Chapter 5

$SU(4)$ symmetric model

In this chapter, we consider the $SU(4)$ symmetric model for graphene, which includes the leading terms from the kinetic and Coulomb terms in the continuum approximation. The model used in this chapter

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_C$$  \hspace{1cm} (5.1)

The kinetic term,

$$\mathcal{H}_0 = \int \Psi^\dagger(r)(v_F \alpha \cdot \pi \otimes 1_4)\Psi(r)$$  \hspace{1cm} (5.2)

The $SU(4)$ symmetric part of electron-electron interaction,

$$\mathcal{H}_C = \frac{1}{2} \int_{r_1,r_2} V_C(|r_1 - r_2|) \left( \Psi^\dagger(r_1)\Psi(r_1)\Psi^\dagger(r_2)\Psi(r_2) - 2\bar{\rho}\Psi^\dagger(r_1)\Psi(r_1) + \bar{\rho}^2 \right)$$  \hspace{1cm} (5.3)

here $\bar{\rho}$ is the average charge density. This has been incorporated to take into account the average background charge due to positive charge of the ions. Both $\mathcal{H}_0$ and $\mathcal{H}_C$ are invariant under $SU(4)$ rotation performed on the field operator, i.e. $\mathcal{U}_{A,B}\Psi(x)_{r,B}$, leaves both terms unchanged.

We will show that, the $SU(4)$ symmetric model spontaneously breaks the $SU(4)$ symmetry to $SU(3) \otimes U(1)$ for Hall conductivity at $\sigma_H = -1$ and $SU(2) \otimes SU(2)$ for Hall...
conductivity $\sigma_H = 0$. It does not throw light on the nature of the ground states of the Hall conductivity for $\sigma_H = 0, \pm 1$. The mean field energies for ground state turns out to be independent of the angle parameters. These angle parameters are responsible for indicating the direction of the ground states in the $SU(4)$ space i.e. the $SU(4)$ polarization of the ground states in not completely specified. In the case of particle-hole excitations also gaps also turns out to be independent of the angle parameters. We will show that leading contributions to the magnitude of the gaps comes from the Coulomb term but the $SU(4)$ component of the excitations are left unspecified.

5.1 Expectation value for symmetric model

In this section we use the two point correlator Eq.(4.67) to compute the expectation value of kinetic and Coulomb term. We will show that the expectation value for the $SU(4)$ symmetric terms is independent of angle parameters that specify the $SU(4)$ polarization. The expectations values are reduced to evaluating the integration of $s$ variable of the correlator, Eq.(4.67), which is done numerically.

5.1.1 Kinetic term

The kinetic term has local fermion field operators and the expectation value can be expressed as,

$$\langle H_0 \rangle = \int \mathcal{H}_r, A; s, B \langle \Psi^\dagger_{r, A}(r) \Psi_{s, B}(r) \rangle$$

From Eq.(5.2), $\mathcal{H}_r, A; s, B = v_F (\alpha \cdot \pi)_{r, s}(1_A, 1_B)$. To compute average of kinetic term we need to take into account the action of operator $h$ which makes it non-local because of the action of conjugate momentum operator. We cannot apply the coincident correlator here instead we compute the action of operator $h$ on the two point correlator and take the
coincident limit.

\[
\langle H_0 \rangle = \int_r \lim_{r \to r_0} \text{Tr}[h \Gamma(r, r_0)]
\]  

(5.5)

Since the operator \(\alpha \cdot \pi\) has only off-diagonal elements, hence

\[
\text{Tr}[h \Gamma(r, r_0)] = \frac{1}{2\pi \ell_c^2} \frac{1}{2} \left( \frac{\hbar v_F}{\ell_c} \right) \sum_{q=1}^{4} \left( \pi_- b_m(q(r, r_0)) + \pi_+ d_m(q(r, r_0)) \right)
\]  

(5.6)

Here \(\pi_\pm = \pi_x \pm i \pi_y\) and its action on the off-diagonal elements of the two-point correlator provides the contributions. \(\pi = p + eA\) is the conjugate momenta in presence of magnetic field. The action of \(\pi_\pm\) can be easily obtained by expressing them as derivatives of complex variable \(z = x + i y\) and its conjugate \(\bar{z}\) as shown in Eq.(4.52) and using the Eq.(4.54) and Eq.(4.55), we obtain

\[
\pi_+((\bar{z} - \bar{z}_0)\zeta_s(z, z_0)) = i \left( -2 - \frac{1}{2} z(\bar{z} - \bar{z}_0) + \frac{1}{2}|z - z_0|^2 (\coth(s) + 1) \right) \zeta_s(z, z_0)
\]

\[
\pi_-((z - z_0)\zeta_s(z, z_0)) = i \left( -2 - \frac{1}{2} \bar{z}(z - z_0) + \frac{1}{2}|z - z_0|^2 (\coth(s) - 1) \right) \zeta_s(z, z_0)
\]

Now taking limit \(z \to z_0\) and we obtain,

\[
\lim_{r \to r_0} \pi_- b_m(q(r, r_0)) = -\frac{1}{2\sqrt{\pi}} \int_s \frac{e^{-sm^2}}{\sqrt{s} \sinh^2(s)}
\]  

(5.7)

\[
\lim_{r \to r_0} \pi_+ d_m(q(r, r_0)) = -\frac{1}{2\sqrt{\pi}} \int_s \frac{e^{-sm^2}}{\sqrt{s} \sinh^2(s)}
\]  

(5.8)

The spatial integration in Eq.(5.5) is trivial and results in \(V\), volume of the system

\[
\langle H_0 \rangle = -\frac{V}{2\pi \ell_c^2} \left( \frac{\hbar v_F}{\ell_c} \right) \frac{1}{2\sqrt{\pi}} \sum_{q=1}^{4} \int_{\frac{1}{2\sqrt{\pi}}}^{\infty} ds \frac{e^{-sm^2}}{\sqrt{s} \sinh^2(s)}
\]  

(5.9)

The integrand in Eq.(5.9), is a diverging function of \(s\) near zero. Although the point of divergence, \(s = 0\), is not part of range of integration but it diverges very rapidly in the proximity of the lower limit of the integration. We note that leading contribution of this integration is independent of variational parameter, which is just a constant from the min-
imization point of view. Hence we remove this constant in the process of computing the coefficients with variational parameter dependence and to keep the integration going out of bounds for numerical computation. The integration can be rearranged in the following way,

\[
\int_1^\infty ds \frac{e^{-sm^2_q}}{\sqrt{s} \sinh^2(s)} = \int_1^\infty ds \frac{1}{\sqrt{s} \sinh^2(s)} - \int_1^\infty ds \frac{(1 - e^{-sm^2_q})}{\sqrt{s} \sinh^2(s)}
\]

The first term in the above equation is independent of variational parameter so we drop it and second one carries the complete variational parameter dependence. The expectation value of the kinetic term that has variational parameter dependence can be expressed as,

\[
\langle H_0 \rangle = \frac{V}{2\pi \ell^2_c} \left( \frac{\hbar v_F}{\ell_c} \right) \sum_{q=1}^4 \eta_t(m_q)
\]

The quantity

\[
\eta_t(m_q) = \frac{4}{\sqrt{\pi}} \int_0^\infty d\xi \frac{(1 - e^{-m^2_q \xi^2})e^{-2\xi^2}}{(1 - e^{-2\xi^2})^2}
\]

is expressed with change of variable which suited best for it to be computed numerically. Also note that the coefficient \(\eta_t(m_q)\) will yield positive values for range of integration and parameter values that are of our interest.

### 5.1.2 Coulomb term

The expectation value of Coulomb term, Eq.(5.3),

\[
\langle H_C \rangle = \frac{1}{2} \frac{e^2}{4\pi \varepsilon} \int_{r_1} \int_{r_2} \frac{1}{|r_1 - r_2|} \left( \langle \Psi_{r,A}^\dagger(r_1) \Psi_{r,A}(r_1) \rangle \langle \Psi_{s,B}^\dagger(r_2) \Psi_{s,B}(r_2) \rangle - \langle \Psi_{r,A}^\dagger(r_1) \Psi_{s,B}(r_2) \rangle \langle \Psi_{s,B}^\dagger(r_2) \Psi_{r,A}(r_1) \rangle - 2\bar{\rho} \langle \Psi_{r,A}^\dagger(r_1) \Psi_{r,A}(r_1) \rangle + \bar{\rho}^2 \right)
\]
In above equation four fermion term has undergone Wick’s decomposition. By definition $\bar{\rho} = \text{Tr}[\Gamma(r, r)]$, the average charge. This leads to cancellation of the first and last two terms. The mean field energy contributions from the Coulomb term comes from the exchange term and can be expressed in terms of the two point correlator,

$$\langle \mathcal{H}_C \rangle = -\frac{1}{2}\frac{e^2}{4\pi\varepsilon} \int_{r_1} \int_{r_2} \frac{1}{|r_1 - r_2|} \text{Tr}[\Gamma(r_1, r_2) \Gamma(r_2, r_1)]$$  \hspace{1cm} (5.13)

We use the fact, $\text{Tr}[P_qP_\bar{q}] = \delta_{q, \bar{q}}$, to evaluate the trace of correlator,

$$\text{Tr}[\Gamma(r_1, r_2) \Gamma(r_2, r_1)] = \frac{1}{(2\pi\ell_c^2)^2} \frac{1}{4} \sum_{q=1}^{4} \left( f_{m_q}(r_1, r_2)f_{m_q}(r_2, r_1) 
+ g_{m_q}(r_1, r_2)g_{m_q}(r_2, r_1) 
+ b_{m_q}(r_1, r_2)b^*_{m_q}(r_2, r_1) 
+ d_{m_q}(r_1, r_2)d^*_{m_q}(r_2, r_1) \right)$$  \hspace{1cm} (5.14)

This indicated that the Coulomb expectation value is independent of the angle parameters.

Now consider the integral

$$\mathcal{I}_1 = \left( \frac{1}{2}\frac{e^2}{4\pi\varepsilon} \right) \frac{1}{(2\pi\ell_c^2)^2} \frac{1}{4} \int_{r_1, r_2} \frac{1}{|r_1 - r_2|} \left( f_{m_q}(r_1, r_2)f_{m_q}(r_2, r_1) 
+ g_{m_q}(r_2, r_1)g_{m_q}(r_1, r_2) \right)$$  \hspace{1cm} (5.15)

Once again we plug in $f_{m_q}(r_1, r_2)$ from Eq.(4.68) and $g_{m_q}(r_1, r_2)$ from Eq.(4.69) in the above equation,

$$\mathcal{I}_1 = \left( \frac{1}{2}\frac{e^2}{4\pi\varepsilon\ell_c} \right) \frac{m_q^2}{(2\pi\ell_c^2)^2} \frac{1}{8\pi} \int_{s_1, s_2} \frac{e^{-(s_1+s_2)m_q^2} \cosh(s_1+s_2)}{\sqrt{s_1 s_2} \sinh(s_1) \sinh(s_2)} \int_{r_1, r_2} \frac{e^{-\frac{1}{2}|r_1-r_2|^2}}{|r_1 - r_2|}$$  \hspace{1cm} (5.16)

The spatial integration involves only the magnitude of relative position coordinates, hence we transform the spatial integration from two position coordinates to center of mass and relative coordinates. The center of mass coordinate is trivial and yields the volume of the
system and the relative coordinate is a gaussian integral.

\[
I_1 = \left( \frac{1}{2} \frac{e^2}{4\pi \varepsilon l_c} \right) \frac{V}{2\pi l_c^2} \frac{m_q^2}{8\sqrt{\pi}} \int_{s_1,s_2} \frac{e^{-(s_1+s_2)m_q^2}}{\sqrt{s_1 s_2} \sinh(s_1) \sinh(s_2) \sqrt{\coth(s_1) + \coth(s_2)}} \cosh(s_1 + s_2)
\]

\[
= \left( \frac{1}{2} \frac{e^2}{4\pi \varepsilon l_c} \right) \frac{V}{2\pi l_c^2} \frac{m_q^2}{8\sqrt{\pi}} \int_{s_1,s_2} \frac{e^{-(s_1+s_2)m_q^2}}{\sqrt{s_1 s_2} \sinh(s_1) \sinh(s_2) \sinh(s_1 + s_2)}
\]

\[
= \left( \frac{1}{2} \frac{e^2}{4\pi \varepsilon l_c} \right) \frac{V}{2\pi l_c^2} \eta_{fg}(m_q)
\]

(5.17)

The variational parameter dependent \( \eta_{fg}(m_q) \) is computed numerically by implementing the double integral

\[
\eta_{fg}(m_q) = m_q^2 \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{d\xi_1}{\sqrt{\xi_1 e^{\xi_1}}} \int_0^{\xi_1} \frac{d\xi_2}{\sqrt{\xi_2 e^{\xi_2}}} \frac{e^{-\xi_1^2 m_q^2}}{\sqrt{1 - e^{2\xi_1^2}}} \frac{e^{-\xi_2^2 m_q^2}}{\sqrt{1 - e^{2\xi_2^2}}}
\]

(5.18)

Now consider the integral,

\[
I_2 = \left( \frac{1}{2} \frac{e^2}{4\pi \varepsilon l_c} \right) \frac{1}{(2\pi l_c^2)^2} \frac{4}{4} \int_{r_1,r_2} \frac{1}{|r_1 - r_2|} \left( b_{m_q}(r_1, r_2) d_{m_q}(r_2, r_1) + b_{m_q}(r_2, r_1) d_{m_q}(r_1, r_2) \right)
\]

(5.19)

Taking \( b_{m_q}(r_1, r_2) \) from Eq.(4.70) and \( d_{m_q}(r_1, r_2) \) from Eq.(4.71) and plugging in above equation,

\[
I_2 = \left( \frac{1}{2} \frac{e^2}{4\pi \varepsilon l_c} \right) \frac{1}{(2\pi l_c^2)^2} \frac{1}{32\pi} \int_{s_1,s_2} \frac{e^{-s_1 m_q^2}}{\sqrt{s_1 \sinh^2(s_1)}} \frac{e^{-s_2 m_q^2}}{\sqrt{s_2 \sinh^2(s_2)}} \int_{r_1,r_2} |r_1 - r_2| e^{-\frac{1}{2} |r_1 - r_2|^2 (\coth(s_1) + \coth(s_2))}
\]

(5.20)

Once again spatial integration done by transforming to center of mass and relative coordinates and done analytically using gamma functions.

\[
I_2 = \left( \frac{1}{2} \frac{e^2}{4\pi \varepsilon l_c} \right) \frac{V}{2\pi l_c^2} \frac{1}{16\sqrt{\pi}} \int_{s_1,s_2} \frac{e^{-s_1 m_q^2}}{\sqrt{s_1 \sinh^2(s_1)}} \frac{e^{-s_2 m_q^2}}{\sqrt{s_2 \sinh^2(s_2)}} \frac{1}{(\coth(s_1) + \coth(s_2))^2}
\]

(5.21)
The double integral over $s$ variable is diverging at lower limit and its leading contribution is independent of variational parameter, a situation similar was seen in computation of expectation value of kinetic term.

\[
\int_{s_1} \int_{s_2} \frac{e^{-s_1 m_q^2}}{\sqrt{s_1 \sinh^2(s_1)}} \frac{e^{-s_2 m_q^2}}{\sqrt{s_2 \sinh^2(s_2)}} \frac{1}{(\coth(s_1) + \coth(s_2))^{3/2}} \]

\[
= \int_{s_1} \int_{s_2} \frac{1}{\sqrt{s_1 \sinh^2(s_1) \sinh^2(s_2)}} \frac{1}{(\coth(s_1) + \coth(s_2))^{3/2}} \]

\[
+ \int_{s_1} \int_{s_2} \frac{(e^{-(s_1+s_2)m_q^2} - 1)}{\sqrt{s_1 \sinh^2(s_1) \sinh^2(s_2)}} \frac{1}{(\coth(s_1) + \coth(s_2))^{3/2}} \quad (5.22)
\]

The first term on the right hand side of the above equation is independent of variational parameter, hence we drop it and only retain the second term.

\[
\mathcal{I}_2 = \left( \frac{1}{2} \frac{e^2}{4\pi \varepsilon \ell_c} \right) \frac{V}{2\pi \ell_c^2} \eta_{bd}(m_q) \quad (5.23)
\]

The coefficient $\eta_{bd}(m_q)$ is computed numerically by implementing the double integral

\[
\eta_{bd}(m_q) = \frac{2\sqrt{2}}{\sqrt{\pi}} \int_{\frac{1}{\sqrt{2}\varepsilon \ell_c}}^{\infty} d\xi_1 \frac{1}{\sqrt{1 - e^{2\xi_1^2}}} \int_{\frac{1}{\sqrt{2}\varepsilon \ell_c}}^{\xi_1} d\xi_2 \frac{(e^{-2(\xi_1^2 + \xi_2^2) - 1})}{\sqrt{1 - e^{2\xi_1^2}(1 - e^{-2(\xi_1^2 + \xi_2^2)})^{3}}} \quad (5.24)
\]

The coefficients $\eta_{fg}(m_q)$ and $\eta_{bd}(m_q)$ both are function of $m_q^2$. We club them together,

\[
\eta_{C}(m_q) = \eta_{fg}(m_q) + \eta_{bd}(m_q) \quad (5.25)
\]

The net variational parameter dependence of Coulomb term can be expressed as,

\[
\langle \mathcal{H}_C \rangle = \frac{V}{2\pi \ell_c^2} \left( \frac{1}{2} \frac{1}{4\pi \varepsilon \ell_c} \right) \sum_{q=1}^{4} \eta_{C}(m_q) \quad (5.26)
\]
5.2 Ground state energy minimization

In this section we compute the ground state energies for Hall conductivity states $\sigma_H = 0$ and $\sigma_H = -1$ for the symmetric model. The general expression from the previous section are applied for each case and minimization is done numerically.

5.2.1 Ground state at $\sigma_H = 0$

The many body ground state has filled Dirac sea and two of four sub-levels of $n = 0$ Landau levels. As we discussed in section 4.3.2, the diagonal mass matrix takes the form $M_D = \{m_o, m_o, -m_u, -m_u\}$, i.e. $m_1 = m_2 = m_o$ the mass for the occupied $n = 0$ Landau levels and $m_3 = m_4 = -m_u$ are for the unoccupied ones.

The mean field energy for the ground state at Hall conductivity $\sigma_H = 0$ for the symmetry model,

$$\mathcal{E} = \langle \mathcal{H}_0 \rangle + \langle \mathcal{H}_C \rangle$$  \hspace{1cm} (5.27)

We only retain the terms that depend on the variational parameters for the ground state energy as other terms are inconsequential for the minimization routine. Using Eq.(5.10) for the kinetic energy and Eq.(5.26) Coulomb energy, and denoting

$$\kappa_t = \left( \frac{\hbar v_F}{\ell_c} \right)$$  \hspace{1cm} (5.28)

$$\kappa_C = \left( \frac{1}{2} \frac{1}{4\pi \varepsilon \ell_c} \right)$$  \hspace{1cm} (5.29)

$$\mathcal{E} = \frac{V}{2\pi \ell_c^2} \left( \kappa_t (\eta_t(m_o) + \eta_t(-m_u)) - \kappa_C (\eta_C(m_o) + \eta_C(-m_u)) \right)$$  \hspace{1cm} (5.30)

The mean field energy is decoupled for variational parameters, $m_o$ and $m_u$. Hence we can
minimize the two equations separately,

\[ \tilde{E}(m_o) = \kappa_t \eta_t(m_o) - \kappa_C \eta_C^2(m_o) \]  

(5.31)

\[ \tilde{E}(-m_u) = \kappa_t \eta_t(-m_u) - \kappa_C \eta_C^2(-m_u) \]  

(5.32)

The coefficients \( \eta_t(m) \) and \( \eta_C^2(m) \) are even functions of \( m \). Hence \( \tilde{E}(-m_u) = \tilde{E}(m_o) \).

This implies that if \( m_o = \tilde{m} \) results in extreme value for \( \tilde{E}(m_o) \) then \( m_u = \tilde{m} \) will be yield same type of extreme value for \( \tilde{E}(-m_u) \), because they are even function of the mass parameter. The diagonal mass matrix for the ground state at Hall conductivity \( \sigma_H = 0 \) take the form

\[ M_D = \{ \tilde{m}, \tilde{m}, -\tilde{m}, -\tilde{m} \} \]  

(5.33)

The angle parameters for the mass matrix \( M \) do not get fixed when working with the \( SU(4) \) symmetric model for Hall conductivity at \( \sigma_H = 0 \).

5.2.2 Ground state at \( \sigma_H = -1 \)

In the case for the ground state at \( \sigma_H = -1 \), there is the filled Dirac sea and one of the sub-levels of the \( n = 0 \) Landau level is occupied. Following the discussion in section 4.3.1, the diagonal mass matrix takes the form, \( M_D = \{ m_o, -m_u, -m_u, -m_u \} \), i.e. the occupied sub-level for \( n = 0 \) Landau level is attributed mass, \( m_1 = m_o \) and the unoccupied ones \( m_2 = m_3 = m_4 = -m_u \).

The mean field energy is computed by collecting variational parameter dependent of the kinetic, \( \langle \mathcal{H}_t \rangle \) using Eq.(5.10) and the Coulomb term, \( \langle \mathcal{H}_C \rangle \), using Eq.(5.26). Using the definition of \( \kappa_t \) in Eq.(5.28) and \( \kappa_C \) in Eq.(5.29), the mean field energy can be arranged as decoupled functions of variational parameters, \( m_o \) and \( m_u \).

\[ \mathcal{E} =\frac{V}{2\pi \ell_C^2} \left( \kappa_t \eta_t(m_o) - \kappa_C \eta_C^2(m_o) + 3 \left( \kappa_t \eta_t(m_u) - \kappa_C \eta_C^2(m_u) \right) \right) \]  

(5.34)
Figure 5.1: This figure shows the variation of dimensionless mass parameter with magnetic field. The mean field energy is minimized by these mass parameter for the particular magnetic field. We have shown the variation of mass parameter with dielectric constant of the substrates. $\varepsilon_r = 1$ corresponds for suspended graphene. The mass parameter is in units of $(\hbar v_F/l_c)$, so $m \to 0$ as $B \to 0$. Here dimensionless constant $\alpha$ is the ratio $\kappa_C/\kappa_L$.

The decoupling of variables $m_o$ and $m_u$ in the above equation yields us similar situation as we had seen in the case for $\sigma_H = 0$. Once again the decoupled equations that needs to minimized are exactly same as we had seen in Eq.(5.31) for parameter $m_o$ and Eq.(5.32). And same argument holds for the extreme values, i.e. $m_o = \tilde{m} = m_u$. Hence in the case for Hall conductivity $\sigma_H = -1$, the diagonal mass matrix takes the form,

$$M_D = \{\tilde{m}, -\tilde{m}, -\tilde{m}, -\tilde{m}\}$$

(5.35)
5.3 Particle-hole gaps

In this section we will compute the particle-hole excitation gaps for the ground states we found for the Hall conductivity states that we found in the previous section. The variational parameters are fixed by the minimization procedure. In the case for the symmetric model, the masses of the Dirac particle get fixed via minimization and the angle parameters are still arbitrary as we saw in the previous section that mean field energy was independent of variational angle parameters. For the particle-hole excitation gaps within the symmetric model, is independent of angle parameters. We will see that the size of the gaps are decided by the symmetric model.

We are considering the particle-hole excitations about the ground state, so in general the excited state can be constructed,

\[ |ES\rangle = \psi_{n_p,l_p,q_p}^{\dagger} \psi_{n_h,l_h,q_h} |GS\rangle \]  

(5.36)

i.e. a hole is created by annihilate a state with quantum numbers \((n_h, l_h, q_h)\), here Landau level index, \(n_h\), of the hole created with \(l_p\) its orbital angular momentum and \(q_h\) the \(SU(4)\) index. And a particle is created by the creation operator with quantum numbers \((n_p, l_p, q_p)\).

The particle-hole activation gap is computed from the expectation value of hamiltonian for excited state and the ground state,

\[ \Delta_{gap} = \frac{1}{2} \left( \langle ES | H | ES \rangle - \langle GS | H | GS \rangle \right) \]  

(5.37)

The ground state expectation value of hamiltonian can be expressed in terms of two point correlator, used for mean field energy calculation. In the similar fashion as we did for ground state computations, we can define two point correlator for excited states,
\( \Upsilon(r_1, r_2) \), which is excited state expectation value for two field operators, defined as

\[
\Upsilon_{r,A; s,B}(r_1, r_2) = \langle ES| \Psi_{s,B}^\dagger(r_2) \Psi_{r,A}(r_1) |ES \rangle
\] (5.38)

This expectation value can be expressed in terms of the wave functions used to construct
the variational state,

\[
\Upsilon_{r,A; s,B}(r_1, r_2) = \Phi_{r,A}^{n_p,l_p,q_p}(r_1) \Phi_{s,B}^{n_p,l_p,q_p}(r_2) \nonumber ^* - \Phi_{r,A}^{n_h,l_h,q_h}(r_1) \Phi_{s,B}^{n_h,l_h,q_h}(r_2) \nonumber ^* + \Gamma_{r,A; s,B}(r_1, r_2)
\] (5.39)

This correlator is 8 x 8 matrix and in compact notation we can write,

\[
\Upsilon(r_1, r_2) = \Gamma^{(p)}(r_1, r_2) - \Gamma^{(h)}(r_1, r_2) + \Gamma(r_1, r_2)
\] (5.40)

Here, the correlator for the particle,

\[
\Gamma^{(p)}(r_1, r_2) = \Phi_{r_1, l_p}^{n_p}(r_1) \Phi_{r_2, l_p}^{n_p}(r_2)
\] (5.41)

and the correlator for the hole,

\[
\Gamma^{(h)}(r_1, r_2) = \Phi_{r_1, l_h}^{n_h}(r_1) \Phi_{r_2, l_h}^{n_h}(r_2)
\] (5.42)

\( \Gamma(r_1, r_2) \) is the two point correlator for the ground state.

In our case, the excited state for the ground states at Hall conductivity at \( \sigma_H = 0, -1 \) has
particle and hole state belong to different sub-levels of \( n = 0 \) Landau level.

\[
|ES \rangle = \psi_{0,l_p,q_p}^\dagger \psi_{0,l_h,q_h}^\dagger |GS \rangle
\] (5.43)
The wave function for the \( n = 0 \) Landau level,

\[
\Phi_{0,l,q}(r) = \begin{pmatrix}
0 \\
\varphi_{0,l}(r)
\end{pmatrix} \chi^q \chi^q \dagger
\]

(5.44)

Here,

\[
\varphi_{0,l}(r) = \frac{1}{\sqrt{2\pi \ell_c^2}} \frac{1}{\sqrt{2\pi}} e^{-i l \theta} \frac{1}{l!} \left( \frac{\bar{z}}{\sqrt{2}} \right)^l e^{-\frac{1}{4} |z|^2}
\]

(5.45)

the wave function expressed in complex variable will be useful for analytic computation of the gaps as we shall see shortly.

The correlator for the particle or hole, \((x = p, h)\)

\[
\Gamma^{(x)}(r_1, r_2) = \Phi^{0,l_x,q_x}(r_1) \Phi^{0,l_x,q_x \dagger}(r_2)
\]

\[
= \frac{1}{2\pi \ell_c^2} \frac{1}{2(1 - \beta)} \frac{1}{l_x!} \left( \frac{\bar{z}_1 z_2}{2} \right)^{l_x} e^{-\frac{1}{4} (|z_1|^2 + |z_2|^2)} P_{q_x}
\]

It is useful for computations to express the above expression in relative coordinates and this achieved by using following relations,

\[
|r_1 - r_2|^2 = |z_1 - z_2|^2 = |z_1|^2 + |z_2|^2 - (\bar{z}_1 z_2 + z_1 \bar{z}_2)
\]

(5.46)

\[
\Gamma^{(x)}(r_1, r_2) = \left( \frac{1}{2\pi \ell_c^2} \right) \frac{1}{2(1 - \beta)} \frac{1}{l_x!} \left( \frac{\bar{z}_1 z_2}{2} \right)^{l_x} e^{-\frac{1}{4} (z_1 z_2 + z_1 \bar{z}_2)} e^{-\frac{1}{4} |z_1 - z_2|^2} P_{q_x}
\]

(5.47)

Note that we have not mentioned anything about the angle parameters for the hole and particle states. Within symmetric model we will show that \( SU(4) \) component of the correlator gets traced out leaving no angle dependence for the activation gaps.
5.3.1 Kinetic term

To compute the contribution to the activation gap from the kinetic terms we need to evaluate

\[ \Delta_t = \frac{1}{2} \left( \langle ES|\mathcal{H}_0|ES \rangle - \langle GS|\mathcal{H}_0|GS \rangle \right) \]  \hspace{1cm} (5.48)

We can express the left hand side of the above equation in terms of the correlator, following the discussion of section 5.1.1.

\[ \Delta_t = \frac{1}{2} \left( \frac{\hbar v_F}{\ell_c} \right) \left( \int r \lim_{r_0 \to r} \text{Tr}[h \Upsilon(r, r_0)] - \int r \lim_{r_0 \to r} \text{Tr}[h \Gamma(r, r_0)] \right) \]  \hspace{1cm} (5.49)

Using the definition of two point correlator for excited state, Eq.(5.40), we find evaluation of correlator for the particle and hole, \( \text{Tr}[h \Gamma^{(p)}(r, r_0)] = 0 \) and \( \text{Tr}[h \Gamma^{(h)}(r, r_0)] = 0 \). And the \( \text{Tr}[h \Gamma(r, r_0)] \) cancels and hence this leads to conclusion that there is no contribution to activation gap from the kinetic term. This is has to do with the fact that both particle and hole states which are \( n = 0 \) Landau levels are same for both massless and massive cases. And here the hamiltonian \( h \) is for massless Dirac particle which have zero eigenvalue for \( n = 0 \) Landau level.

5.3.2 Coulomb term

The contribution to the activation gap from the Coulomb term is computed by evaluating,

\[ \Delta_C = \frac{1}{2} \left( \langle ES|\mathcal{H}_C|ES \rangle - \langle GS|\mathcal{H}_C|GS \rangle \right) \]  \hspace{1cm} (5.50)

Here \( \mathcal{H}_C \) is taken from Eq.(5.3). And use two point correlator to evaluate the above expression in a similar fashion as we accomplished for mean field energy computation in section 5.1.2.
The direct term contributions for $\Delta_C$

$$\frac{1}{2} \left( \frac{1}{2} \frac{e^2}{4\pi \varepsilon} \right) \int_{r_1, r_2} \frac{1}{|r_1 - r_2|} \left( \text{Tr}[\Gamma^{(p)}(r_1, r_1) - \Gamma^{(h)}(r_1, r_1)] \right) \right)$$

$$\left( \text{Tr}[\Gamma^{(p)}(r_2, r_2) - \Gamma^{(h)}(r_2, r_2)] \right)$$  \hspace{1cm} (5.51)

The exchange contributions

$$\frac{1}{2} \left( \frac{1}{2} \frac{e^2}{4\pi \varepsilon} \right) \int_{r_1, r_2} \frac{1}{|r_1 - r_2|} \left( \text{Tr}[\left( \Gamma^{(p)}(r_1, r_2) - \Gamma^{(h)}(r_1, r_2) \right) \Gamma(r_2, r_1)] \ight.$$

$$\left. + \text{Tr}[\left( \Gamma^{(p)}(r_2, r_1) - \Gamma^{(h)}(r_2, r_1) \right) \Gamma(r_1, r_2)] \ight.$$ 

$$\left. + \text{Tr}[\left( \Gamma^{(p)}(r_1, r_2) - \Gamma^{(h)}(r_1, r_2) \right) \left( \Gamma^{(p)}(r_2, r_2) - \Gamma^{(h)}(r_2, r_2) \right)] \right)$$  \hspace{1cm} (5.52)

On collecting the direct and exchange contributions together to find the final expression for excitation gap, we find terms

$$\text{Tr}[\Gamma^{(p)}(r_1, r_1)]\text{Tr}[\Gamma^{(p)}(r_2, r_2)] - \text{Tr}[\Gamma^{(p)}(r_1, r_2)\Gamma^{(p)}(r_2, r_1)]$$

and

$$\text{Tr}[\Gamma^{(h)}(r_1, r_1)]\text{Tr}[\Gamma^{(h)}(r_2, r_2)] - \text{Tr}[\Gamma^{(h)}(r_1, r_2)\Gamma^{(h)}(r_2, r_1)]$$

on spatial integration have no contribution as the direct and exchange terms cancel each other. The terms

$$\text{Tr}[\Gamma^{(p)}(r_1, r_2)\Gamma^{(h)}(r_2, r_1)] = 0$$

by virtue of orthonormal $SU(4)$ components of the particle and hole wave functions.

In our simplified picture of activation process we are assuming that the hole is created at one end of the sample and the particle is created on the other end. The overlap of particle and hole wave functions, whose centers are separated by large distances can neglected.
And the term
\[
\iint_{r_1, r_2} \frac{1}{|r_1 - r_2|} \text{Tr}[\Gamma^{(p)}(r_1, r_1)] \text{Tr}[\Gamma^{(h)}(r_2, r_2)]
\]
which is essentially overlap of particle and hole wave functions with a weight factor of inverse of distance between them, i.e. we are not considering the possibility that particle and hole states can form a bound state. Hence we can neglect this integral.

The activation gap in SU(4) symmetric model comes from the exchange terms only,

\[
\frac{1}{2} \left( \frac{e^2}{2} \right) 2 \int \int_{r_1, r_2} \frac{1}{|r_1 - r_2|} \left( \text{Tr}[\Gamma^{(h)}(r_1, r_2) \Gamma(r_2, r_1)] - \text{Tr}[\Gamma^{(p)}(r_1, r_2) \Gamma(r_2, r_1)] \right)
\]

\[
\text{(5.53)}
\]

The activation gap from the Coulomb term,

\[
\Delta_C = \frac{1}{2} \left( \frac{e^2}{2} \right) 2 \sum_{q} \frac{1}{\sqrt{\pi}} \int \frac{1}{l!} \left( \bar{z}_1 z_2 \right)^l \left( e^{-\frac{1}{4}(\bar{z}_1 z_2 + z_1 \bar{z}_2)} - e^{-\frac{1}{4}|z_1 - z_2|^2} g_{m_q}(z_2, z_1) \right)
\]

\[
\text{(5.55)}
\]

Using the particle and hole correlator from Eq.(5.47) and the correlator for filled Dirac sea from Eq.(4.67). And we convert the integrals to complex coordinates as we did earlier.

\[
\Delta_C = \frac{1}{2} \left( \frac{e^2}{2} \right) 2 \sum_{q=1}^{4} \frac{1}{\sqrt{\pi}} \int \frac{1}{l!} \left( \bar{z}_1 z_2 \right)^l \left( e^{-\frac{1}{4}(\bar{z}_1 z_2 + z_1 \bar{z}_2)} - e^{-\frac{1}{4}|z_1 - z_2|^2} g_{m_q}(z_2, z_1) \right)
\]

\[
\text{(5.56)}
\]

After plugging in \( g_{m_q}(z_2, z_1) \)

\[
\Delta_C = \left( \frac{1}{2} \left( \frac{e^2}{2} \right) 2 \sum_{q=1}^{4} \frac{1}{\sqrt{\pi}} \int \frac{1}{l!} \left( \bar{z}_1 z_2 \right)^l \left( e^{-\frac{1}{4}(\bar{z}_1 z_2 + z_1 \bar{z}_2)} - e^{-\frac{1}{4}|z_1 - z_2|^2} g_{m_q}(z_2, z_1) \right) \right)
\]

\[
\text{(5.56)}
\]
Figure 5.2: This figure shows the variation of activation gap with applied magnetic field. The gaps in meV and magnetic field in Tesla. The gaps for the Hall conductivity at $\sigma_H = 0$ and $\sigma_H = -1$ are same. The points are values for the gap obtained from our calculations where filled Dirac sea is taken into account and solid line curve is obtained when lowest Landau level projection is considered. The thin solid line with the points show the best fit. The best fit is function of magnetic field of the form $a\sqrt{B} + bB + c$, with $a$, $b$ and $c$ are best fit parameters. We have shown the variation of gaps with change in the dielectric constant of the substrate. The dielectric constant $\epsilon_r = 1$ corresponds to the suspended graphene. The best fit showed the dominant $\sqrt{B}$ contribution and linear $B$ decreases as the dielectric constant of substrate increased. The constant term in the best fit was negligible. Along with dielectric constant we have presented the value $\alpha = \kappa_C/\kappa_I$.

The spatial integrals are solved analytically using the general solution from Appendix G.

$$\Delta_C = \left(\frac{e^2}{4\pi \epsilon_c}\right) \frac{1}{2} \sum_{q=1}^{4} \text{Tr}[P_h P_q - P_p P_q] \frac{m_q}{2\sqrt{\pi}} \int_s e^{-s(m_q^2-1)} \frac{\pi}{\sqrt{s} \sinh(s)} \sqrt{(1 + \coth(s))}$$ \hspace{1cm} (5.57)

Using the fact from the energy minimization $m_h = \tilde{m}$ and $m_p = -\tilde{m}$, the contribution to gap from filled Dirac sea,

$$\Delta_C = \left(\frac{e^2}{2\pi \epsilon_c}\right) \frac{\tilde{m}}{2} \int_s \frac{e^{-s\tilde{m}^2}}{\sqrt{s} \sinh(s)} \frac{e^{\tilde{m}^2}}{\sqrt{s} \sinh(s)} = \left(\frac{e^2}{2\pi \epsilon_c}\right) \eta C_1(\tilde{m})$$ \hspace{1cm} (5.58)
The coefficient $\eta_{C_1}$ in numerically implemented as following

$$\eta_{C_1} = \tilde{m} \sqrt{2} \int_{\sqrt{2} \kappa_C}^{\infty} \frac{d\xi}{\sqrt{1 - e^{-2\xi^2}}}$$  \hspace{1cm} (5.59)

The activation gap for the symmetric model for the Hall conductivity at $\sigma_H = 0$ and $\sigma_H = -1$,

$$\Delta_{\text{gap}} = \Delta_C$$  \hspace{1cm} (5.60)

The variation of particle-hole gap with magnetic field is shown in Fig.5.2. The values of gap were computed numerically and the result was best fitted to a curve of the form $a\sqrt{B} + bB + c$. Here $a, b, c$ are the best fit coefficients. We observe that dominant contribution comes from the $\sqrt{B}$ contribution and few percent contribution from the linear term and the constant term was very small compared to $\sqrt{B}$ contribution. We have compared results of our calculations where filled Dirac sea is taken into account with that of lowest Landau level projection. In Fig.5.2, we have also presented the variation of gaps with dielectric constant of the substrate. It clearly shows decrease in gaps as dielectric constant increases and also the linear magnetic field dependence of our best fit of the gaps. The magnitude of gaps that we obtained from our computations is approximately double of what is seen in the gap measurements for the suspended graphene [1].

### 5.4 Summary

We here summarize the results of our symmetric model calculations,

1. We have showed that the Coulomb interaction breaks the $SU(4)$ symmetry spontaneously for the ground states for Hall conductivity at $\sigma_H = 0$ and $\sigma_H = -1$.

2. The order parameter for spontaneous symmetry breaking is the mass of the Dirac particle which is proportional to a dimensionless $\alpha = \kappa_C/\kappa_1$, which depends on
dielectric constant.

3. The order parameter is proportional to magnetic field and tends to zero as magnetic field goes to zero which indicates spontaneous symmetry breaking of $SU(4)$ symmetry by Coulomb interaction in presence of magnetic field.

4. The particle-hole gaps from symmetric model showed a square root dependence on the applied magnetic field. Our symmetric model without disorder taken into account over estimates the gaps when compared with experimental values.