Arg}[\Gamma(i\lambda - \frac{E\alpha}{\eta})] + \mathrm{Arg}[\nu + \frac{\alpha}{\eta}(m+E) - i\lambda] + \lambda \ln(2\eta a) + p\pi = \mathrm{Arg}[\Gamma(1+2i\lambda)]$

  where p is a positive integer.
- This condition gives the quasibound state energy spectrum of gapped graphene cone with zigzag edge boundary condition.

Quasibound state energy spectrum

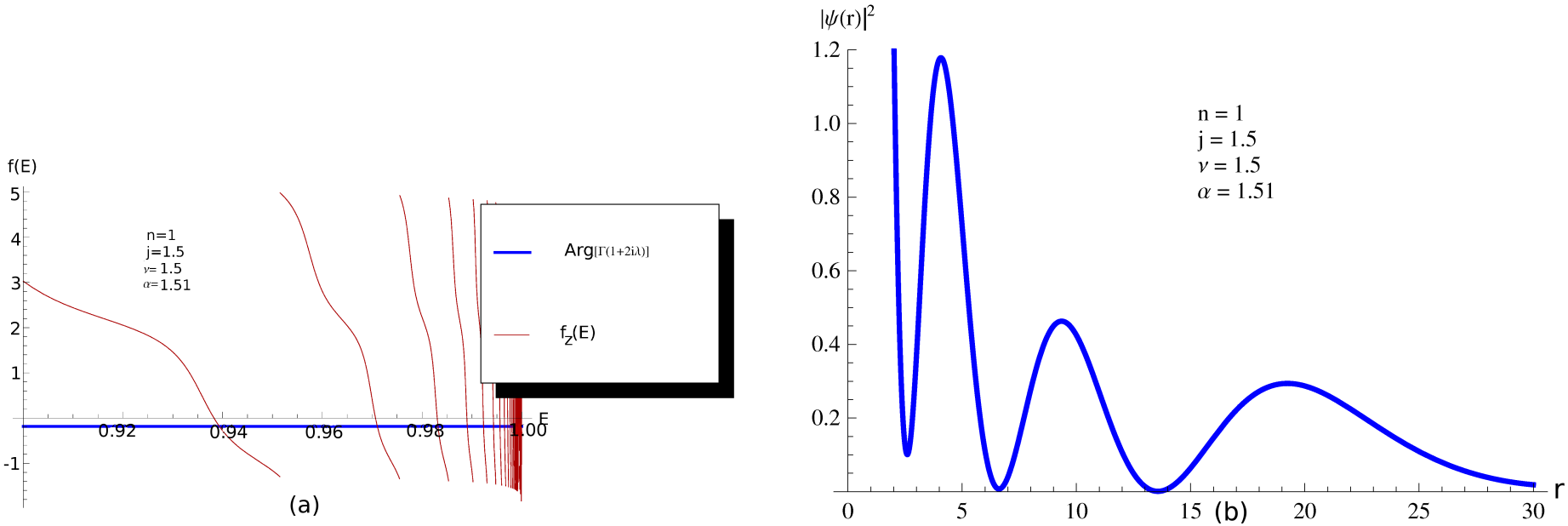


Figure 11: (a)Quasibounstate energy spectrum with zigzag edge boundary condition is shown. Here the blue line represents Arg$[\Gamma(1+2i\lambda)]$ and the dashed and the dark red line represents RHS of $f(E)$). (b)Dependence of $|\Psi(r)|^2$ on the distance r from the charge impurity placed at the apex of the gapped graphene cone is shown for a particular energy $E = 0.94m$ obtained from the plot of the quasiboundstate energy spectrum.

Comparison : Energy spectrum

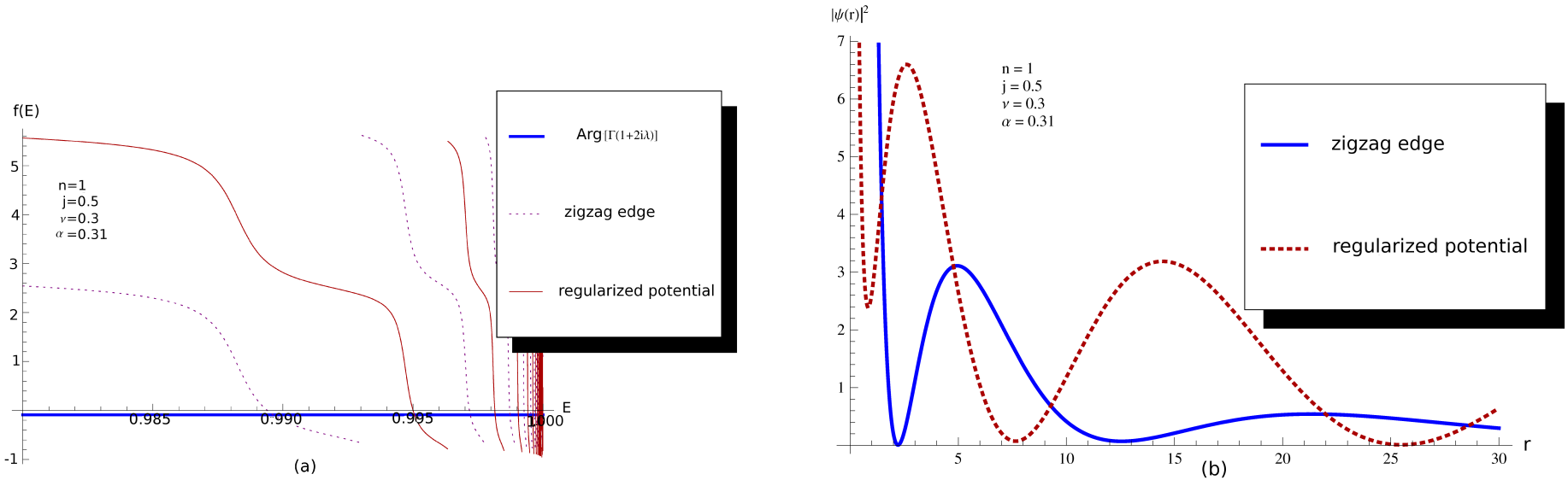


Figure 12: (a)Quasibounstate energy spectrum with zigzag edge boundary condition and regularized Coulomb potential. Here the blue line represents Arg$[\Gamma(1+2i\lambda)]$ and the dashed and the solid line represents RHS of Equations giving $f(E)$. (b)Dependence of $|\Psi(r)|^2$ on the distance r from the charge impurity placed at the apex of the gapped graphene cone is shown at a particular energy. The values of energy are obtained from the quasibound-state energy spectrum. From Fig.(a) we can see that for zigzag edge boundary condition a possible bound state energy is $E = 0.9895m$ and for regularized potential a possible energy is $E = 0.995m$.

Comparison : Critical charge

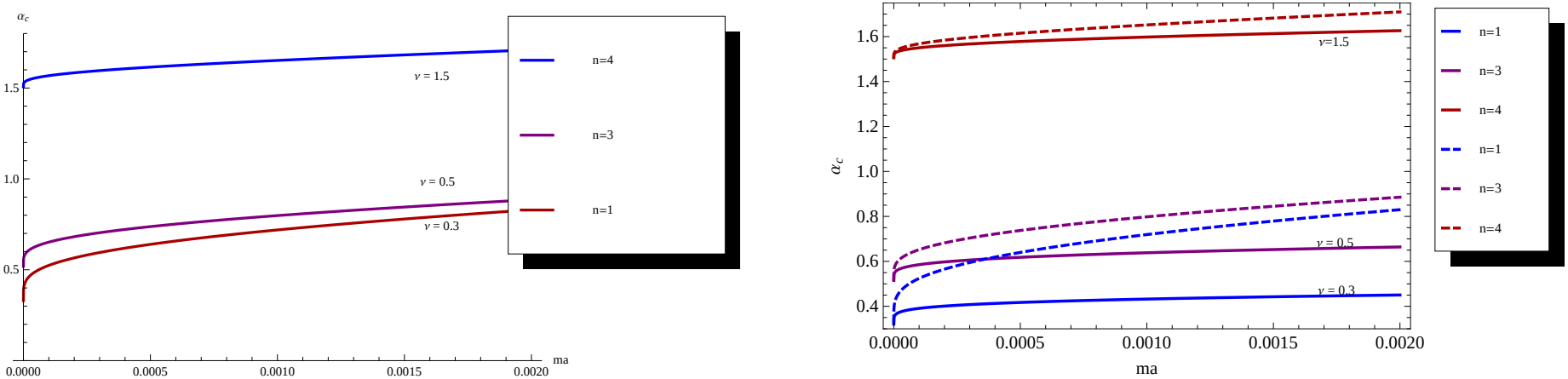


Figure 13: (a)Dependence of critical charge on the nonzero mass and cutoff parameter are shown for regularized Coulomb potential for different opening angles of the gapped graphene cone. (b)Dependence of critical charge on the nonzero mass and cutoff parameter are shown for both zigzag edge boundary 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.

Gapped graphene cone : Subcritical region

- In the subcritical region γ is always real.
- Bound states occur when $\gamma - \frac{\alpha E}{\eta} = -p$.where

$$p = \begin{cases} 0, 1, 2, ..., & \text{when } \nu > 0, \\ 1, 2, 3...., & \text{when } \nu < 0. \end{cases}$$

- The corresponding bound state spectra is obtained as $E_p = \frac{m\ \text{sgn}(\alpha)}{\sqrt{1+\frac{\alpha^2}{(p+\gamma)^2}}}$.
- The energy should be of the same sign (positive or negative) as α because otherwise the value of p will become negative and in our range of interest, it is not allowed

Gapped graphene cone : Subcritical region

- In the scattering sector the parameter $\eta = \sqrt{m^2 - E^2}$ becomes purely imaginary, i.e. $\eta = iq,$ where the real parameter q is defined as $q = \sqrt{E^2 - m^2}$.
- Using the $r \to \infty$ limit of the scattering states the scattering matrix is obtained as

$$S(q) = (2iq)^{\frac{2i\alpha E}{q}} \frac{\left(\gamma + i\frac{E\alpha}{q}\right)}{\left(\nu - i\frac{m\alpha}{q}\right)} \frac{\Gamma\left(1 + \gamma - i\frac{\alpha E}{q}\right)}{\Gamma\left(1 + \gamma + i\frac{E\alpha}{q}\right)} e^{i\pi\left(\gamma + i\frac{\alpha E}{q}\right)}.$$

- Now the self adjointness of the Dirac Hamiltonian is checked for the subcritical region by using the self-adjoint extension procedure prescribed by von Neumann to consider the effect of topology and short range or singular interactions.

Introduction to Self-adjoint Extension

- We know that in quantum mechanics the observables must have real eigenvalues.
- The operators corresponding to these observables are conventionally called self-adjoint operators.
- Whether an operator is self-adjoint or not depends on its boundary conditions.
- Those possible boundary conditions can be obtained from the principles formulated by von Neumann on self-adjoint extentions of operators.

Introduction to Self-adjoint Extension

- Let the inner product of two elements $\alpha, \beta \in H$ be denoted by (α, β).
- Here H denotes the Hilbert space.
- An operator T with domain $D(T)$ is called a **symmetric operator** if it obeys the relation

$$(\phi, T\psi) = (T\phi, \psi), \tag{2}$$

for all elements $\phi, \psi \in D(T)$.

- The symmetric operator T is self-adjoint if and only if

$$T = T^* \text{ and } D(T) = D(T^*). \tag{3}$$

where T^* denote the operator adjoint to T.

Introduction to Self-adjoint Extension

- To check whether T is self-adjoint or not we consider the equations

$$T^*\phi_+ = +i\phi_+ \tag{4}$$

$$T^*\phi_- = -i\phi_- \tag{5}$$

- 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.

Domain of Self-adjointness

- The operator T can be classified in terms of the deficiency indices as follows:
  - T is essentially self-adjoint iff $(n_+, n_-) = (0, 0)$.
  - T is not self-adjoint but has self-adjoint extensions iff $n_+ = n_- = n \neq 0$.
  - 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

$$D_U(T) = \left\{ \phi + \phi_+ + U\phi_- \middle| \phi \in D(T) \right. \\ \left. \text{and } U \text{ is a } n \times n \text{ unitary matrix} \right\}. \quad (6)$$

Application in Graphene

- In case of gapped graphene cone it can be shown that for the range $0 < \gamma < \frac{1}{2}$, $n_+ = n_- = 1$.
- H_r admits a one parameter family of self-adjoint extensions.
- According to von Neumann's analysis domain in which H_r is self-adjoint is given by $D_z(H_r) = D(H_r) \oplus \{e^{i\frac{z}{2}}\Psi_+ + e^{-i\frac{z}{2}}\Psi_-\}$.
- Here $z \in R(\text{mod } 2\pi)$ is the self-adjoint extension parameter.
- Physically, the domain $D_z(H_r)$ provides the boundary conditions for which the radial Dirac operator for graphene is self-adjoint and we see that the boundary conditions are labelled by the parameter z.
- We would now like to find the spectrum of the system in a range of ν and the effective subcritical Coulomb strength α such that $0 < \gamma < \frac{1}{2}$.

Bound State Spectrum

- In terms of the system parameters and the self-adjoint extension parameter z the spectrum is determined by the equation

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

$$= \frac{\chi_1 \cos\left(\phi_1+\frac{z}{2}\right)}{\chi_2 \cos\left(\phi_2+\frac{z}{2}\right)}.$$

- Each choice of z corresponds to a different boundary condition described by the domain $\mathcal{D}_z(H_\rho)$ and leads to an inequivalent quantum theory. However the choice of z for a particular system is determined empirically as the theory cannot predict its value.

- Though the equation cannot be solved analytically, from a typical plot of $f(E)$ it can be obtained numerically.

Plot : Bound state spectrum

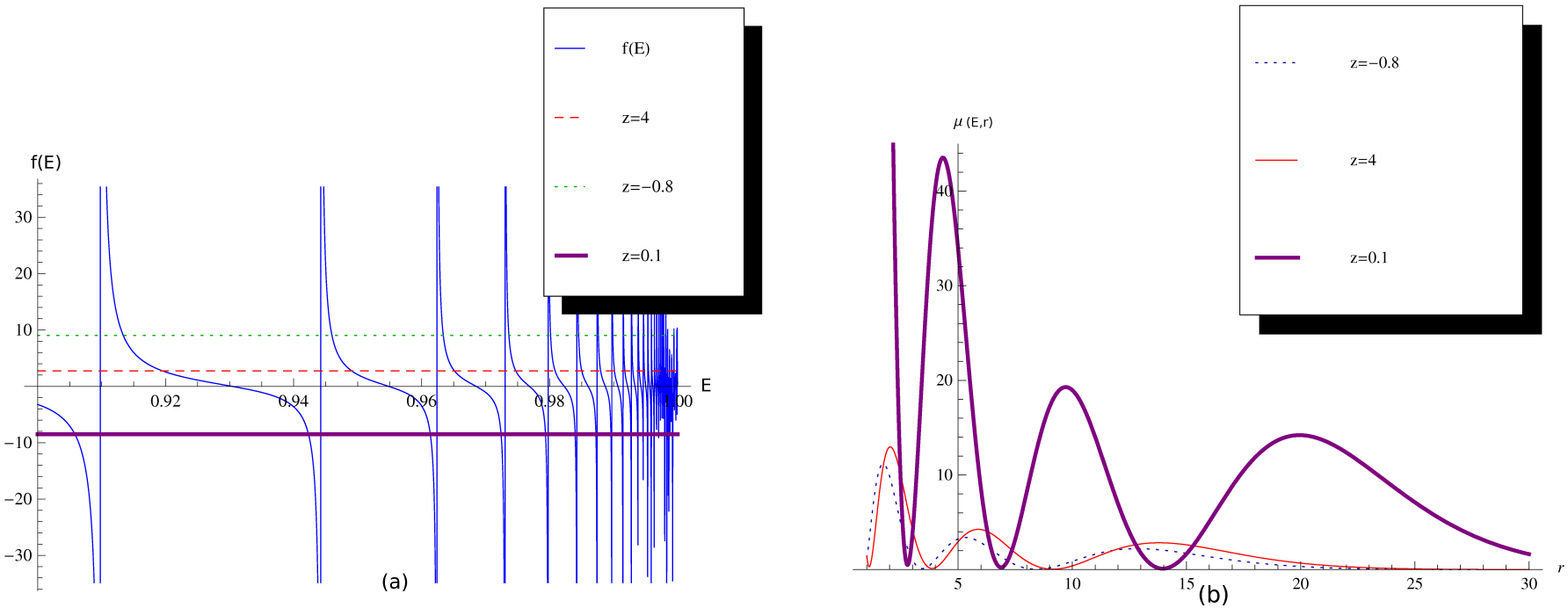


Figure 14: (a)Plot of $f(E)$ is shown for system parameters $j = \frac{3}{2},\ n = 1,\ \alpha = 1.48$ and $m = 1$. The three horizontal line corresponds to the three different values of the self adjoint extension parameter $z = 4, 0.1, -0.8$. (b) Dependence of LDOS in the bound state sector of the gapped 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.

Plot : Bound state spectrum

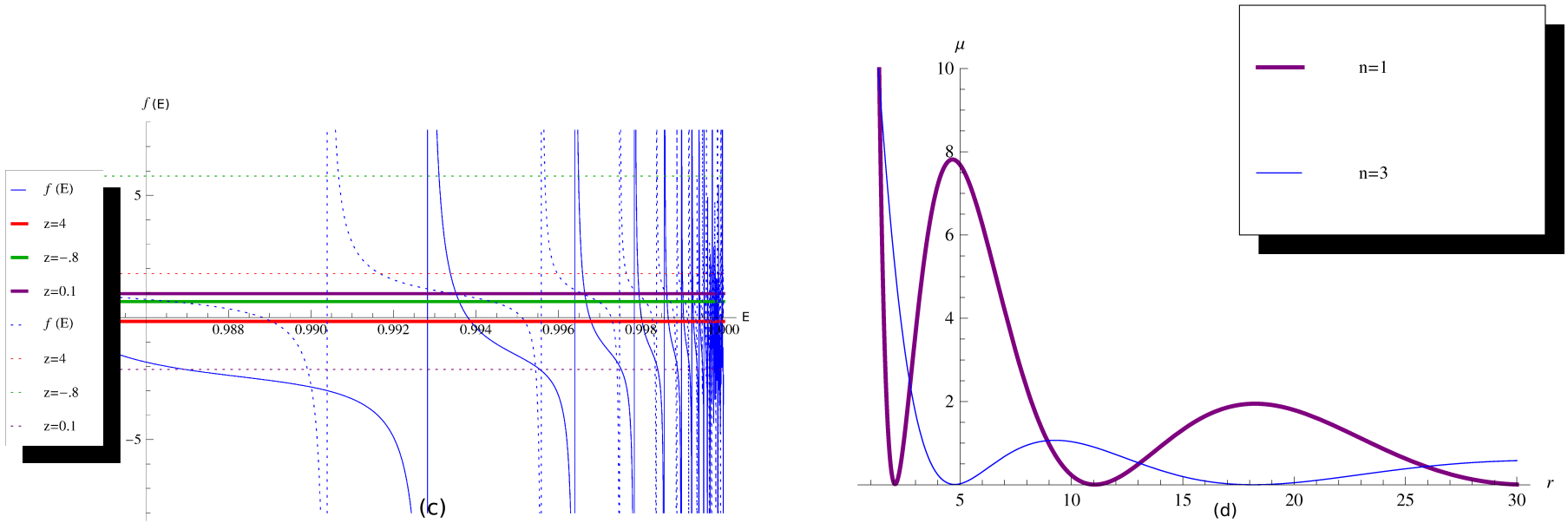


Figure 15: (c) Plot of $f(E)$ is shown for two different values of $n = 1$ (dotted) and $n = 3$ (solid) with system parameters $j = \frac{1}{2}$, $\alpha = 0.29$ and $m = 1$. The three horizontal line corresponds to the three different values of the self adjoint extension parameter $z = 4, 0.1, -0.8$. (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 $z = 0.1$.

Scattering Matrix

- The $\mathbf{S}$ matrix for gapped graphene cone for the parameter range $0 < \gamma < \frac{1}{2}$ is given by

$$\mathbf{S}(q) = (2iq)^{2i\frac{\alpha E}{q}} \frac{C_1}{C_2}$$

where

$$C_1 = -\frac{\chi_1 \cos(\phi_1 + \frac{z}{2})}{\chi_2 \cos(\phi_2 + \frac{z}{2})} (2\eta_1)^{2\gamma} (2\eta)^{-2\gamma} \frac{1+f_2}{1+f_1} f_1 \frac{\Gamma(1+2\gamma)}{\Gamma(1+\gamma+i\frac{\alpha E}{q})} + f_2 \frac{\Gamma(1-2\gamma)}{\Gamma(1-\gamma+i\frac{\alpha E}{q})}$$

and

$$C_2 = -\frac{\chi_1 \cos(\phi_1 + \frac{z}{2})}{\chi_2 \cos(\phi_2 + \frac{z}{2})} (2\eta_1)^{2\gamma} (2\eta)^{-2\gamma} \frac{1+f_2}{1+f_1} \frac{\Gamma(1+2\gamma)}{\Gamma(1+\gamma-i\frac{\alpha E}{q})} e^{-i\pi(\gamma+i\frac{\alpha E}{q})}$$

$$+ \frac{\Gamma(1-2\gamma)}{\Gamma(1-\gamma-i\frac{\alpha E}{q})} e^{-i\pi(-\gamma+i\frac{\alpha E}{q})},$$

where

$$f_1 \equiv \frac{\gamma - \frac{\alpha E}{\eta}}{\nu + \frac{m\alpha}{\eta}}, \quad f_2 \equiv \frac{-\gamma - \frac{\alpha E}{\eta}}{\nu + \frac{m\alpha}{\eta}}.$$

Plot : Scattering phase shift

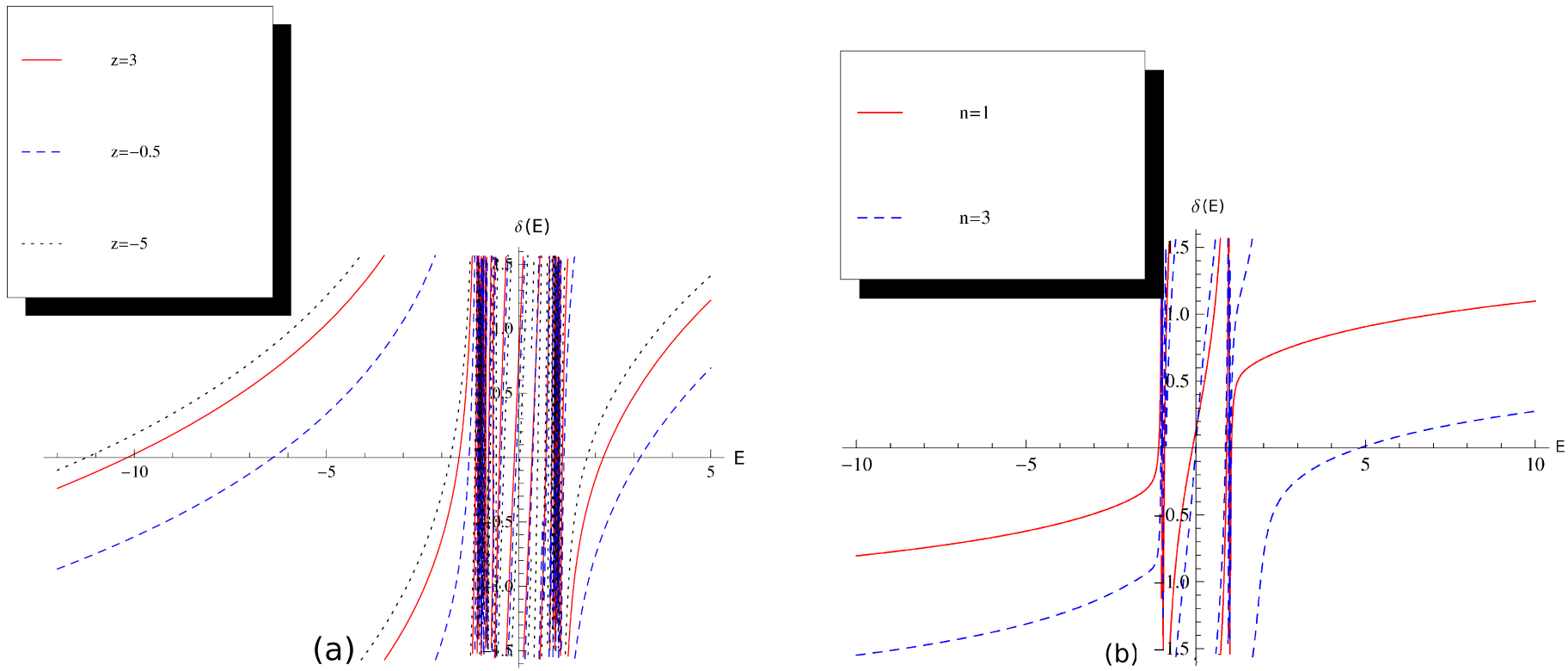


Figure 16: (a)Phase shifts in the gapped graphene cone is shown for three different values of the self adjoint extension parameter $z = 3, -0.5, -5$ where the system parameters are $n = 1, j = \frac{3}{2}, \alpha = 1.48$, and $m = 1$. (b) Scattering phase shifts are shown for different angles of the gapped graphene cone with the sae parameter $z = -0.5$ and system parameters $j = \frac{1}{2}, \alpha = 0.29$ and $m = 1$.

LDOS

- To determine the LDOS of the system we use the following expression $\mu(E,r) = \frac{4}{\pi\hbar v_F}\sum_j |\Psi^{(j)}(k,r)|^2$.
- We have observed that LDOS depend on the values of self adjoint extension parameter z and also on the topology of the system.
- Measurement of LDOS using scanning tunneling microscopy can give us information about the self adjoint extension parameter and the topology of the system.

Plot : LDOS

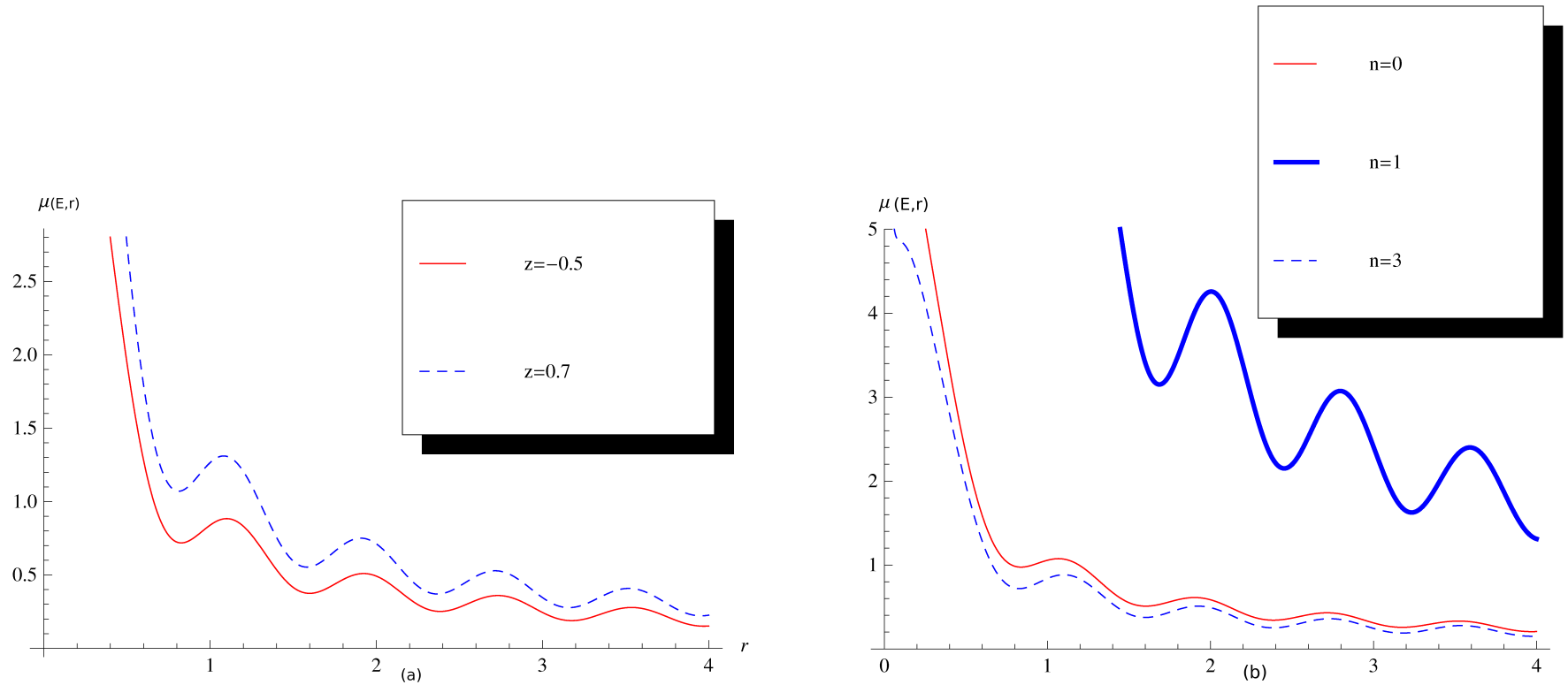
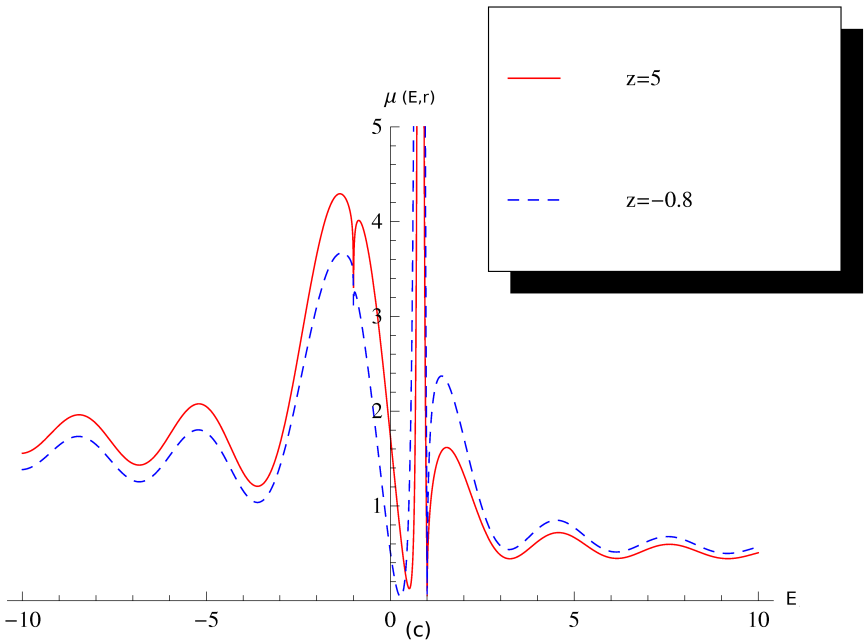


Figure 17: (a)Dependence of LDOS on the distance r from the Coulomb impurity is shown for two different values of sae parameter $z = -0.5, 0.7$ and a particular value of $E = 4$ and with $j = \frac{1}{2}$, $n = 3$, $\alpha = 0.29$ and $m = 1$. (b) Effect of topology on r dependence of LDOS is shown for sae parameter $z = -0.5$, $E = 4$ and with sam system parameters.

Plot : LDOS



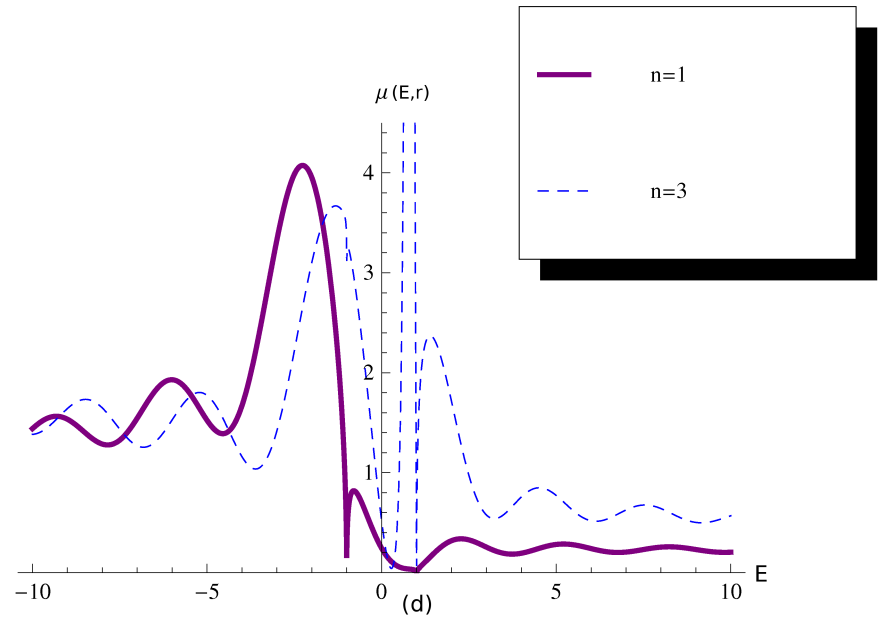


Figure 18: (c)Energy dependence of LDOS is shown for two different values of sae parameter $z = 5,\ -0.8$ at a distance $r = 1$ from the external Coulomb impurity. The system parameters used for the plot are $\alpha = 0.29$ and $m = 1$ and contribution coming from the angular momentum channel $j = \frac{1}{2}$ is considered. (d) Effect of topology on the energy dependence of LDOS is shown for sae parameter $z = -0.8$, angular momentum channel $j = \frac{1}{2}$ and system parameters $\alpha = -0.29,\ n = 1, 3$ and $m = 1$.

Conclusions

- The system of a graphene cone with an external Coulomb charge at its apex has been described by the combination of the Coulomb charge and a suitable magnetic flux tube passing through the apex.
- The quantities of physical interest such as the scattering phase shifts, the LDOS and the quasi-bound state energies depend explicitly on the topology.
- The existence of the quasi-bound states in gapless graphene cone indicates the possibility of the localization of the wavefunctions in the presence of a supercritical charge. Our analysis shows that the nature and extent of the localization depends on the spatial topology of the gapless graphene sample.
- We have given qualitative arguments which shows that under the RG flow and for $\nu \neq 0$, the supercritical charge in the gapless graphene cone tends to its critical value. If this argument can be extended for $\nu = 0$, for which the critical charge vanishes, that would lead to complete shielding of the external charge. This issue and the related electronic properties are currently under investigation.

Conclusions

- For gapped graphene cone the above analysis has been done in both the subcritical and supercritical regime.
- The critical value of the Coulomb charge has been observed to depend on the sample topology and the Dirac mass.
- In the supercritical region we obtained the condition for the appearance of bound states with both the zigzag boundary condition and the regularized Coulomb potential.
- In the subcritical region for a certain range of the parameter γ we have shown that the corresponding Hamiltonians are not self-adjoint. However they can be made self-adjoint by choosing suitable boundary conditions.
- These boundary conditions introduce a self-adjoint extension parameter z. For each value of z we obtained an inequivalent quantization and spectral data for the conical system.
- The physically interesting quantities in this system include the scattering phase shifts, the S matrix, the LDOS and the bound state energies. We have shown that all these quantities depend on the parameter z explicitly.

Conclusions

- From the nature of dependence of the LDOS plots on z, the parameter can be determined empirically.
- We have considered the effect of a conical topology and observed how the LDOS plots for different angles of the cone, depends on the self-adjoint extension parameter.

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THANK YOU