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Two Stream Instability in Graphene

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TWO STREAM INSTABILITY IN GRAPHENE

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Abstract

We investigate the unstable modes of the two-stream instability in graphene to determine if they can occur. This instability occurs when a population of electrons streams past another inside graphene. We obtain the unstable modes by numerically determining the zeros of the non-equilibrium graphene dielectric function using MATLAB. The dielectric function used in this study, in contrast to previous studies, includes the effects of the particle-hole excitation continuum (PHEC) that normally quells the evolution of unstable plasmons. MATLAB's built in zero solver is employed to solve the sixth order polynomial and determine its roots. For some range of parameters, the zeros are found to exist in the upper half of the complex plane. This indicates that there is a range of unstable modes that exists even with the incorporation of PHEC. The presence of these unstable modes signifies that the plasmons' amplitudes increase with time.

Introduction

In order to understand the two-stream instability in graphene, there are several important concepts that need to be explained. First and foremost, it is important to understand what graphene is. Graphene is a 2D material comprised of carbon atoms arranged in a hexagonal lattice; these films can be anywhere from one to ten atoms thick due to the fact that at ten layers, graphene begins to behave like a 3D solid [1]. Due to its unique electronic properties, many theoretical and experimental studies have been conducted in order to investigate graphene, including previous studies on the two-stream instability [2].

Second, it is crucial to understand what the two-stream instability is and how it occurs. The two-stream instability normally occurs within plasmas when one species of charge carriers drifts with respect to another. This causes charge density perturbations to occur that grow exponentially in amplitude; these are called unstable modes. This can be more easily understood by first considering the effect of the particle-hole excitation continuum (PHEC) called Landau damping, the process that causes plasma waves to decay over time [2]. When a plasma is in an equilibrium state, there is a net transfer of energy from plasmons to charged particles that results in the decay of the plasmons due to the loss of energy [2]. The most popular heuristic explanation for the two-stream instability is the surfer example [3] (**Fig 1.1**).

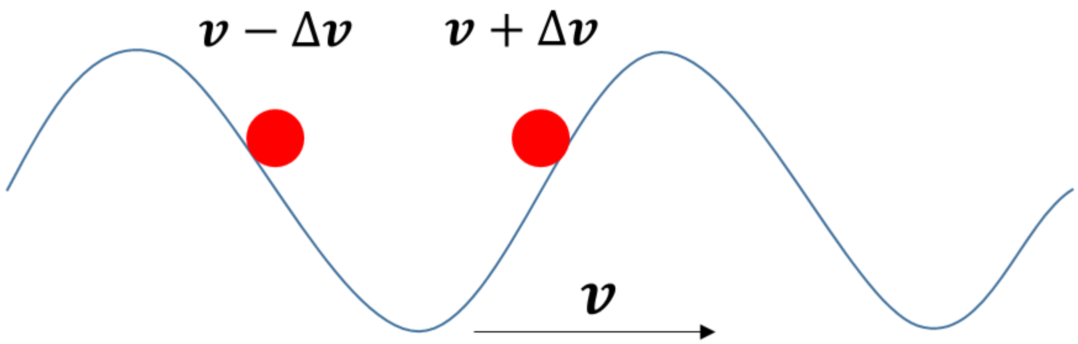


Figure 1.1 Surfer example. The red balls represent particles, or "surfers", and the wave represents a charge density perturbation wave. The wave is traveling to the right with a velocity v and the particles are traveling to the right with their respective velocities indicated in the image. The particle with velocity $v + \Delta v$ is moving slightly faster than the wave and the particle with velocity $v - \Delta v$ is moving slightly slower than the wave.

Imagine a particle as a surfer on a wave. In a non-equilibrium situation in a plasma, i.e. when one species of charge carriers drifts relative to another, if the surfer is moving slightly faster than the wave, they will catch up to the wave and push it along. This gives energy to the wave, leading to unstable modes. If the surfer is moving slightly slower than the wave, the wave will catch up to them and push them along. This gives energy to the particle and causes the wave to decay. In other words, if there are more high energy particle than low energy particles, the charge density perturbations will grow exponentially. This is because there are more particles pushing the wave and giving energy to it, than there are particles being pushed by the wave, taking energy away from it. Conversely, if there are more low energy particles than high energy particles, the perturbations will decay over time. There have been previous studies done regarding the two-stream instability in graphene; however, these studies did not incorporate the effects of the particle-hole excitation continuum (PHEC), also known as Landau damping.

Model

The system investigated in this study consisted of a doped monolayer of graphene and a beam of electrons injected across its surface. As discussed in the introduction, when the injected electrons stream relative to the electrons in the graphene, unstable modes occur. This is due to a feedback loop that takes place when the charge carriers drift with respect to each other. A diagram showing this loop can be seen below in figure 2.1.

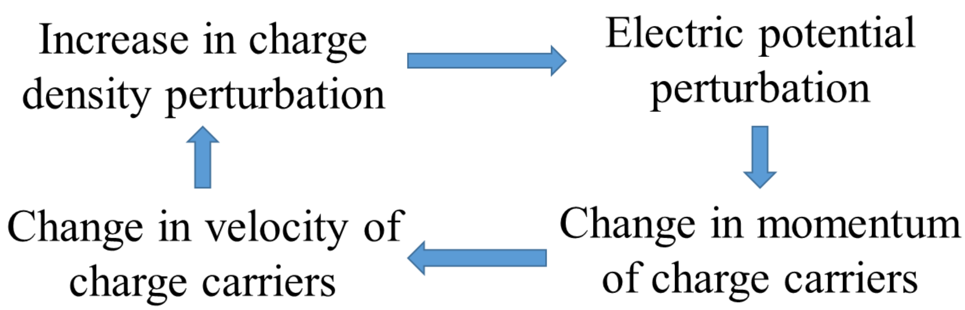


Figure 2.1 The positive feedback loop. This feedback loop occurs as a result of charge carriers drifting with respect to one another. In this non-equilibrium situation, the feedback loop causes a net transfer of energy to the charge density perturbations. This causes them to grow exponentially in amplitude as time goes on.

Due to the transfer of energy from the charge carriers to the charge density waves, there is an increase in the charge density perturbations that take place in the graphene. It is easiest to think about this by imagining a line of particles with a longitudinal wave traveling through it. There will be some regions with particles very close to one another and other regions with particles spaced far apart. This causes an increase in electric potential perturbations which changes the momentum of the charge carriers in the material. In systems with parabolic bands, in which the velocity of the particle is proportional to the momentum, this causes a change in the velocity of the particles. Graphene does not have parabolic bands; instead, it has linear bands (**Fig 2.2** & **2.3**). This means that the speed of the particles is independent of the momentum of the particles, creating an apparent breakdown in the feedback loop. However, the direction of the velocity is dependent on the direction of the momentum, thus keeping the feedback loop intact. The change in velocity then continues to increase the charge density perturbations, creating a positive feedback loop.

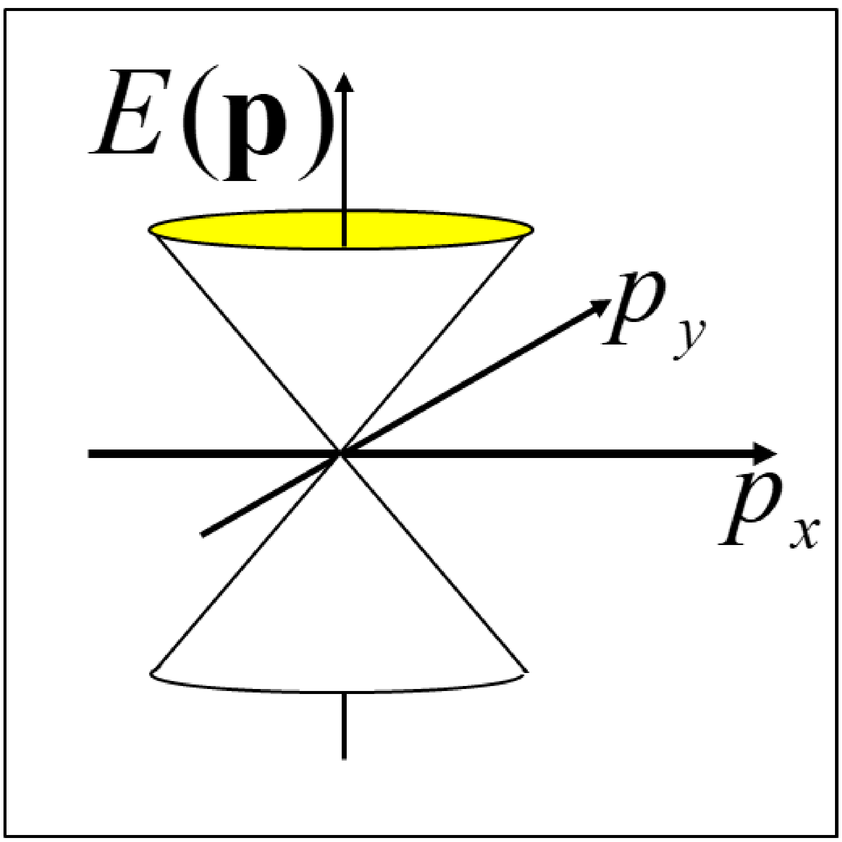


Figure 2.2 Band structure of graphene. This figure displays the band structure of graphene around the Dirac points, *K* and *K'*, which shows that graphene has linear bands rather than parabolic bands. This is important to note because, as discussed above, this creates an apparent break in the feedback loop due to the fact that the speed of a particle is not proportional to the momentum.

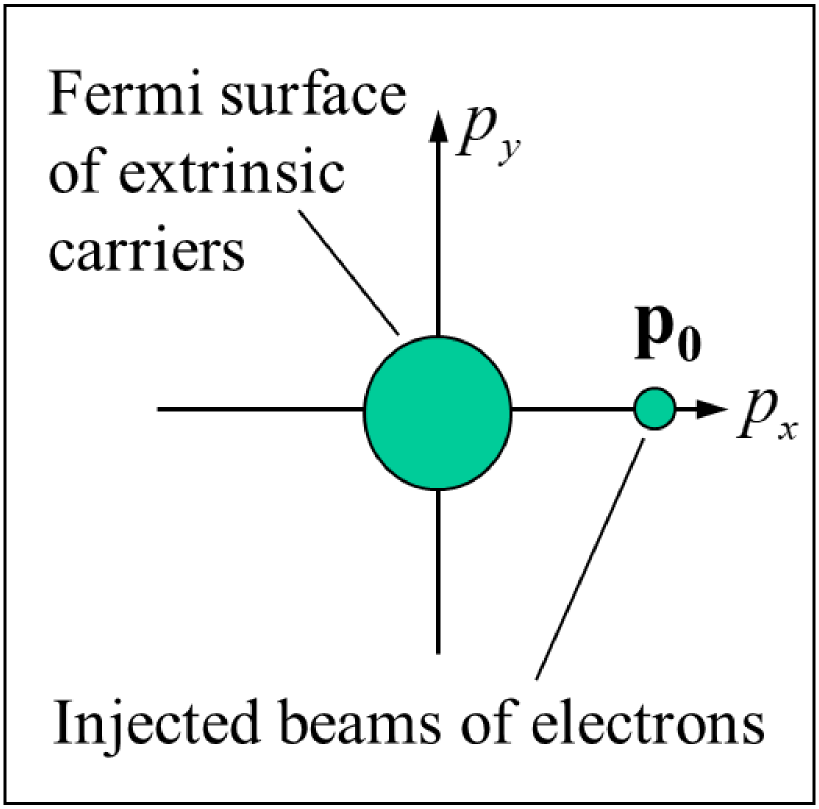


Figure 2.3 Fermi surfaces. This image shows the fermi surfaces for the injected electrons and the extrinsic charge carriers in graphene as a top-down view of figure 2.2. In this model it is assumed that the charge density of the extrinsic charge carriers is larger than the charge density of the injected electrons.

When unstable modes occur, the oscillations in the charge density inside the graphene are described by the wave vector, $\boldsymbol{q}$, and have frequency, $\omega(\boldsymbol{q})$. The frequency has a real and imaginary portion and can be written as the following.

$$\omega(\boldsymbol{q}) = \omega_r + i\,\omega_i$$

$$\Rightarrow \exp(-i\omega t) = \exp(-\mathrm{i}\omega_r t)\exp(-i^2\omega_i t)$$

$$\Rightarrow \exp(-i\omega t) = \exp(-\mathrm{i}\omega_r t)\exp(\omega_i t) \quad \ldots\ldots\ldots\ldots\ldots\ldots \textbf{Eqn.}\ (1)$$

The real part of $\omega(\boldsymbol{q})$ describes the angular frequency of the charge density perturbations while the imaginary part describes the growth rate of the amplitude. Looking at equation (1) above, if the imaginary part of $\omega(\boldsymbol{q})$ is positive, there will be an exponential growth in the amplitude of the perturbations.

These unstable modes arise when the dielectric function is equal to zero. The dielectric function of a material describes its permittivity and is defined as the ratio between the Fourier components of the externally applied potential, $\tilde{V}_{\text{ext}}(\boldsymbol{q},\omega)$, and the total potential of the system, $\tilde{V}_{\text{tot}}(\boldsymbol{q},\omega)$.

$$\varepsilon(\boldsymbol{q},\omega) = \frac{\tilde{V}_{\text{ext}}(\boldsymbol{q},\omega)}{\tilde{V}_{\text{tot}}(\boldsymbol{q},\omega)}$$

Rearranging this equation and plugging in zero for $\varepsilon(\boldsymbol{q},\omega)$ yields the following.

$$\tilde{V}_{\text{tot}}(\boldsymbol{q},\omega) \times (0) = \tilde{V}_{\text{ext}}(\boldsymbol{q},\omega)$$

This means that when $\varepsilon(\boldsymbol{q},\omega) = 0$, there can be a total potential without having to apply an external potential, indicating that the system is self-oscillating. Solving for $\varepsilon(\boldsymbol{q},\omega) = 0$ gives the values of $\omega(\boldsymbol{q})$ at which unstable modes occur. By determining the imaginary parts of these solutions, it can be determined if exponential growth occurs.

The improved dielectric function for graphene, incorporating the effects of the PHEC is shown below in equation (2).

<u>Eqn.</u> <u>(2)</u>

$$\varepsilon(\boldsymbol{q},\omega) = 1 - V_c(q)\Bigg[\underbrace{\frac{2n_{\text{ext}}}{v_0 p_F}\left(-1 + \frac{\omega}{\sqrt{\omega^2 - (qv_0)^2}}\right)}_{\textbf{(A)}} + \underbrace{\frac{q^2 v_0 n_{\text{beam}} \sin^2\theta}{p_0(\omega - qv_0\cos\theta)^2}}_{\textbf{(B)}}\Bigg] = 0$$

In this equation, q is the magnitude of the wave vector, $\boldsymbol{q}$, that describes the oscillation of the charge density in graphene. In addition to this, v_0 is the speed of an electron in graphene, p_0 is the momentum of the injected particle, and θ is the angle $\boldsymbol{q}$ makes with respect to the direction of the drifting electrons. p_F is the magnitude of the momentum of particles at the Fermi level with respect to the Dirac point, n_{ext} is the density of the charge carriers in graphene, n_{beam} is the density of the charge carriers being injected into the graphene, and $V_c(q)$ is the Fourier transform of the Coulomb potential in two dimensions. Part (**A**) of this equation includes the damping effects caused by the PHEC. It indicates that there are charge carriers already present in the graphene that respond to externally applied perturbations. Part (**B**) of this equation describes the response of charge carriers in the injected beam to externally applied perturbations.

It is helpful to compare equation (2) to the dielectric function previously used to explore the possibility of the two-stream instability in graphene. This function can be seen below in equation (3).

<u>**Eqn.** (3)</u>

$$\varepsilon(\boldsymbol{q},\omega) = 1 - V_c(q)\frac{q^2 v_0}{p_F}\Bigg[\underbrace{\frac{n_{\text{ext}}}{\omega^2}}_{(\mathbf{C})} + \underbrace{\frac{p_F n_{\text{beam}} \sin^2\theta}{p_0(q v_0 \cos\theta - \omega)^2}}_{(\mathbf{D})}\Bigg] = 0$$

By comparing part (**A**) of equation (2) to part (**C**) of equation (3), it can be seen that (**C**) is much more simplistic. Equation (2) provides a better description of the extrinsic charge carrier’s response to externally applied perturbations than equation (3). On the other hand, when comparing part (**B**) to part (**D**), it is easy to see that these terms are the same.

<u>Method</u>

In order to properly explore the two-stream instability in graphene, a MATLAB program was written to numerically solve for the roots of the previously discussed, improved dielectric function for graphene (**Eqn.** (2)). Equation (2) was first simplified and put into the following form.

<u>Eqn.</u> <u>(4)</u>

$$z^4(z-\lambda)^4 = \frac{\Gamma^4}{4\epsilon^2}[(z-\lambda)^2-1]^2(z-\lambda)^4 + \frac{\Gamma^2}{\epsilon}[(z-\lambda)^2-1](z-\lambda)^4 + (z^2-\Gamma^2)(z-\lambda)^4$$

The variables in this equation were defined by Aryal and Hu [2] as follows.

<u>Eqn. set</u> <u>(5)</u>

$$\epsilon = \frac{n_{\text{ext}} p_0}{n_{\text{beam}} p_F \sin^2\theta}$$

$$z = \omega\sqrt{\frac{\kappa p_0}{2\pi e^2 v_0 n_{\text{beam}} q}}\frac{1}{\sin\theta} = \frac{\omega}{\omega^*(q)}$$

$$\omega^*(q) = \sqrt{\frac{2\pi e^2 v_0 n_{\text{beam}} q}{\kappa p_0}}\sin\theta$$

$$\lambda = \sqrt{\frac{\kappa p_0 v_0 q}{2\pi e^2 n_{\text{beam}}}}\cot\theta = \frac{q v_0 \cos\theta}{\omega^*(q)}$$

$$\Gamma = \sqrt{\frac{\kappa p_0}{2\pi e^2 v_0 n_{\text{beam}} q}}\frac{q v_0}{\sin\theta} = \frac{q v_0}{\omega^*(q)}$$

In these equations, κ is the dielectric constant and e is the charge of an electron. Equation (4) was then foiled out into a sixth order polynomial and set equal to zero. After this, the following constants were defined using Gaussian units in order to be used in calculations.

$$v_0 = 1.0 \times 10^8 \text{ cm/s}$$

$$n_{\text{ext}} = 1.0 \times 10^{12} \text{ cm}^{-2}$$

$$n_{\text{beam}} = 1.0 \times 10^{11} \text{ cm}^{-2}$$

$$\kappa = 3$$

$$e = 4.803 \times 10^{-10} \text{ esu}$$

$$E_{\text{beam}} = 130\ meV = 2.1 \times 10^{-13} \text{ erg}$$

$$p_0 = \frac{E_{\text{beam}}}{v_0}$$

$$p_F = \hbar\sqrt{2\pi n_{\text{ext}}}$$

In this list of variables, it is important to note that E_{beam} is the energy of the electrons being injected into the system, $\hbar = 1.05 \times 10^{-27}\,\text{erg} \cdot \text{s}$ is the reduced Planck's constant in Gaussian units, q is an array of values from 0.1 to $9 \times 10^6\ \text{cm}^{-1}$, and $\theta = 10°, 45°$. Using the equations shown in equation set (5) and the list of variables, the program stepped through the array of q values and calculated $\omega^*(q), \epsilon, \lambda, \Gamma,$ and z. MATLABs built-in root finder was then implemented to solve the sixth order polynomial for values of $\omega(\boldsymbol{q})$ that would yield $\varepsilon(\boldsymbol{q}, \omega) = 0$. For each value of q, there are six root, two of which are complex numbers. This investigation is only interested in the roots with positive imaginary values as these are the only solutions that cause exponential growth. The program then looped through the six roots for every value of q and found those with positive imaginary portions. The real and imaginary parts of the solutions were then put into arrays and graphs displaying the real and imaginary parts of $\omega(\boldsymbol{q})$ as a function of q were created. These graphs show the values of q that give unstable modes and the growth rate of the corresponding charge density perturbations.

Results and Discussion

Using the method described above, it was determined that unstable modes can arise in graphene when incorporating the effects of PHEC. The graph shown on the next page in figure 3.1 displays the real and imaginary parts of ω as a function of q. To obtain these results, an angle of θ = 10° with respect to the direction of drifting electrons, was used. The line representing the imaginary results shows that there is a wide range of q values that lead to unstable modes. At approximately $q = 7.3 \times 10^6\ \text{cm}^{-1}$, the imaginary line goes to zero indicating that there is no exponential growth and that the charge density perturbations will continue to oscillate with the same amplitude indefinitely in the model. The red line representing the absolute values of the real part of $\omega(\boldsymbol{q})$ increases rapidly as q increases and breaks into two curves where the imaginary solutions go to zero. Due to the fact that there are no longer complex solutions after a certain wave number, there are no longer complex conjugates for solutions that share a real part. Once the solutions become strictly real, they bifurcate into two real solutions.

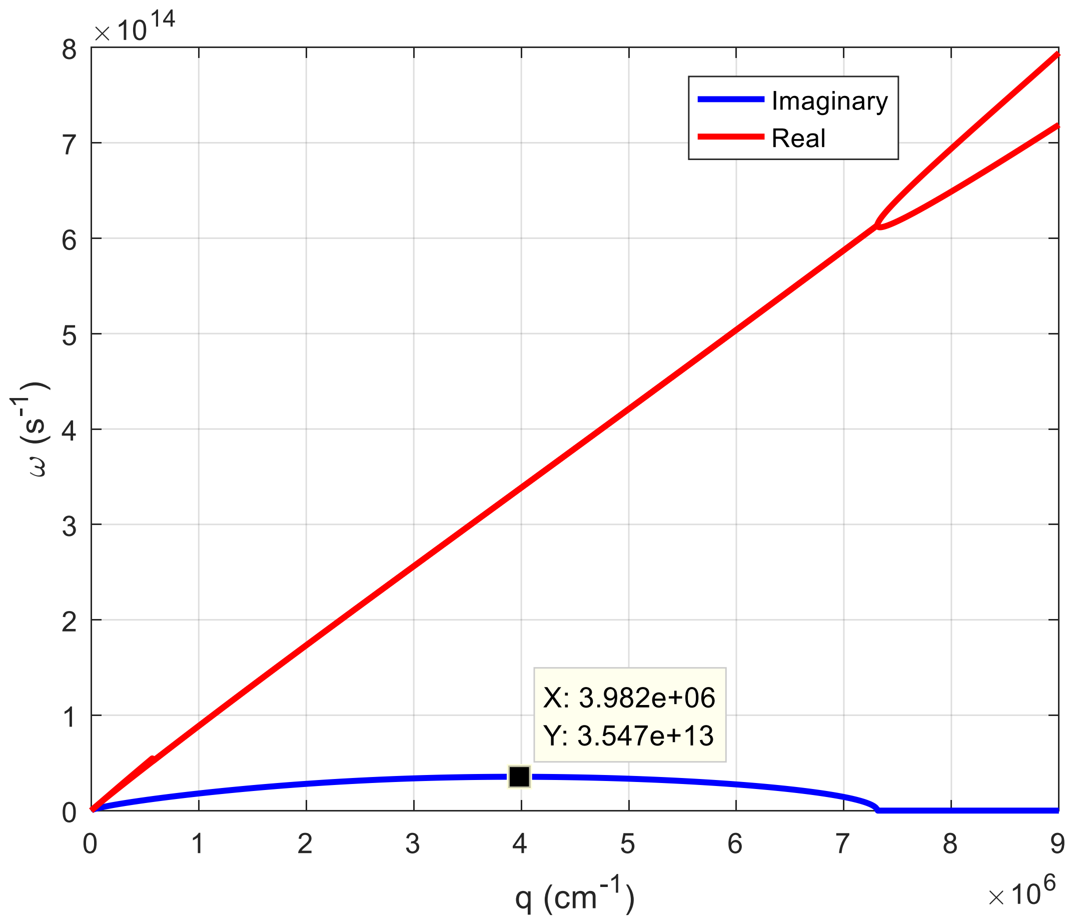


Figure 3.1 Graphene two-stream instability angular frequencies and growth rates using improved dielectric function for an angle $\theta = 10°$. The blue curve represents the positive imaginary part of $\omega(\boldsymbol{q})$ and the red curve represents the absolute value of the real part of $\omega(\boldsymbol{q})$. Positive imaginary solutions indicate unstable modes. The imaginary curve peaks at $\omega_i = 3.547 \times 10^{13}\ \mathrm{s}^{-1}$.

To better understand the effects of using the more sophisticated dielectric function, equation (2), these results must be compared to results obtained using the old dielectric function, equation (3). Figure 3.2 below displays a graph of the solutions to the same system as in figure 3.1, but using equation (3).

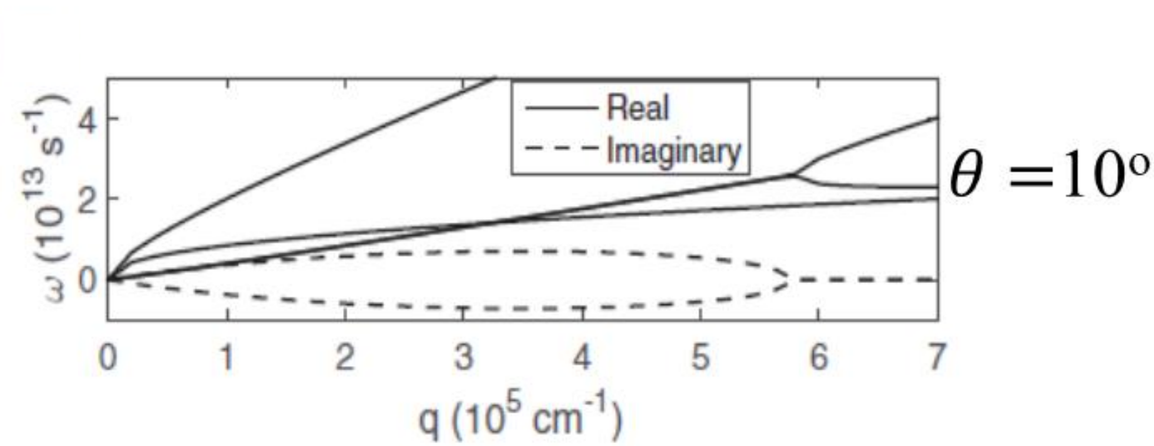
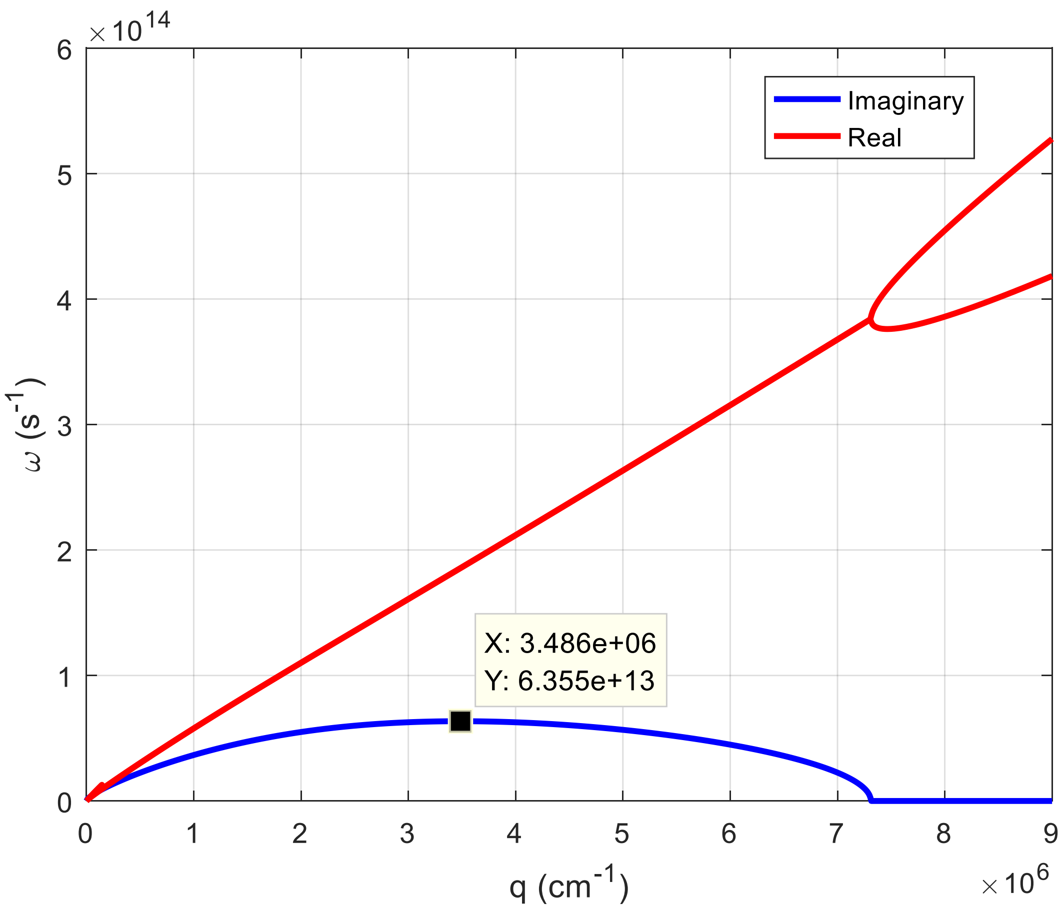


Figure 3.2 [2] Graphene two-stream instability dispersion and growth rates using old dielectric function for an angle $\theta = 10°$. Here, the dashed lines show the positive and negative imaginary parts of $\omega(\boldsymbol{q})$ while the forked solid line shows the corresponding real part of $\omega(\boldsymbol{q})$. As before, positive imaginary solutions indicate exponential growth while negative imaginary solutions indicate exponential decay. The other two curves are strictly real solutions to equation (3).

Comparing figure 3.1 to figure 3.2, the range of q values for figure 3.2 is smaller than the range for figure 3.1. In addition to this, the real part of figure 3.1 increases much faster than in figure 3.2 meaning that the PHEC causes charge density perturbations to have higher angular frequencies. Furthermore, in figure 3.1, the imaginary curve peaks roughly at $\omega_i = 3.547 \times 10^{13}\ \text{s}^{-1}$ and in figure 3.2, the imaginary curve peaks at approximately $\omega_i = 1.0 \times 10^{13}\ \text{s}^{-1}$. In other words, the maximum growth rate for the amplitude of the charge density perturbations is greater when incorporating the damping effects of the PHEC. This was not the expected result as one would think that a damping effect would quell the growth rate.

The program was then run using an angle of $\theta = 45°$ and the graph shown in figure 3.3(a) below was produced. Once again, to see the effects of the improved dielectric equation, this data will be compared to data acquired by Aryal and Hu [2] for the same system, described with the old dielectric function. These solutions can be seen in figure 3.3(b) below.

(a)



(b)

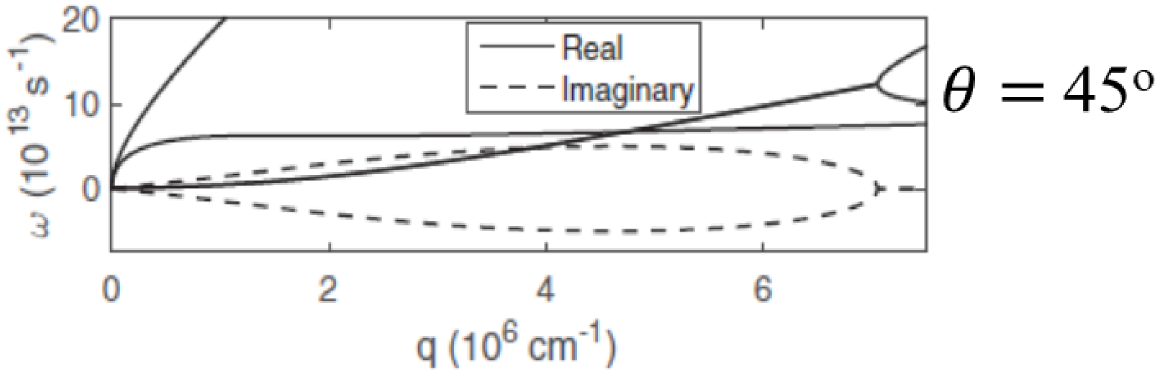


Figure 3.3 (a) Two-stream instability angular frequencies and growth rates using improved dielectric function for an angle $\theta = 45°$. As in figure 3.1 the real and imaginary parts of $\omega(\boldsymbol{q})$ that cause exponential growth of the charge density perturbations are plotted as a function of q, the magnitude of the wave vector, $\boldsymbol{q}$. **(b)** [2] Two-stream instability dispersion and growth rates using old dielectric function for an angle $\theta = 45°$. This graph displays the growth rates and angular frequencies for unstable modes found using equation (3).

In the case where $\theta = 45°$, equation (2) and (3) have a range of q values where unstable modes occur that is about equal. As before, the real part of $\omega(\boldsymbol{q})$ increases much faster for equation (2), meaning PHEC causes charge density perturbations to have higher angular frequencies. As shown in figures 3.3(a), the peak of the imaginary solution curve is at $\omega_i = 6.355 \times 10^{13}\ \mathrm{s}^{-1}$ while the peak of the imaginary curve for figure 3.3(b) is approximately $\omega_i = 5.0 \times 10^{13}\ \mathrm{s}^{-1}$. This signifies that in a more realistic system, not only are unstable modes possible, but they may grow at a greater exponential rate than previously thought.

These results are interesting because it was expected that the maximum growth rate would decrease with the more accurate representation of the damping effects caused by the PHEC. This is certainly something that needs deeper exploration, but speculation about what would cause this to happen is made on the next page.

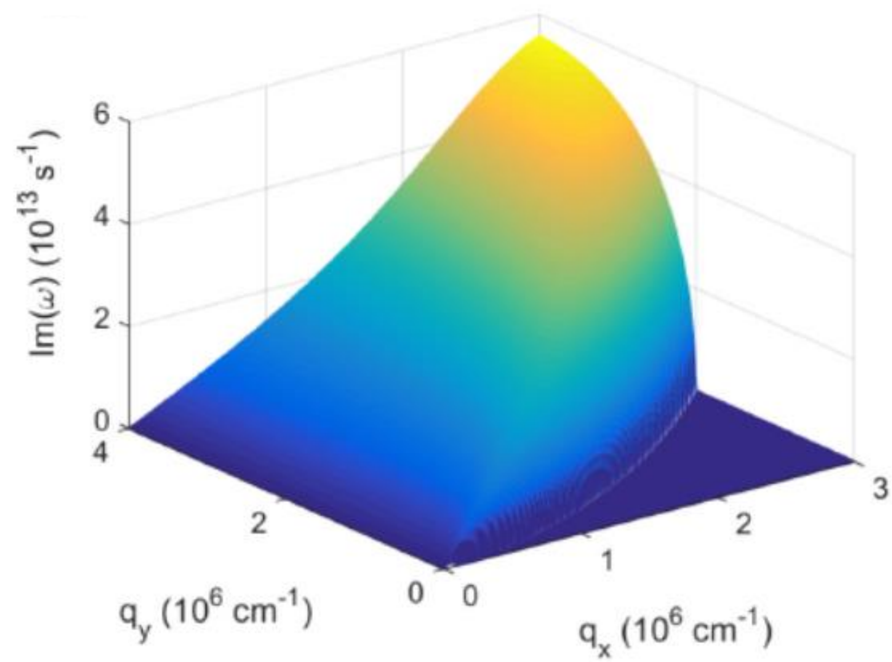


Figure 3.4 [2] Surface plot that plots the imaginary part of $\omega(\boldsymbol{q})$ as a function of $\boldsymbol{q}$. This surface plot was obtained by numerically solving for the roots of equation (3) at some angle.

Figure 3.4 shows a surface plot of the imaginary part of $\omega(\boldsymbol{q})$ as a function of the x and y components of $\boldsymbol{q}$. This figure was obtained by Aryal and Hu [2] using equation (3) at some angle θ. If using equation (2) caused a shift in this curve towards the x-axis, then larger growth rates would be obtained.

Conclusion

The purpose of this investigation was to determine if unstable modes could form in graphene when using a more sophisticated version of the dielectric function to more accurately describe the effects of PHEC on the charge density perturbations. MATLAB's built in root solver was used to numerically solve the sixth order polynomial dielectric function, producing values of $\omega(\boldsymbol{q})$ that gave $\varepsilon(\boldsymbol{q}, \omega) = 0$ which had positive imaginary parts. This indicates that unstable modes could occur which give rise to an exponential growth rate in the charge density perturbations in graphene. It was also determined that incorporating a more accurate representation of the damping effects of PHEC leads to larger growth rates. It is speculated that this could be due to a shift in the contours of the surface plot of the imaginary part of $\omega(\boldsymbol{q})$ as a function of $\boldsymbol{q}$. This is something that requires further investigation and is a great topic for future research. In addition to this, future research could also deal with attempting to reproduce these effects experimentally or determining if there are any other two dimensional materials in which the two-stream instability can occur.

References

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[2] C. M. Aryal, B. Y.-K. Hu, and A.-P. Jauho, Phys. Rev. B **94**, 115401 (2016).

[3] F. Chen, *Introduction to Plasma Physics and Controlled Fusion*, Vol.1, 2nd ed. (Plenum, New York, 1984).