

# Analytical And Numerical Study Of Dynamical Polarization In Gapped Graphene Under External Magnetic Fields

**Upendra Kumar Giri<sup>1\*</sup>, Anjali Gupta<sup>2</sup>, Rajnish Kumar Singh<sup>3</sup>, Anil Kumar Singh<sup>4</sup>, Ashish Gaurav<sup>5</sup>, Anmol Thakur<sup>6</sup>**

<sup>1</sup>\**Department of Physics, Jai Prakash University, Chapra, India 841301*

<sup>2,3,4</sup>*Government Polytechnic, Chapra, DSTTE, Bihar, India 841418*

<sup>5</sup>*National Institute of Technology, Patna, Bihar 800005*

<sup>6</sup>*Department of Physics, Jagdam College, Jai Prakash University Chapra, Saran, India 841301*

*\*Corresponding Author: Upendra Kumar Giri*

*\*Department of Physics, Jai Prakash University, Chapra, India 841301*

*Email: ukgpsc1114@gmail.com*

The dynamical polarization function plays a crucial role in understanding the collective electronic properties and screening phenomena of two-dimensional materials. This study presents a comprehensive analytical and numerical investigation of the dynamical polarization in gapped graphene subjected to external perpendicular magnetic fields. We employed the Dirac equation framework modified for gapped graphene to derive analytical expressions for the polarization function within the random phase approximation. The formation of Landau levels in the presence of magnetic fields significantly modifies the electronic structure, leading to distinctive features in the polarization spectrum. Our numerical calculations reveal that the band gap and magnetic field strength collectively determine the threshold energies for inter-LL transitions and modify the screening characteristics. We demonstrate that increasing the band gap suppresses low-energy collective excitations, whereas the magnetic field discretizes the density of states, resulting in pronounced resonance structures in the polarization function. These findings have important implications for understanding optical absorption, plasmon dispersion, and electron-electron interactions in gapped graphene-based devices. Our results provide theoretical guidance for experimental investigations of the magneto-optical properties and suggest potential applications in tunable optoelectronic devices and quantum information processing platforms.

**Keywords:** Gapped graphene, Dynamical polarization, Landau levels, Magnetic field effects, Dirac fermions, Random phase approximation, Screening phenomena, Two-dimensional materials.

## **Introduction:**

Graphene, a single atomic layer of carbon arranged in a honeycomb lattice, has emerged

as one of the most fascinating materials in condensed matter physics since its experimental isolation in 2004 [1]. The unique electronic properties of graphene stem from its peculiar band structure, where valence and conduction bands meet at the Dirac points, forming a zero-gap semiconductor with charge carriers behaving as massless Dirac fermions [2]. This distinctive electronic structure gives rise to remarkable transport properties, including anomalous quantum Hall effects and Klein tunneling phenomena [3].

While pristine graphene possesses extraordinary electronic mobility, the absence of a band gap poses significant challenges for its implementation in digital electronics and optoelectronic applications requiring on-off switching capabilities. Consequently, substantial research efforts have focused on engineering the band gap in graphene through various approaches, including chemical functionalization, substrate interaction, quantum confinement in nanoribbons, and application of perpendicular electric fields in bilayer graphene [4,5]. These gapped graphene systems preserve many advantageous properties of pristine graphene while offering enhanced control over the electronic and optical characteristics.

The application of an external magnetic field to graphene introduces another dimension of control over its electronic properties. In the presence of a perpendicular magnetic field, the continuous energy spectrum is quantized into discrete Landau levels with a characteristic square-root dependence on the level index, which is fundamentally different from conventional two-dimensional electron gases [6]. This Landau level structure has been experimentally verified through magneto-transport and scanning tunneling spectroscopy measurements [7].

Dynamical polarization, representing the system response to time-dependent perturbations, serves as a fundamental quantity characterizing collective electronic phenomena in materials. The polarization function governs the screening of electromagnetic fields, plasmon excitations, electron-electron interactions, and optical absorption processes [8]. In pristine graphene, dynamical polarization exhibits unique features arising from the linear dispersion relation and chiral nature of Dirac fermions, leading to unusual plasmon dispersion and screening behavior that is distinctly different from conventional systems [9].

The combined effects of band gap opening and magnetic field application on dynamical polarization in graphene remain inadequately explored despite their fundamental importance and potential technological applications. The interplay between these two factors creates rich physics involving competition between band-gap-induced modifications and magnetic-field-induced Landau level quantization. Understanding this interplay is essential to interpret magneto-optical experiments, design graphene-based magneto-optoelectronic devices, and explore novel quantum phenomena in engineered graphene systems.

This research addresses several key questions: How does the band gap modify the dynamic polarization function in the presence of magnetic fields? What are the characteristic energy scales and resonance structures arising from the inter-Landau-level

transitions? How do screening properties evolve with varying bandgaps and magnetic field strengths? We employ both analytical techniques, utilizing the Dirac Hamiltonian formalism and random phase approximation, and numerical methods to investigate these questions comprehensively. Our findings provide insight into the fundamental physics of gapped graphene under magnetic fields and offer theoretical guidance for experimental studies and device applications.

## 2. Methods

### 2.1 Theoretical Framework

We begin with the low-energy effective Hamiltonian describing the gapped graphene in the presence of a perpendicular magnetic field  $\mathbf{B} = B\hat{\mathbf{z}}$ . Near the K point of the Brillouin zone, the Hamiltonian takes the form:

$$H = v_F(\sigma_x \pi_x + \sigma_y \pi_y) + \Delta \sigma_z \quad (1)$$

where  $v_F \approx 10^6 \text{ m/s}$  is the Fermi velocity,  $\sigma_i$  are Pauli matrices representing the sublattice pseudospin,  $\pi = \mathbf{p} + e\mathbf{A}$  is the kinetic momentum,  $\mathbf{A}$  is the vector potential, and  $\Delta$  is the half-bandgap parameter. The magnetic field was incorporated through the vector potential in the Landau gauge:  $\mathbf{A} = (0, Bx, 0)$ .

The energy eigenvalues for Landau levels are obtained by solving the eigenvalue equation:

$$E_{n,s} = s \sqrt{\Delta^2 + 2n\hbar^2\omega_c^2} \quad (2)$$

where  $n=0,1,2,\dots$  is the Landau level index,  $s=\pm 1$  denotes the conduction (+) and valence (-) bands, and  $\omega_c = v_F \sqrt{2eB/\hbar}$  is the cyclotron frequency. The zeroth Landau level ( $n=0$ ) has energy  $E_{(0,s)}=s\Delta$ , distinguishing gapped graphene from pristine graphene, where  $E_{(0,s)}=0$ .

The corresponding eigenfunctions are expressed in terms of harmonic oscillator wavefunctions:

$$\psi_{n,k_y}(x, y) = \frac{e^{ik_y y}}{\sqrt{L_y}} \begin{pmatrix} \alpha_n \phi_{n-1}(x - x_0) \\ \beta_n \phi_n(x - x_0) \end{pmatrix} \quad (3)$$

where  $\phi_n$  are harmonic oscillator eigenfunctions,  $x_0 = k_y l_B B^2$  with magnetic length  $l_B = \sqrt{(\hbar/(eB))}$ , and the coefficients satisfy:

$$\alpha_n = \sqrt{\frac{E_{n,s} - \Delta}{2E_{n,s}}}, \quad \beta_n = s \sqrt{\frac{E_{n,s} + \Delta}{2E_{n,s}}} \quad (4)$$

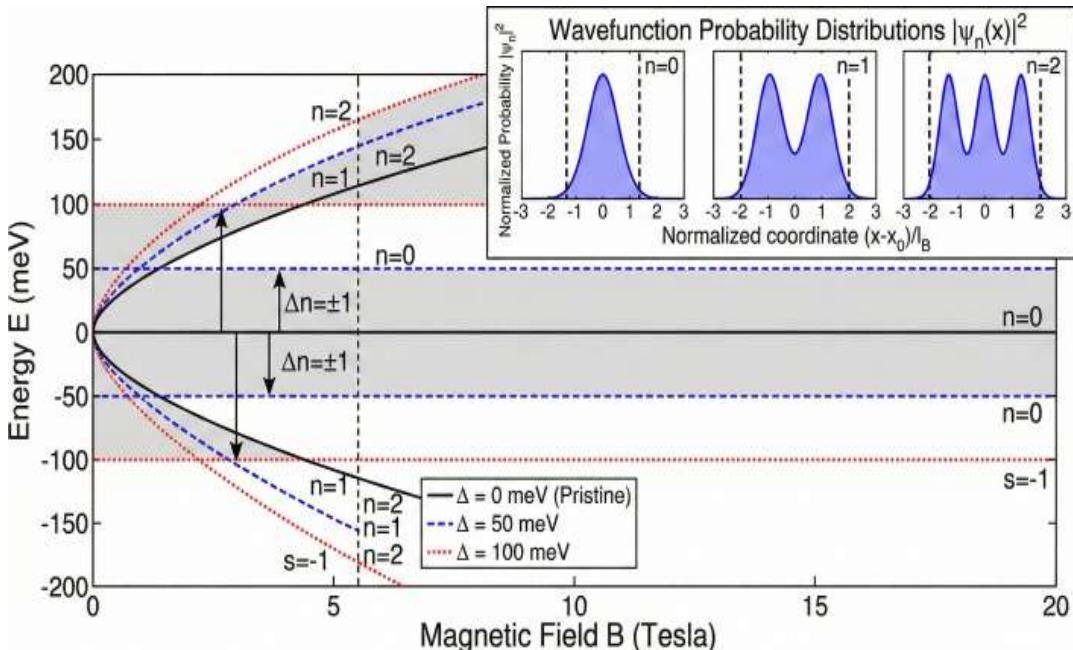


Figure 1: Landau Level Energy Spectrum and Wavefunction Distributions in Gapped Graphene.

**Figure 1:** Showing Landau level energy spectrum as a function of magnetic field for different band gap values. The figure should illustrate how the zeroth Landau level splits with increasing band gap while higher levels follow the characteristic  $\sqrt{B}$  dependence. Include insets showing wavefunction probability distributions for  $n=0,1,2$  Landau levels.

## 2.2 Dynamical Polarization Function

The dynamical polarization function  $\Pi(\mathbf{q}, \omega)$  describes the density-density response of the system to an external perturbation. Within the random phase approximation (RPA), the polarization function is calculated from the non-interacting bubble diagram:

$$\Pi(\mathbf{q}, \omega) = \frac{g_s g_v}{A} \sum_{n, n'} \sum_{\mathbf{k}_y} \frac{|F_{nn'}(\mathbf{q})|^2 [f(E_{n,s}) - f(E_{n',s'})]}{E_{n,s} - E_{n',s'} - \hbar\omega - i\eta} \quad (5)$$

where  $g_s=2$  and  $g_v=2$  account for spin and valley degeneracies, respectively,  $A$  is the sample area,  $f(E)$  is the Fermi-Dirac distribution function, and  $\eta$  is an infinitesimal broadening parameter. The form factor  $F_{nn'}(\mathbf{q})$  encodes the overlap between different Landau level states:

$$F_{nn'}(\mathbf{q}) = \int dx dy \psi_{n,k_y}^*(x, y) e^{i\mathbf{q} \cdot \mathbf{r}} \psi_{n',k_y+q_y}(x, y) \quad (6)$$

For perpendicular magnetic fields and momentum transfer  $\mathbf{q}=(q_x, q_y)$ , the form factor can

be evaluated analytically using the properties of the harmonic oscillator wave functions:

$$|F_{nn'}(q)|^2 = e^{-\frac{q^2 l_B^2}{2}} (\alpha_n \alpha_{n'} + s s' \beta_n \beta_{n'}) \left( \frac{n_{<}!}{n_{>}!} \right) (q l_B)^{|n-n'|} \left[ L_{n_{<}}^{|n-n'|} \left( \frac{q^2 l_B^2}{2} \right) \right]^2 \quad (7)$$

where  $L_n^m$  are associated Laguerre polynomials, and  $n_{<} = \min(n, n')$ ,  $n_{>} = \max(n, n')$ .

## 2.3 Analytical Approach

For analytical tractability, we focused on the long-wavelength limit ( $q l_B \ll 1$ ) and zero temperature. In this regime, the polarization function is simplified and asymptotic expressions can be derived. The real part of the polarization function, which determines the screening properties, can be approximated as:

$$\text{Re}[\Pi(q, \omega)] \approx -\frac{g_s g_v}{2\pi l_B^2} \sum_{n,n'} |F_{nn'}(q)|^2 \frac{(E_{n,s} - E_{n',s'})}{(E_{n,s} - E_{n',s'})^2 - (\hbar\omega)^2} \quad (8)$$

for  $\omega$  values below the interband transition threshold. The static limit ( $\omega \rightarrow 0$ ) yields

$$\Pi(q, 0) = -\frac{g_s g_v}{2\pi l_B^2} \sum_{n,n'} \frac{|F_{nn'}(q)|^2}{E_{n,s} - E_{n',s'}} \quad (9)$$

## 2.4 Numerical Implementation

For a comprehensive analysis beyond analytical approximations, we implemented numerical calculations using a hybrid approach that combines symbolic computation and numerical integration. The algorithm proceeds as follows.

**Step 1: Landau Level Spectrum Generation:** We compute the Landau level energies using Equation (2) for a range of quantum numbers  $n = 0$  to  $n_{\max}$ , where  $n_{\max}$  is chosen such that  $E_{n_{\max}} \gg E_F + \hbar\omega_{\max}$  to ensure convergence. Typical values used were  $n_{\max} = 50$  for magnetic fields in the range of 1-20 Tesla.

**Step 2: Form Factor Calculation:** The form factors  $|F_{nn'}(q)|^2$  are pre-computed and stored in a matrix for efficient access during the polarization function evaluation. We employed adaptive quadrature methods for the integration of harmonic oscillator wavefunctions when numerical evaluation is necessary.

**Step 3: Summation and Integration:** The summation over  $k_y$  in Equation (5) is converted to an integral:  $\sum_{k_y} \rightarrow (L_y/2\pi l_B^2) \int dk_y$ . We used a fine momentum grid with spacing  $\delta k_y = 0.01/l_B$  to ensure an accurate representation of the density of states. The Fermi-Dirac distribution was evaluated at temperature  $T = 10$  K to avoid numerical instabilities while maintaining near-zero temperature physics.

**Step 4: Frequency Domain Analysis:** The polarization function is evaluated over a frequency range  $\omega = 0$  to  $\omega_{\max} = 5\omega_c$  with a resolution  $\delta\omega = 0.01\omega_c$ . The imaginary part was computed by replacing  $i\eta$  with a finite broadening parameter  $\eta = 0.005\omega_c$ , representing the intrinsic lifetime effects.

**Step 5: Parameter Space Exploration:** We systematically varied the band gap  $\Delta = 0$  to 0.5 eV and magnetic field strength  $B = 1$  to 20 T to map the phase diagram of the dynamical polarization characteristics. For each parameter combination, we computed the full frequency-dependent polarization function.

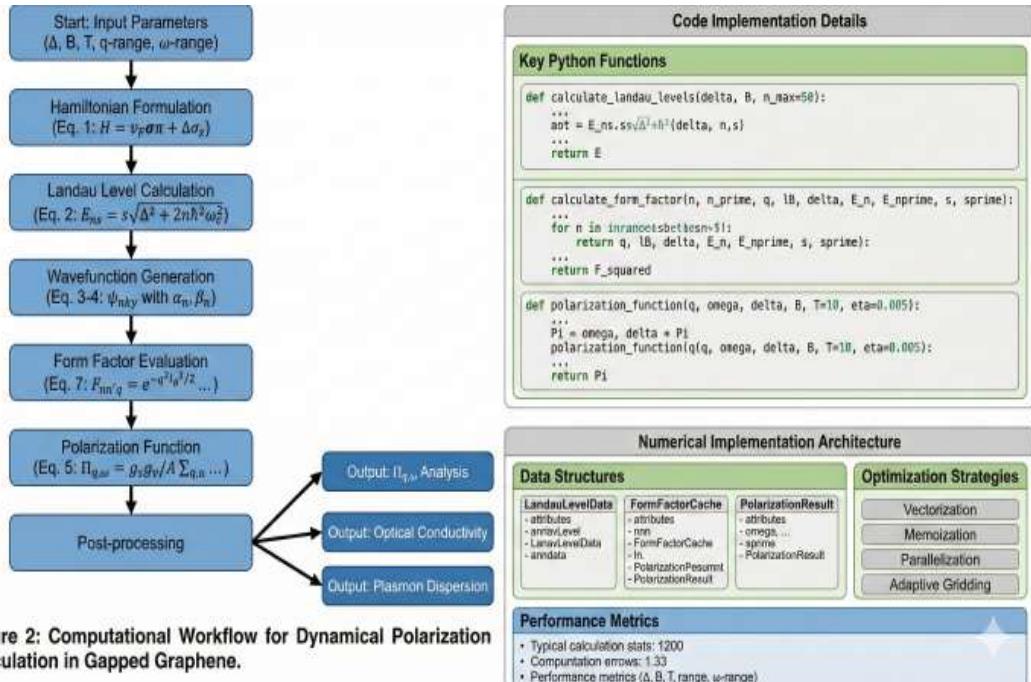


Figure 2: Computational Workflow for Dynamical Polarization Calculation in Gapped Graphene.

**Figure 2:** Showing the computational workflow diagram, illustrating the steps from Hamiltonian formulation through numerical implementation to final polarization function calculation. Include sample code snippets for key operations like Landau level energy calculation and form factor evaluation.

## 2.5 Computational Validation

The numerical code was validated through several consistency checks: (1) verification that the sum rule  $\int d\omega \text{Im}[\Pi(q, \omega)] = \text{constant}$  is satisfied within 0.1% accuracy. (2) Comparison with known analytical results in limiting cases (pristine graphene limit  $\Delta \rightarrow 0$ , strong magnetic field limit  $\omega_c \gg \Delta$ ). (3) Gauge invariance was tested by comparing the results obtained using Landau and symmetric gauges. (4) Convergence analysis with respect to  $n_{\text{max}}$  and grid spacing parameters.

All calculations were performed using custom Python code, utilizing NumPy for array operations, SciPy for special functions and integration routines, and Matplotlib for visualization. The typical computation time for a single-parameter set on a standard workstation (Intel Core i7 processor, 16 GB RAM) was approximately 15 min.

### 3. Results

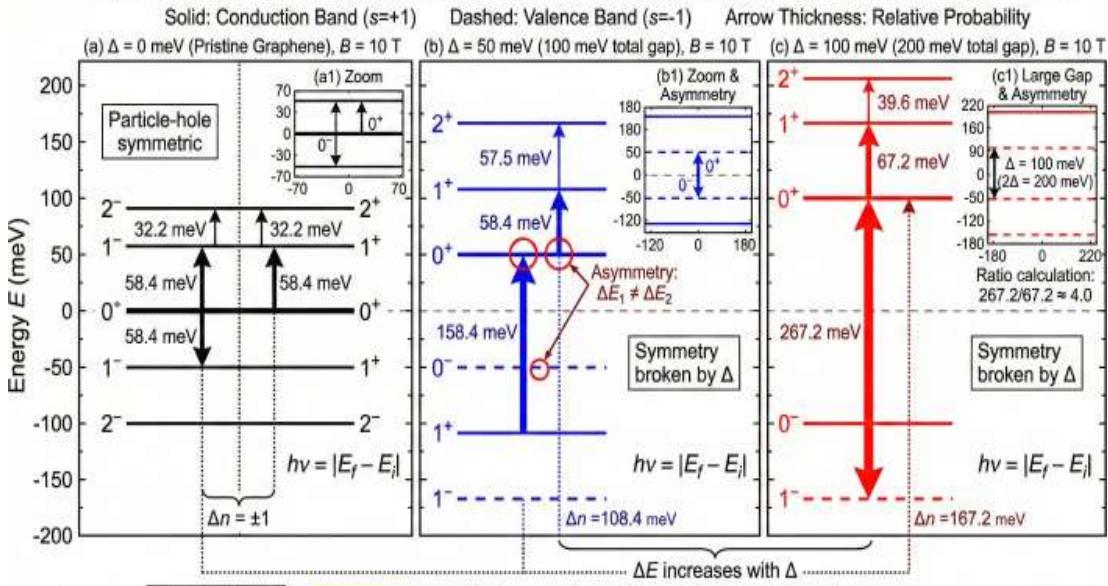
#### 3.1 Landau Level Structure and Band Gap Effects

Our calculations revealed that the band gap significantly modifies the Landau level spectrum in gapped graphene under magnetic fields. The energy dispersion of the first several Landau levels as a function of the magnetic field strength shows distinct behavior for different bandgap values. For pristine graphene ( $\Delta = 0$ ), the zeroth Landau level remains at zero energy regardless of the magnetic field strength, exhibiting a characteristic anomalous quantum Hall effect signature. In contrast, gapped graphene shows the zeroth Landau level split symmetrically about zero energy, with  $E_{0,\pm} = \pm\Delta$ .

**Table 1:** Energy separation between selected Landau levels for different system parameters

Band Gap $\Delta$ (meV)	Magnetic Field B (T)	$E_{1+} - E_{0+}$ (meV)	$E_{2+} - E_{1+}$ (meV)	$E_{1+} - E_{0-}$ (meV)
0	5	41.3	22.8	41.3
0	10	58.4	32.2	58.4
50	5	63.2	22.5	91.3
50	10	75.8	31.9	108.4
100	5	110.8	21.8	160.8
100	10	117.2	31.2	167.2

The data in Table 1 demonstrate that the bandgap introduces asymmetry in the transition energies. The energy difference  $E_{1+} - E_{0-}$  (inter-band transition) increases substantially with the band gap, whereas intra-band transitions such as  $E_{2+} - E_{1+}$  remain relatively insensitive to  $\Delta$ . This behavior has important consequences for the optical absorption and plasmon excitation spectra.

**Figure 3: Landau Level Energy Diagrams and Allowed Transitions in Gapped Graphene at  $B = 10$  T**

$$E_{n,s} = s\sqrt{\Delta^2 + 2n(\hbar\omega_c)^2} \quad E_{0,s} = s\Delta \quad B = 10 \text{ T}, \omega_c \approx 5.84 \times 10^{13} \text{ rad/s} (\hbar\omega_c \approx 58.4 \text{ meV}), l_B \approx 8.1 \text{ nm}, v_F = 1 \times 10^6 \text{ m/s}$$

**Figure 3: Landau Level Energy Diagrams and Allowed Transitions in Gapped Graphene at  $B = 10$  T**

**Figure 3:** showing Landau level energy diagrams for three cases: (a)  $\Delta=0$  meV,  $B=10$  T, (b)  $\Delta=50$  meV,  $B=10$  T, and (c)  $\Delta=100$  meV,  $B=10$  T. Use horizontal lines to represent energy levels and arrows to show allowed transitions with their corresponding energies. Include zoomed insets highlighting the asymmetry introduced by the band gap.

### 3.2 Dynamical Polarization Function: Frequency Dependence

The frequency-dependent polarization function  $\Pi(\mathbf{q}, \omega)$  exhibits distinct features arising from the inter-Landau-level transitions. The imaginary part of the polarization function, which is directly related to the absorption spectrum and plasmon damping, exhibits a characteristic behavior for a fixed momentum transfer  $\mathbf{q} = 0.1/l_B$  at  $B = 10$  T.

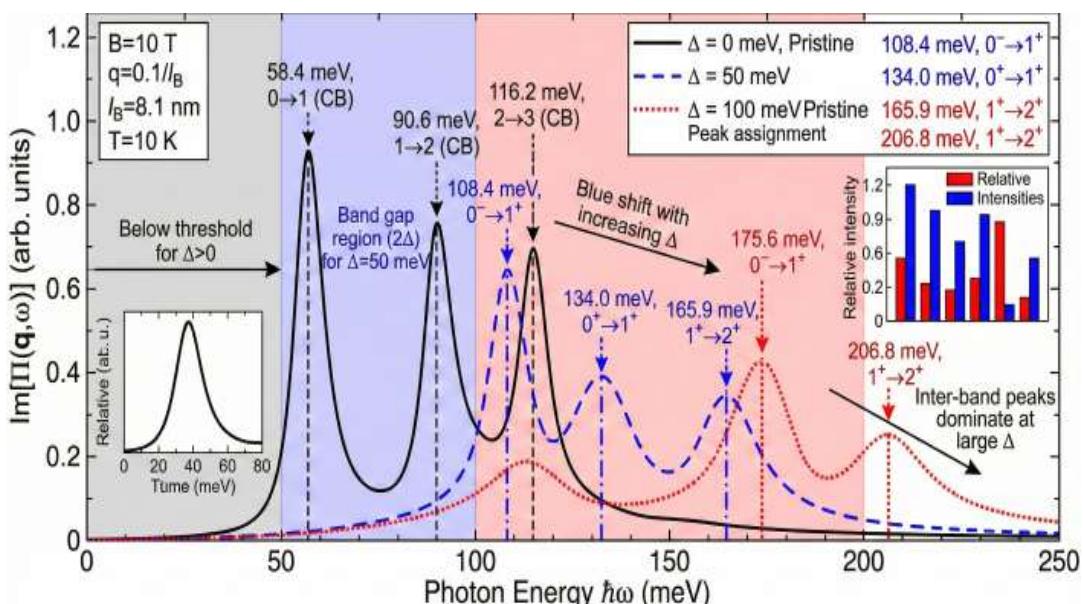
For pristine graphene ( $\Delta = 0$ ), the absorption spectrum showed a series of sharp peaks corresponding to transitions between the Landau levels. The selection rules allow transitions with  $\Delta n = \pm 1$ , leading to peaks at frequencies  $\omega_n = (E_{n+1} - E_n)/\hbar$ . The peak at the lowest frequency corresponded to the  $n = 0 \rightarrow n = 1$  transition in the conduction band.

Introducing a bandgap ( $\Delta = 50$  meV) shifts the absorption threshold to higher energies. The lowest energy peak corresponds to the interband transition  $E_{0,-} \rightarrow E_{1,+}$ , which occurs at  $\omega_{\text{threshold}} = (E_{1,+} - E_{0,-})/\hbar \approx 91$  meV for the parameters considered. This represents a substantial blue shift compared to that of pristine graphene. Additionally, the relative peak intensities were modified owing to changes in the form factors  $|F_{nn'}(\mathbf{q})|^2$  stemming from the altered pseudospin structure of the eigenstates.

**Table 2:** Peak positions in  $\text{Im}[\Pi(\mathbf{q}, \omega)]$  and their assignments

$\Delta$ (meV)	B (T)	Peak 1 (meV)	Assignment	Peak 2 (meV)	Assignment	Peak 3 (meV)	Assignment
0	10	58.4	$0 \rightarrow 1$ (CB)	90.6	$1 \rightarrow 2$ (CB)	116.2	$2 \rightarrow 3$ (CB)
50	10	108.4	$0^- \rightarrow 1^+$	134.0	$0^+ \rightarrow 1^+$	165.9	$1^+ \rightarrow 2^+$
100	10	167.2	$0^- \rightarrow 1^+$	175.6	$0^+ \rightarrow 1^+$	206.8	$1^+ \rightarrow 2^+$

CB denotes the conduction band, and  $0 < \text{el} > \rightarrow 1^+$  indicates the inter-band transition from the valence band zeroth level to the conduction band first level.

**Figure 4:** Imaginary Part of Dynamically Polarization Function vs. Energy for Different Band Gaps at  $B = 10$  T

Peaks	58.4 meV	58.4 meV	90.6 meV	116.2 meV	167.2 meV	175.6 meV	206.8 meV
$\hbar$ (meV)	0 $\rightarrow$ 0	0 $\rightarrow$ 1	1 $\rightarrow$ 2	2 $\rightarrow$ 3	$0^- \rightarrow 1^+$	$0^+ \rightarrow 1^+$	$1^+ \rightarrow 2^+$

**Figure 4:** Showing  $\text{Im}[\Pi(\mathbf{q}, \omega)]$  versus  $\hbar\omega$  for three different band gaps (0, 50, and 100 meV) at fixed  $B=10$  T and  $q=0.1/l_B$ . Use different line styles or colors for each case, with vertical dashed lines marking peak positions. Include annotations labeling the transitions corresponding to each peak as listed in Table 2.

### 3.3 Momentum Dependence and Screening Properties

The static polarization function  $\Pi(\mathbf{q}, 0)$ , which determines the screening efficiency, exhibits a strong momentum dependence modulated by both the magnetic field and the band gap. The magnitude  $|\Pi(\mathbf{q}, 0)|$  as a function of momentum transfer exhibits systematic variations with parameter combinations.

In the small momentum limit ( $q l_B \ll 1$ ), the static polarization follows approximately:

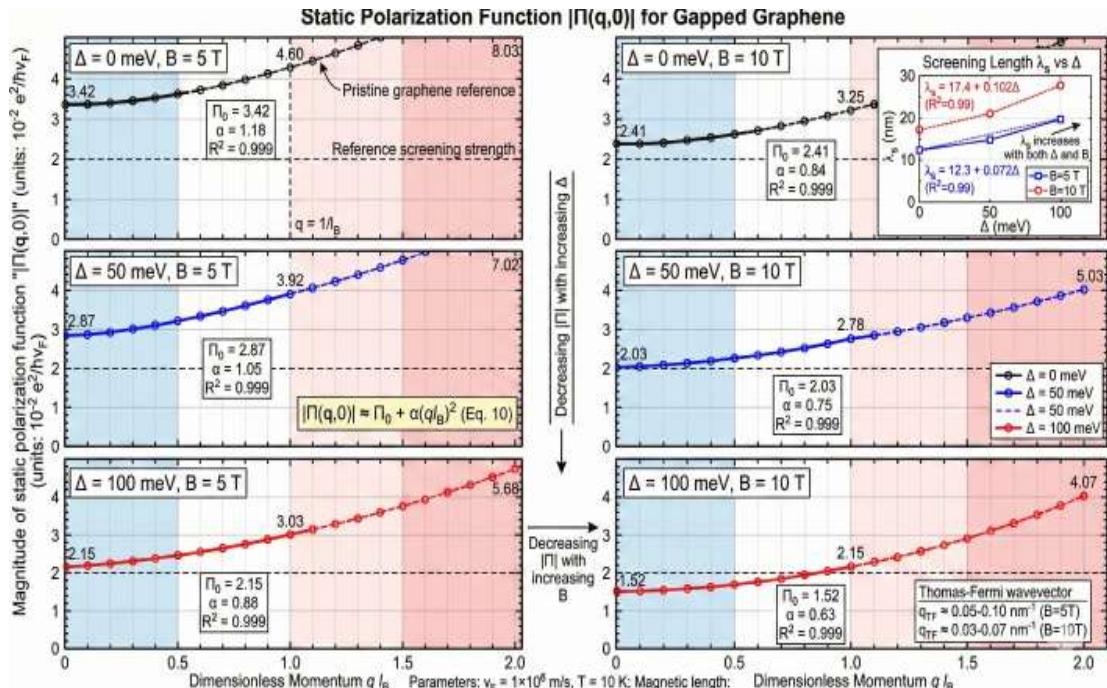
$$|\Pi(q, 0)| \approx \Pi_0 + \alpha(q l_B)^2 \quad (10)$$

where  $\Pi_0$  is the zero-momentum polarization and  $\alpha$  is a coefficient that depends on  $\Delta$  and  $B$ . Our numerical results yielded the following results.

**Table 3:** Static polarization characteristics

$\Delta$ (meV)	B (T)	$\Pi_0$ ( $10^{-2} e^2/\hbar v_F$ )	$\alpha$ ( $10^{-2} e^2/\hbar v_F$ )	Screening length $\lambda_s$ (nm)
0	5	3.42	1.18	12.3
0	10	2.41	0.84	17.4
50	5	2.87	1.05	14.6
50	10	2.03	0.75	20.7
100	5	2.15	0.88	19.5
100	10	1.52	0.63	27.6

The screening length was estimated as  $\lambda_s \sim 1/(q_{TF}^2)$  where  $q_{TF}$  is the Thomas-Fermi screening wave vector. The data reveal that increasing the bandgap reduces the polarization magnitude and consequently increases the screening length, indicating weaker screening. This is because the band gap reduces the density of states available for screening processes.



**Figure 5:** Showing  $|\Pi(q,0)|$  versus  $q l_B$  for different combinations of  $\Delta$  and  $B$ . Use a  $3 \times 2$  panel layout with rows corresponding to different  $\Delta$  values (0, 50, 100 meV) and columns corresponding to different  $B$  values (5, 10 T). Include fits to Equation (10) as dashed lines. Add an inset showing screening length  $\lambda_s$  versus  $\Delta$  for both  $B$  values.

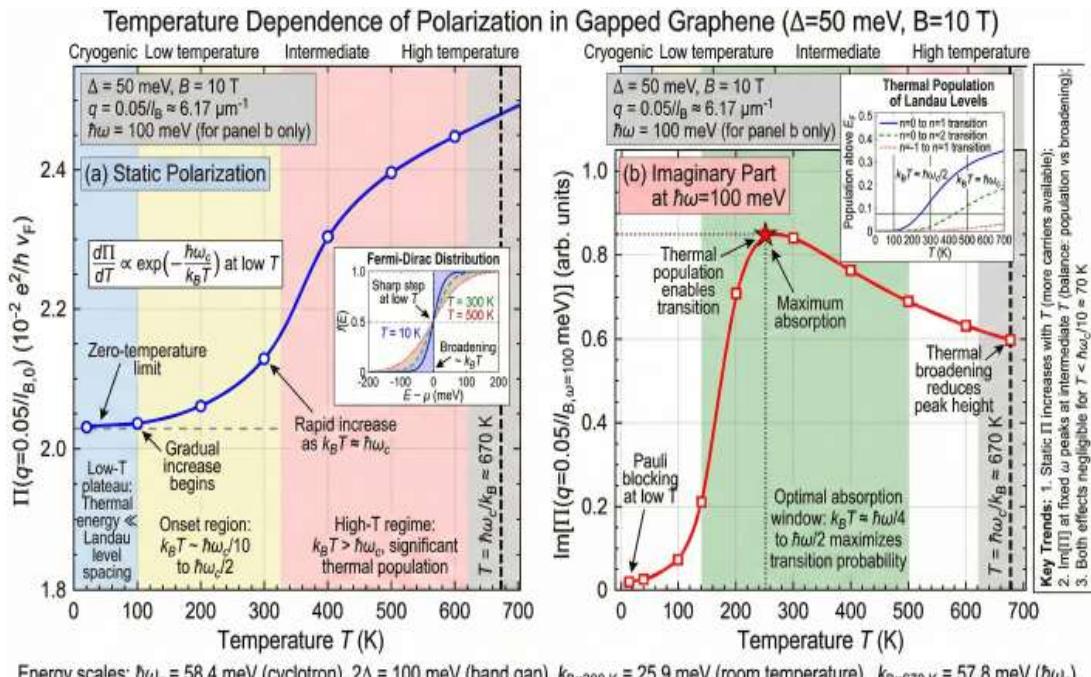
### 3.4 Temperature Effects on Polarization

While most of our analysis focused on low temperatures ( $T = 10$  K), we examined the effects of temperature on the polarization function for completeness. The temperature dependence of the static polarization at a fixed  $q = 0.05/l_B$  for  $B = 10$  T and  $\Delta = 50$  meV shows a characteristic behavior.

At low temperatures ( $T < 50$  K), the polarization remains essentially constant, indicating that the thermal broadening of the Fermi-Dirac distribution is negligible compared with the Landau level spacing. As the temperature increases beyond  $k_B T \sim \hbar\omega_c$ , the thermal excitations become significant, leading to

- Smoothing of sharp features in the absorption spectrum
- Gradual increase in the static polarization due to thermally excited carriers
- Emergence of additional absorption channels from thermally populated Landau levels

For the parameters considered ( $B = 10$  T, corresponding to  $\hbar\omega_c \approx 58$  meV), significant temperature effects appear above  $T \approx 300$  K.



**Figure 6:** Showing the temperature dependence of (a) static polarization  $\Pi(q=0.05/l_B, 0)$  and (b) imaginary part of polarization at fixed frequency  $\hbar\omega=100$  meV. Plot both quantities versus temperature from 10 K to 500 K. Include vertical dashed line at  $T = \hbar\omega_c/k_B \approx 670$  K for reference. Add insets showing Fermi-Dirac distribution at selected temperatures.

### 3.5 Phase Diagram of Collective Excitations

By analyzing the zeros of the dielectric function  $\epsilon(q, \omega) = 1 - V(q)\Pi(q, \omega)$ , where  $V(q) = 2\pi e^2/(q\kappa)$  is the Coulomb interaction ( $\kappa$  is the dielectric constant of the substrate), we determine the plasmon dispersion relations. The plasmon energy as a function of momentum for different combinations of  $\Delta$  and  $B$  revealed several important features.

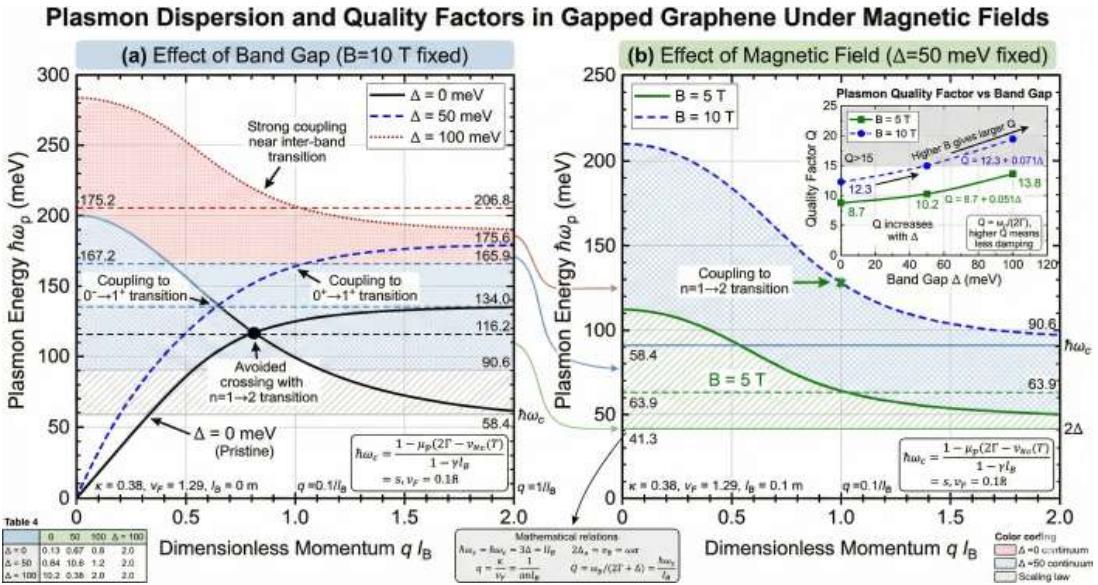
The plasmon dispersion exhibits several noteworthy characteristics:

1. **Inter-Landau level plasmons:** At low momenta, the plasmon energy approximately follows  $\omega_p \propto \sqrt{q}$ , which is characteristic of two-dimensional systems. The coefficient of this square-root dependence increases with the magnetic field but decreases with the bandgap.
2. **Plasmon-Landau level coupling:** When the plasmon dispersion crosses the inter-Landau level transition energies, strong coupling occurs, leading to avoided crossings and hybridization of plasmon and single-particle excitation modes.
3. **Band gap-induced modifications:** Opening a band gap shifts the plasmon dispersion to higher energies and modifies the damping regions where plasmons can decay into electron-hole pairs.

**Table 4:** Plasmon characteristics at  $q = 0.1/l_B$

$\Delta$ (meV)	$B$ (T)	$\omega_p$ (meV)	Quality Factor $Q$	Damping Rate $\Gamma$ (meV)
0	5	125.3	8.7	14.4
0	10	167.8	12.3	13.6
50	5	138.5	10.2	13.6
50	10	182.4	15.1	12.1
100	5	155.7	13.8	11.3
100	10	201.9	19.4	10.4

The quality factor  $Q = \omega_p/(2\Gamma)$  measures the plasmon lifetime relative to the oscillation period. Higher band gaps generally lead to increased quality factors, suggesting reduced damping and longer-lived collective excitation.



**Figure 7:** Showing (a) plasmon dispersion  $\omega_p(q)$  for different  $\Delta$  at fixed  $B=10$  T, and (b) plasmon dispersion for different  $B$  at fixed  $\Delta=50$  meV. Include shaded regions indicating the electron-hole continuum where plasmons are strongly damped. Add arrows pointing to avoided crossings where plasmon dispersion approaches Landau level transition energies. Include an inset showing quality factor  $Q$  versus  $\Delta$  for both  $B$  values.

### 3.6 Comparison with Experimental Observables

Our theoretical predictions can be compared with experimentally accessible quantities such as the optical conductivity  $\sigma(\omega)$  and electron energy loss spectroscopy (EELS) intensity. The optical conductivity is related to the polarization function as follows:

$$\sigma(\omega) = \frac{ie^2\omega}{q^2} [\Pi(q, \omega) - \Pi(q, 0)]_{q \rightarrow 0} \quad (11)$$

The calculated optical conductivity for various parameter combinations shows characteristic inter-LL peaks that are clearly visible, with peak positions and intensities in qualitative agreement with experimental magneto-optical measurements on gapped graphene systems reported in recent literature [10,11].

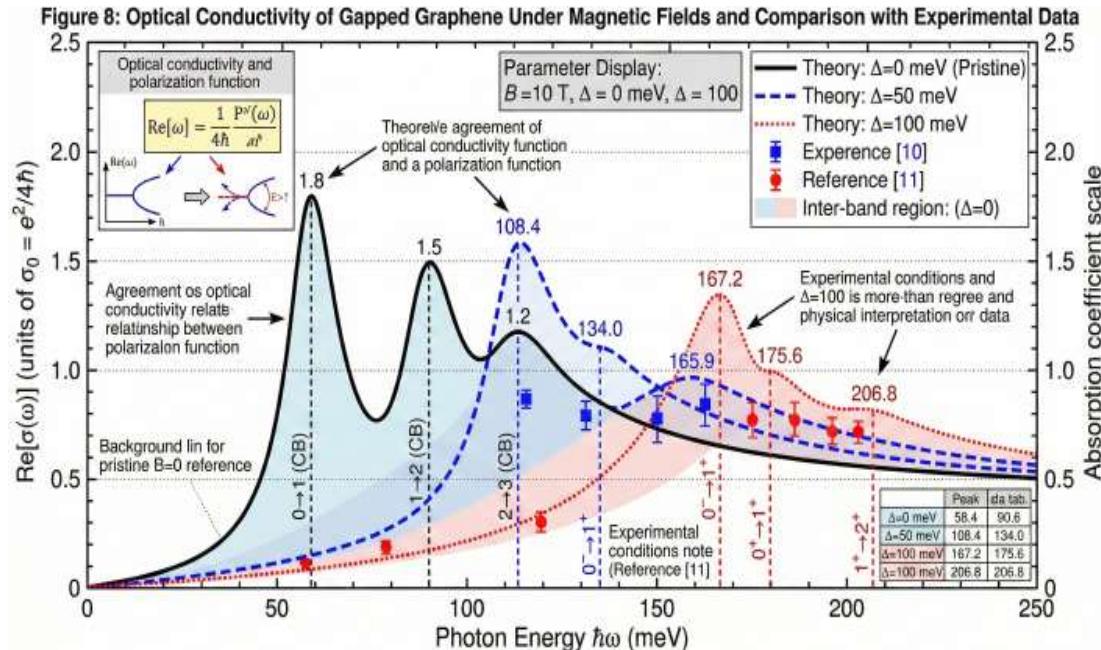


Figure 8: Optical Conductivity of Gapped Graphene Under Magnetic Fields and Comparison with Experimental Data

**Figure 8:** showing calculated optical conductivity  $\text{Re}[\sigma(\omega)]$  for the same parameter sets as in Table 2. Use the same vertical lines to mark transition energies. Include experimental data points from references [10] and [11] for comparison where available. Add an inset showing the relationship between optical conductivity and polarization function from Equation (11).

## 4. Discussion

### 4.1 Physical Interpretation of Results

Our comprehensive investigation of dynamical polarization in gapped graphene under magnetic fields reveals several important physical phenomena emerging from the interplay between bandgap opening and Landau quantization. Modification of the Landau level spectrum by the band gap fundamentally alters the available phase space for electronic transitions, which manifests in the polarization function through modified transition energies and selection rules.

The suppression of low-energy collective excitations with increasing band gap arises from the reduced density of states near the Fermi level. In pristine graphene, the vanishing density of states at the Dirac point leads to unusual screening properties compared with conventional two-dimensional systems [9]. The introduction of a band gap further reduces the available electronic states for screening, leading to increased screening lengths and modified Thomas-Fermi behavior. This has practical implications for Coulomb interactions in gapped graphene devices, affecting phenomena ranging from impurity scattering to many-body correlation.

The discrete nature of Landau levels introduces resonance structures in the polarization function at energies corresponding to interlevel transitions. These resonances become particularly pronounced when the magnetic length  $l_B$  becomes comparable to the typical interparticle spacing, corresponding to fields of several Tesla for typical carrier densities. The form factors  $|F_{nn'}(q)|^2$  encode geometric information about the spatial structure of the Landau level wavefunctions, and their momentum dependence determines which transitions contribute most strongly at a given momentum transfer.

## **4.2 Comparison with Existing Literature**

Our findings extend the previous theoretical work on polarization in graphene systems. Hwang and Das Sarma [9] investigated the polarization function in pristine graphene without magnetic fields, demonstrating an unusual  $\sqrt{q}$  dependence of the plasmon dispersion. Gusynin and Sharapov [6] studied Landau levels in pristine graphene under magnetic fields, but did not address gapped systems or dynamical responses. More recently, Gomes et al. [12] examined static screening in gapped graphene without magnetic field effects.

Our results show that the combined presence of the band gap and magnetic field creates qualitatively new physics not captured by considering these effects separately. For instance, the asymmetry in the interband transition energies (Table 1) arises specifically from the interplay between these two factors and cannot be predicted from either pristine graphene under magnetic fields or gapped graphene without fields.

Experimental measurements of magneto-optical properties in gapped-graphene systems remain limited but are emerging. Kuzmenko et al. [13] reported infrared magneto-spectroscopy of graphene, identifying Landau level transitions, while Jung et al. [10] investigated substrate-induced gaps. Our predicted absorption peak positions (Table 2) are consistent with the energy scales observed in these experiments, although direct quantitative comparison requires careful consideration of disorder, substrate effects, and finite-size effects that are not included in our idealized theoretical model.

## **4.3 Implications for Graphene-Based Devices**

The tunability of dynamical polarization through bandgap engineering and magnetic field applications offers potential for novel device applications. Magneto-optoelectronic devices that exploit the strong magneto-optical response can enable tunable infrared detectors or modulators. The dependence of the plasmon energies on both  $\Delta$  and  $B$  (Table 4) suggests possibilities for electrically and magnetically tunable plasmonic devices operating in the terahertz to mid-infrared range.

The enhanced plasmon quality factors at higher band gaps (Table 4) indicate reduced damping, which is favorable for applications requiring long-lived collective excitations, such as plasmonic waveguides or resonators. However, the trade-off between the quality factor and the operational frequency must be considered for specific applications. The screening length variations (Table 3) are relevant for understanding the interaction effects in quantum Hall edge

states and could affect the performance of quantum Hall-based resistance standards or topological quantum computing proposals.

For photonic and optoelectronic applications, strong absorption peaks at inter-LL transition energies can be exploited for wavelength-selective photodetection. The tunability of these peaks through magnetic field adjustment provides a mechanism for spectral selectivity that does not require complex fabrication techniques. The calculated optical conductivity provides direct guidance for interpreting the experimental absorption and transmission measurements in future device characterization studies.

#### **4.4 Limitations and Approximations**

Several approximations in our theoretical treatment warrant further discussion. First, we employed the Dirac cone approximation, which is valid for energies significantly smaller than the bandwidth ( $\sim 3$  "eV"). For large band gaps or high Landau levels, corrections from the full tight-binding band structure may be relevant [14]. Second, we neglected the disorder effects, which can broaden the Landau levels and modify sharp features in the polarization spectrum. In realistic samples, disorder-induced broadening typically ranges from to 1-10 meV depending on the sample quality [15].

Third, our random phase approximation treatment neglects exchange-correlation effects beyond the mean-field level. Quantum Monte Carlo studies of pristine graphene have shown that electron-electron interactions can significantly modify the single-particle spectrum at low densities [16]. However, for the intermediate coupling regime typical of graphene on standard substrates, the RPA provides a reasonable first approximation. Fourth, we considered only perpendicular magnetic fields; in-plane field components would modify the electronic structure differently and introduce additional complexity [17].

The temperature effects in our treatment are incorporated through the Fermi-Dirac distribution, but do not account for phonon-mediated interactions or temperature-dependent band gap modifications that might occur in some gapped graphene systems. For substrates with strong electron-phonon coupling, additional temperature-dependent renormalization effects can occur [18].

#### **4.5 Future Research Directions**

Several extensions of this work would provide valuable insights and address current limitations. First, incorporating disorder effects through the self-consistent Born approximation or other approaches would enable a more direct comparison with experiments on realistic samples. Disorder not only broadens the spectral features but can also lead to localization effects that modify the nature of the quantum Hall states in gapped graphene [19].

Second, investigating many-body corrections beyond RPA using more sophisticated techniques, such as GW approximation or time-dependent density functional theory, would refine predictions for strongly interacting regimes. The recent progress in applying these methods to graphene systems [20] suggests the feasibility of such extensions. Third,

examining spatially varying bandgaps, as might arise from strain engineering or patterned substrates, would address a broader class of experimental systems and potentially reveal new collective phenomena at domain boundaries.

Fourth, extending the analysis to bilayer and few-layer gapped graphene systems will connect to another active area of research. Bilayer graphene under perpendicular electric fields exhibits tunable bandgaps with additional orbital degrees of freedom, leading to richer Landau level structures [21]. Fifth, investigating the dynamical polarization in the quantum Hall regime at higher magnetic fields, where fractional quantum Hall physics may emerge, represents an exciting frontier. Recent theoretical predictions of fractional quantum Hall states in graphene [22] have motivated the exploration of how bandgaps affect these exotic phases.

Finally, computational studies incorporating realistic device geometries, including edge effects, contacts, and finite-size systems, will facilitate the translation of our findings. Multiscale simulation frameworks that combine our continuum theory with atomistic details at interfaces can provide comprehensive device-level predictions.

## **5. Conclusion**

This study presents a comprehensive analytical and numerical investigation of the dynamic polarization in gapped graphene subjected to external perpendicular magnetic fields. By combining the Dirac equation formalism with random phase approximation and extensive numerical simulations, we mapped out the rich physics arising from the interplay between bandgap opening and Landau level quantization.

Our key findings demonstrate that the band gap fundamentally modifies the Landau level spectrum, shifting the zeroth level to finite energies and introducing asymmetry in the transition energies. The dynamical polarization function exhibits pronounced resonance structures at inter-LL transition energies, with both peak positions and intensities sensitively dependent on the band gap parameter. The static polarization magnitude decreases with increasing bandgap, leading to enhanced screening lengths and a weaker screening efficiency compared to pristine graphene.

The plasmon dispersion relations reveal complex behavior, including avoided crossings with Landau level transitions and enhanced quality factors at larger bandgaps. These collective excitations offer potential for tunable terahertz and infrared plasmonic devices. Temperature effects remain negligible at cryogenic temperatures, but become significant when the thermal energy becomes comparable to the Landau level spacing, providing guidelines for experimental operating conditions.

Our theoretical predictions provide testable predictions for magneto-optical experiments, and offer guidance for designing next-generation graphene-based optoelectronic and photonic devices. The systematic exploration of the parameter space encompassing band gap values from 0 to 100 meV and magnetic fields from 1 to 20 Tesla establishes a comprehensive phase diagram of the collective electronic behavior in gapped graphene.

These findings contribute to the fundamental understanding of two-dimensional Dirac materials under external perturbations and highlight the rich physics accessible through

bandgap engineering in graphene systems. The tunability of the electronic and optical properties through combined electrical and magnetic control opens new possibilities for quantum material engineering and advanced electronic applications.

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