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# THE EFFECT OF NON-LOCAL ELECTRICAL CONDUCTIVITY ON NEAR-FIELD RADIATIVE HEAT TRANSFER BETWEEN GRAPHENE SHEETS

By

Behrad Zeinali Tajani

M.Sc. in Mechanical Engineering, University of Zanjan, 2017

#### A THESIS

Submitted in Partial Fulfillment of the Requirements for the Degree of Master of Science (in Mechanical Engineering)

> The Graduate School The University of Maine August 2021

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# THE EFFECT OF NON-LOCAL ELECTRICAL CONDUCTIVITY ON NEAR-FIELD RADIATIVE HEAT TRANSFER BETWEEN GRAPHENE SHEETS

By Behrad Zeinali Tajani

Thesis Advisor: Dr. Sheila Edalatpour

An Abstract of the Thesis Presented in Partial Fulfillment of the Requirements for the Degree of Master of Science (in Mechanical Engineering) August 2021

Every object above zero kelvin emits electromagnetic radiation with the dominant wavelength determined using the Wien's law (10 microns at room temperature). These waves can transfer energy and hence are the foundation of radiative heat transfer (RHT). RHT consists of two regimes: far-field and near-field. If the distance between the heat exchanging media is more than the dominant wavelength, the regime is far-field and is limited to the ideal Planck's blackbody, and only propagating waves contribute to heat transfer. On the other hand, when the distance is less than the dominant wavelength, the regime is called the near-field. In near-field radiative heat transfer (NFRHT), the contribution of evanescent waves becomes more significant than the propagating ones, and this causes a spike in the spectral RHT that exceeds Planck's blackbody limit by several orders of magnitude. If the thermal emitter supports surface modes, NFRHT can become monochromatic.

These surface modes can be surface phonon polaritons (SPhP) and surface plasmon polaritons (SPP). Materials such as silicon carbide support SPhP and graphene is an example of a material that support SPPs. These surface modes cause the quasi-monochromatic behavior that can be exploited for applications such as thermophotovoltaic devices and thermal rectifiers. Graphene is one of the few materials that support surface modes in the infrared where these modes can be thermally excited. Another characteristic of graphene SPPs is their tunability using gate voltage or chemical doping which has transformed graphene into a revolutionary material for NFRHT applications in mid-to far-infrared regions.

Graphene has been studied both theoretically and experimentally. However, in most NFRHT studies, graphene has been investigated theoretically for its application in NFRHT. NFRHT for graphene is calculated using its electrical conductivity. The studies in NFRHT have utilized a local method for graphene's electrical conductivity called the Kubo formula. However, graphene is a non-local material that has non-local conductivity and dielectric response, hence it is not clear whether a local model such as the Kubo formula can capture the non-local behavior of graphene. In this thesis, a non-local model called the Lindhard formula is used to calculate graphene's conductivity, and the radiative conductance between two graphene sheets. The Lindhard predictions are compared with the results obtained from the Kubo formula. It is found that at low chemical potential both methods agree, while by increasing the chemical potential of graphene, the Kubo formula overestimates the radiative conductance between two graphene sheets by several orders of magnitude. Increasing the gap size and reducing temperature would increase the difference. It is concluded that the observed differences are due to the simplification involved when deriving the Kubo formula, and therefore it is recommended to use the Lindhard formula in NFRHT studies.

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### CHAPTER 1 INTRODUCTION

#### 1.1 Background

Every material with a temperature above zero Kelvin or absolute zero emits electromagnetic waves with a maximum intensity at wavelength of  $\lambda_{max}$ . According to Wien's law [1],  $\lambda_{max}$  is equal to 10 microns at room temperature. The emission of these electromagnetic waves can transfer energy from an object to another, and this process is called the radiative heat transfer (RHT) [2]. The RHT is divided into two distinct regimes called the near-field and far-field regimes. If the distance between the heat exchanging media is more than the dominant wavelength  $\lambda_{max}$ , the heat transfer regime is called the far-field regime. The far-field regime is described by Planck's theory [3] and RHT in this regime is limited to that for blackbodies. As proposed in Max Planck's theory of RHT, the blackbody limit is a great tool for quantifying the rate of RHT because it represents the maximum possible RHT between objects in the far-field. In a far-field regime, only propagating modes contribute to RHT (refer to Fig.1.1). Far-field radiative heat transfer (FFRHT) is modeled using the radiative transfer equation and geometric optic.

The other regime of RHT is called the near-field radiative heat transfer (NFRHT). In this regime, the distance between the objects is less than the dominant wavelength (refer to Fig.1.1). At such small gaps, the contribution of frustrated evanescent modes and surface evanescent modes becomes the dominant RHT method [4, 5, 6, 7, 8]. As shown in Fig.1.1, frustrated evanescent modes are propagative in the emitting medium but they are evanescent in the free space. Surface evanescent modes such as surface phonon polaritons (SPhP) [9, 10] and surface plasmon polaritons (SPP) [11, 12] are evanescent in both the

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emitting medium and the free space. SPhPs and SPPs result from the strong coupling between EM waves and phonons or plasmons, respectively [13].

NFRHT is described using the theory of fluctuational electrodynamics [14]. In this theory, the thermally agitation of the charged particles within the emitting medium (which is the source of thermal emission) is modeled using the stochastic current density which is added to Maxwell's equations.



Figure 1.1. FFRHT is dominated by propagating modes while NFRHT includes the contribution of frustrated evanescent modes and surface evanescent modes.

Polder and Van Hove [15] used the formulation in Rytov's work [16] to study the effect of evanescent waves on radiative heat transfer and, upon doing so, paved the way for the emergence of the famous NFRHT. It was theoretically predicted that radiation between closely spaced surfaces could exceed that of blackbody [15, 17, 18, 19, 20], and it was attributed to constructive interference of propagating waves or tunneling of evanescent waves [4]. Evanescent waves can enhance near field radiative heat transfer by several orders of magnitude [4, 5]. The tunneling of evanescent waves decays exponentially with increasing the distance between the heat exchanging media (refer to Fig.1.1); hence their contribution vanishes if the separation gap is larger than the dominant thermal wavelength  $(\lambda_{max} = 10 \,\mu m$  at room temperature) [21].

The enhanced RHT in near-field has many applications and this concept is being employed in a variety of technologies such as thermal diodes [22, 23], thermophotovoltaics [24, 25, 26], contactless cooling [27, 28, 29] and thermal rectification [30]. Near-field thermophotovoltaic devices have been experimentally demonstrated recently and are proven to enhance power output by 40-fold compared to the far-field ones [26]. The enhancement of RHT in the near-field regime has also been capitalized on for photonic cooling and solid-state refrigeration [29]. It has also been shown that the surface modes in near-field can achieve a very high thermal rectification ratio of up to 23.7 [30].

Many of these near-field applications rely on spectrally-selective thermal emission that is made possible because of the narrow-band surface polaritons [31]. When most of NFRHT occurs in a very narrow frequency band, RHT is called monochromatic. If the medium supports SPPs or SPhPs, then the NFRHT can be quasi-monochromatic [31, 32, 33].

Polaritonc materials that support SPhPs and SPPs in the near to mid-infrared region are of utmost value since these modes can be thermally excited [26, 29, 30, 31]. The limited number if materials that support SPhPs and SPPs in the near to mid-infrared is the main limitation in taking advantage of the surface evanescent modes in the NFRHT applications. To overcome such deficiency, various metamaterials [34, 35, 36, 37] have been proposed. However, utilizing metamaterials for tuning the spectrum of NFRHT involves significant computational and fabrication costs for design and nanofabrication of these man-made materials.

One of the few materials supporting SPPs in the near and mid-infrared region is graphene [38, 39, 40]. Graphene is an one-atom-thick and two-dimensional allotrope of carbon arranged in a honeycomb lattice. It was discovered in 2004 [41] and has been studied extensively for potential applications in optics, plasmonics, and energy conversion due to its unique thermal, and optical properties [42, 43, 44, 45, 46, 47]. Graphene has proven to be a revolutionary material with massless charge carriers [48, 49] that equips it with surface plasmons in the near and mid-infrared region that can be actively tuned using electric gate voltage and chemical doping [41, 42, 50]. Due to supporting SPPs, graphene

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NFRHT can be quasi-monochromatic. Optical and thermal radiation properties of graphene are determined from its electrical conductivity. Two well-known formulas for predicting the electrical conductivity of graphene are Kubo formula and Lindhard formula.

The Kubo formula for graphene's conductivity is a local model that is a function of chemical potential, temperature and frequency [51, 52, 53, 54, 55, 56, 57, 58, 59]. The Kubo model neglects the wavevector dependency of graphene's electrical conductivity.

Another model for calculating the electrical conductivity of graphene is the Lindhard formula which is determined using the framework of Random Phase Approximation (RPA) formula [48, 60, 61, 62]. This model is not only a function of chemical potential, frequency, and temperature, but also considers the wavevector dependency of electrical conductivity and hence provides a great tool to quantify the nonlocal effect of graphene's electrical conductivity. It is worth saying that the Kubo formula is often referred to as the local-RPA as well.

In the next section, a literature review on graphene in the context of NFRHT is provided.

#### 1.2 Literature Review

#### **1.2.1** Theoretical studies

The highly tunable surface plasmons in graphene has a variety of applications in NFRHT. Due to the thinness of graphene sheet, it can be easily placed on dissimilar dielectric materials to enhance their RHT. The surface plasmons in graphene can not only enhance RHT but also can suppress it. This RHT modulation is evident in the work of Joulain et al.[6], and Ilic et al.[56] who reported that a mismatch between SPP frequencies in two media can result in reduced RHT between the two media. For this reason, graphene has been extensively proposed for modulating NFRHT. Based on modulation characteristics of graphene SPPs, it has been proposed as thermal switch [58, 59, 63, 64, 65, 66] and fast non-contact cooling devices [67]. The versatility of graphene application in NFRHT has been evaluated by calculating the NFRHT between graphene and different material with different dielectric constant such as MoS<sub>2</sub>, SiO<sub>2</sub>, anisotropic magneto-dielectric hyperbolic metamaterials (AMDHM), black phosphorene and amorphous SiO<sub>2</sub> [68, 69, 70, 71, 72, 73, 74].

Graphene supports SPPs in the infrared region. An SPP resonance frequency in the infrared is of high interest for nano-gap thermophotovoltaic devices, as these frequencies can be thermally excited [46, 53, 75]. Numerical investigation of this phenomenon has shown that applying graphene sheet on a nano-gap TPV cell can enhance energy output significantly [46, 53, 75].

The electrical conductivity of graphene can be tuned in these ways: By changing the chemical potential of graphene that is done by applying gate voltage or chemical doping [35, 76, 77], by applying magnetic field [78] and by applying stress to graphene sheets [79].

Graphene was also studied as a component of metamaterials. One of the drawbacks of metamaterials for NFRHT application is their lack of tunability. Using graphene in metamaterial has been proposed in recent studies and it is shown that the coupling of graphene plasmons with surface modes of other metamaterial components can serve as a mechanism for active tuning of radiative properties of metamaterials [80, 81, 82, 83, 84, 85]. The same mechanism of tuning exists for graphene covered gratings [86].

Graphene/vacuum multi-layers have also been studied in the context of NFRHT, and it has been reported that they demonstrate different characteristic than graphene sheets and metamaterials that include graphene [87, 88]. Increasing the number of sheets can not only blueshift the peak frequency of NFRHT, but it also can increase it as well. Another

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observation is that increasing the distance between the sheets can smoothen the temperature gradient between them. This change of temperature gradient can be explained by ultrafast heat transfer between graphene sheets in the near-field regime.

#### 1.2.2 Experimental studies

So far, there are only four experimental studies on NFRHT between graphene sheets or graphene-covered substrates. Experimental work in graphene has proven the findings of existing theoretical investigation. Zwol et al. [89] experimentally demonstrated that when surface plasmons are thermally excited in a system comprising of doped silicon and graphene on SiC, NFRHT is increased by almost 25% at distance smaller than 200 nm.

Another experimental work successfully observes the super-Planck heat transfer in the presence of graphene. The graphene sheets were deposited on silicon substrates in TPV cells and proven to enhance the efficiency of the TPV cell by almost two orders of magnitude at temperature differences above 300 [90].

Recently, another experimental investigation [91] has studied the feasibility of a thermal switch using graphene by applying gate voltage as a mechanism for changing the chemical potential. They separated optical flat coated with graphene and a graphene-coated silicon wafer by 560 nm and imposed two 0 and 35 V gate voltages and shown that the heat flux when bias is imposed is modulated by about 3 to 5%. Another aspect of the proposed device, is that this device is operable in a wide range of temperatures and no moving element exists in that structure. Applying higher gate voltage can also change the behavior of the proposed system. The change of reflectance, transmittance and electrical conductivity of graphene in a wide range of gate voltage is experimentally studied by Li et al. [92]. They observed as gate voltage is increased, the amplitude of change in the electrical conductivity of graphene also increases.

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Finally, it is worth noting that due to the Lindhard formula's complexity, most researchers opt for a simplified model called Kubo formula [51, 52, 53, 54, 55, 56, 57, 58, 59, 60].

#### **1.3** Approach and Contributions

As it is discussed in Section 1.2, graphene is a very promissing materials for applications such as heat transfer enhancement, active control and modulation of heat transfer, thermal switches, nano-gap thermophotovoltaic devices, as well as ultra fast cooling. However, many of these application are being proposed theoretically using a local formula for electrical conductivity of graphene (i.e., the Kubo formula). It is not clear how non-local electrical conductivity of graphene can modify its NFRHT magnitude and SPP resonance frequency. To answer this question, we model near-field radiative conductance of two graphene sheets separated by a vacuum gap using the Kubo formula as well as the Lindhard formula, which is a non-local model. we compared the radiative conductance of graphene sheets obtained using the two formula to understand the non-local effects on NFRHT between graphene sheets.

The results of this study, provides insight into the differences between the two local and non-local modeling approaches. The differences observed between the Kubo and Lindhard formulas results suggest that the non-local effects on NFRHT are significant in most cases.

#### 1.4 Thesis Outline

This thesis is organized as follows. The theoretical background on graphene conductivity formulas is provided in chapter 2. The radiative conductance and dispersion relation expressions are also discussed in this chapter. The research method and the results of the present study are presented in chapter 3. Conclusion and recommendations are discussed in the fourth chapter.

## CHAPTER 2 THEORETICAL BACKGROUND

In this chapter, the fluctuational electrodynamics framework, which is used for modeling near-field radiative heat transfer is discussed. the NFRHT between two graphene covered media is then formulated by applying the fluctuating electrodynamics theory. Next, the surface plasmon polariton modes and their existence in graphene have been discussed.

we discuss how the thermal fluctuations are incorporated into Maxwell's equations. The thermal radiation is then formulated by applying the fluctuating electrodynamics theory, and the NFRHT equations are achieved. The geometry under study is then introduced, and the constituents of the NFRHT equation for the problem under consideration, Fresnel coefficients, are set forth.

#### 2.1 Fluctuational Electrodynamics for Describing Thermal Radiation

Energy flux due to thermal emission of electromagnetic wave, can be found using Poynting vector. The average of Poynting vector over time is expressed as [93]:

$$\langle \mathbf{S}(\mathbf{r},\omega) \rangle = 4 \times \frac{1}{2} \operatorname{Re} \left\{ \mathbf{E} \times \mathbf{H}^* \right\}$$
 (2.1)

The **E** and **H** in Eq. 2.1 are the thermally emitted electric and the magnetic fields, respectively. Superscript \* denotes complex conjugate and  $\omega$  is the frequency in rad/s. The factor 4 is included in Eq. 2.1 to account for the fact that only the positive frequencies are considered in the Fourier decomposition of the electromagnetic fields [94, 95]. **E** and **H** are obtained from Maxwell's equations when augmented by the source of thermal emission [93].

The source of thermal emission is the random motion of charge particles in the matter caused by thermal agitation. From a macroscopic paint of view, this random motion can be modelled using an stochastic current density,  $\mathbf{J}^r$ , which is added to Maxwell equations. The resulting Maxwell's equations are referred to as the stochastic Maxwell's equations, This framework for modelling thermal radiation is called fluctuational electrodynamics.

$$\nabla \times \mathbf{E}(\mathbf{r}, \omega) = i\omega\mu_0 \mathbf{H}(\mathbf{r}, \omega) \qquad (Faraday's law)$$

$$\nabla \times \mathbf{H}(\mathbf{r}, \omega) = -i\omega\varepsilon \mathbf{E}(\mathbf{r}, \omega) + \mathbf{J}^r(\mathbf{r}, \omega) \qquad (Ampere's law)$$

$$\nabla \cdot \mathbf{E}(\mathbf{r}, \omega) = 0 \qquad (Gauss's law)$$

$$\nabla \cdot \mathbf{H}(\mathbf{r}, \omega) = 0 \qquad (Gauss's law)$$

where  $\mu_0 = 1.257 \times 10^{-6}$  H/m is the permeability of vacuum,  $\varepsilon$  is the complex permittivity of the materials, **r** is the position vectors, and **J**<sup>r</sup> is the stochastic current density due to thermally fluctuation of charged particles. The thermally emitted electric and magnetic fields can be written in terms of dyadic Green's function and the fluctuating current as:

$$\mathbf{E}(\mathbf{r},\omega) = i\omega\mu_0 \int_V dV' \overline{\overline{\mathbf{G}}}^E (\mathbf{r},\mathbf{r}',\omega) \cdot \mathbf{J}^r (\mathbf{r}',\omega) = i\omega\mu_0 \int_V dV' G_{in}^E J_n^r$$

$$\mathbf{H}(\mathbf{r},\omega) = \int_V dV' \overline{\overline{\mathbf{G}}}^H (\mathbf{r},\mathbf{r}',\omega) \cdot \mathbf{J}^r (\mathbf{r}',\omega) = i\omega\mu_0 \int_V dV' G_{in}^H J_n^r$$
(2.3)

In Eq. 2.3,  $\overline{\overline{\mathbf{G}}}^{E}(\mathbf{r}, \mathbf{r}', \omega)$  and  $\overline{\overline{\mathbf{G}}}^{H}(\mathbf{r}, \mathbf{r}', \omega)$  are the DGF for electric and magnetic field, respectively and n is the state polarization of the fields observed at  $\mathbf{r}$ . The DGF can be viewed as a transfer function relating the electric field at point  $\mathbf{r}$  to the fluctuating current at point  $\mathbf{r}'$  (refer to Fig. 2.1). The electric and magnetic DGFs are obtained by solving the Maxwell equations for a point source located at location  $\mathbf{r}'$ .

Using the relations established between the stochastic current density and the magnetic and electric fields, the energy flux can be obtained by inserting Eq. 2.3 into Eq. 2.1, as:

$$\langle \mathbf{S}(\mathbf{r},\omega) \rangle$$

$$= 4 \times \frac{1}{2} \operatorname{Re} \left\{ \mathbf{E}(\mathbf{r},\omega) \times \mathbf{H}^{*}(\mathbf{r},\omega) \right\}$$

$$= 2\omega\mu_{0} \operatorname{Re} \left\{ i \int_{V} dV' \int_{V} dV'' G_{n\alpha}^{E} \left(\mathbf{r},\mathbf{r}',\omega\right) G_{n\beta}^{H^{*}} \left(\mathbf{r},\mathbf{r}'',\omega'\right) \left\langle J_{\alpha}^{r} \left(\mathbf{r}',\omega\right) J_{\beta}^{r^{*}} \left(\mathbf{r}'',\omega'\right) \right\rangle \right\}$$

$$(2.4)$$



Figure 2.1. DGF can be viewed as a transfer function relating the thermally fluctuating current at location  $\mathbf{r}$ ' to the electric field at location  $\mathbf{r}$ .

Since the thermal fluctuations of charged particles cause the stochastic current density  $\mathbf{J}^r$ , the ensemble average of the correlation function of the fluctuating current, i.e., the term  $\langle J^r_{\alpha} (\mathbf{r}', \omega) J^{r^*}_{\beta} (\mathbf{r}'', \omega') \rangle$ , that is the source of thermal radiation should be related to the temperature of the emitter. This relation is established by the fluctuation-dissipation theorem [96]. Under the same assumptions as of the Maxwell equations and assuming that the material is in thermal equilibrium, the ensemble average of the correlation function of the fluctuating current is given by:

$$\left\langle J_{\alpha}^{r}\left(\mathbf{r}',\omega\right)J_{\beta}^{r^{*}}\left(\mathbf{r}'',\omega'\right)\right\rangle = \frac{\omega\varepsilon_{0}\varepsilon''}{\pi}\Theta(\omega,T)\delta(\mathbf{r}'-\mathbf{r}'')\delta(\omega-\omega')$$
(2.5)

where  $\Theta(\omega, T) = \hbar \omega / (\exp(\hbar \omega / k_B T) - 1)$  is the mean energy of a Planck oscillator [82, 84, 97],  $\varepsilon''$  is the imaginary part of the dielectric function of the material,  $\varepsilon_0 = 8.854 \times 10^{-12}$  F/m is the permittivity of the vacuum,  $\hbar = h/2\pi = 1.0546 \times 10^{-3} J.s$  is the reduced Planck constant and  $k_B = 1.381 \times 10^{-23} J/K$  is the Boltzmann constant. Therefore, by applying the fluctuation-dissipation theorem to Eq. 2.4 and using ergodic hypothesis, the radiative heat flux is found as:

$$\langle \mathbf{S}(\mathbf{r},\omega) \rangle =$$

$$\frac{2k_0^2 \Theta(\omega,T)}{\pi} \operatorname{Re} \left\{ i \varepsilon_r''(\omega) \int_V dV' G_{n\beta}^E(\mathbf{r},\mathbf{r}',\omega) G_{n\alpha}^{H^*}(\mathbf{r},\mathbf{r}'',\omega') \right\}$$

$$(2.6)$$

In Eq. 2.6,  $k_0 = \omega/c_0$  is the wavevector in the vacuum, where  $c_0 = \sqrt{\varepsilon_0 \mu_0}$  is the speed of light in vacuum.

### 2.2 Near-Field Radiative Heat Transfer Between Two Graphene Covered Semi-Infinite Media

In this section, NFRHT between two graphene-covered planar bodies is derived. The schematic of the problem under consideration is shown in Fig. 2.2 where two semi-infinite media are covered with graphene sheets. It is realistically assumed that graphene sheets' temperature is equal to the medium's temperature on which they are placed. The emitter and the receiver are kept at the constant temperatures of  $T_1$  and  $T_3$ , respectively, and a vacuum gap of length D separates the two media.



Figure 2.2. Schematic of the problem under consideration. Two graphene-covered media (media 1 and 3), with permittivities  $\varepsilon_1$  and  $\varepsilon_3$  are kept at temperatures  $T_1$  and  $T_3$ , respectively, and they are separated by a vacuum gap (medium 2) of size D,  $\varepsilon_2 = 1$ .

The NFRHT flux from medium 1 to medium 3 is calculated using Eq. 2.6 in which the only unknowns are Green's functions  $G_{13}^E(\mathbf{r}, \mathbf{r}', \omega)$  and  $G_{13}^H(\mathbf{r}, \mathbf{r}', \omega)$ . For the

one-dimensional geometry shown in Fig. 2.2, the DGFs in the free space (Eq. 2.3) are the solution of the following equation [97]:

$$\nabla \times \nabla \times \overline{\overline{\mathbf{G}}}^{E}(\mathbf{r}, \mathbf{r}', \omega) - k^{2} \overline{\overline{\mathbf{G}}}^{E}(\mathbf{r}, \mathbf{r}', \omega) = \overline{\overline{\mathbf{I}}} \delta(\mathbf{r} - \mathbf{r}')$$
(2.7)

In Eq. 2.7,  $\overline{\overline{\mathbf{I}}}$  is the identity matrix. The solution for the magnetic DGF can be obtained using the solution of the electric DGF as  $\overline{\overline{\mathbf{G}}}^{H}(\mathbf{r},\mathbf{r}',\omega) = \nabla \times \overline{\overline{\mathbf{G}}}^{E}(\mathbf{r},\mathbf{r}',\omega)$ . Since the geometry under consideration has azimuthal symmetry, the polar coordinate will be utilized instead of the Cartesian coordinate. The solution of Eq. 2.7 is provided in Ref. [98]. After using this solution for  $G_{13}^{E}(\mathbf{r},\mathbf{r}',\omega)$  and  $G_{13}^{H}(\mathbf{r},\mathbf{r}',\omega)$ , the integral term in Eq. 2.6 can be written as [99]:

$$\int_{V_1} dV' G^E_{13i\alpha} \left( \mathbf{r}, \mathbf{r}', \omega \right) G^{H^*}_{13j\alpha} \left( \mathbf{r}, \mathbf{r}', \omega \right) =$$

$$\int_{-\infty}^{\infty} \frac{d\mathbf{k}_{\rho}}{(2\pi)^2} \int_z dz' g^E_{13i\alpha} \left( k_{\rho, z}, z', \omega \right) g^{H^*}_{13j\alpha} \left( k_{\rho, z}, z', \omega \right)$$
(2.8)

where  $g_{13i\alpha}^E$  and  $g_{13j\alpha}^H$  are the Weyl components of DGF [98, 99],  $k_{\rho}$  is the parallel component of the wavevector (refer to Fig. 2.3) and z and z' are the z components of the location vectors **r** and **r'** (See Fig. 2.1). The complex wavevectors in medium 1 and 3 are  $k_1$  and  $k_3$ , respectively with  $k_1^2 = \varepsilon_1 k_0^2$  and  $k_3^2 = \varepsilon_3 k_0^2$ . The normal component of the wavevector in medium j is calculated as  $k_{zj} = \sqrt{k_j^2 - k_\rho^2}$ . The parallel component of the wavevector which has components along x and y directions can be written as  $\mathbf{k}_{\rho} = k_x \hat{\mathbf{x}} + k_y \hat{\mathbf{y}}$ . By expressing  $\mathbf{k}_{\rho}$  in the polar coordinate system and considering azimuthal symmetry,  $\int_{-\infty}^{\infty} d\mathbf{k}_{\rho}$  can be written as [93]:

$$\int_{-\infty}^{\infty} d\mathbf{k}_{\rho} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dk_x dk_y = \int_{k_{\rho}=0}^{\infty} \int_{\phi=0}^{2\pi} k_{\rho} dk_{\rho} d\phi = 2\pi \int_{k_{\rho}=0}^{\infty} k_{\rho} dk_{\rho}$$
(2.9)



Figure 2.3. The complex wavevector in medium 1 and 3 has a component parallel to the surface of the medium  $(k_{\rho})$  and a normal component  $(k_z)$ .

Substituting Eq. 2.8 and 2.9 into Eq. 2.6, the near-field radiative heat flux from medium 1 to medium 3 is equal to [100]:

$$q_{\omega,13}^{\prime\prime} = \frac{k_0^2 \Theta(\omega, T_1)}{\pi^2} \times \operatorname{Re} \left\{ i \varepsilon_1^{\prime\prime} \int_{k_\rho=0}^{\infty} k_\rho dk_\rho \int_z dz^{\prime} \left[ \begin{array}{c} g_{13\rho\alpha}^E\left(k_\rho, z, z^{\prime}, \omega\right) g_{13\rho\alpha}^{H^*}\left(k_\rho, z, z^{\prime}, \omega\right) \\ -g_{13\theta\alpha}^E\left(k_\rho, z, z^{\prime}, \omega\right) g_{13\rho\alpha}^{H^*}\left(k_\rho, z, z^{\prime}, \omega\right) \end{array} \right] \right\}$$
(2.10)

The integral over  $k_{\rho}$  from 0 to  $\infty$  (i.e.,  $\int_{k_{\rho}=0}^{\infty}$ ) in Eq. 2.10 can be divided into two parts: an integral from 0 to  $k_0$  ( $\int_{k_{\rho}=0}^{k_0}$ ) and an integral from  $k_0$  to  $\infty$  ( $\int_{k_{\rho}=k_0}^{\infty}$ ). The first integral is over EM wares with  $k_{\rho} < k_0$ . Therefore, these wave are propagative in the Vacuum gap. The flux of heat transferred by these propagating wares is referred to as  $q_{\omega}^{\prime\prime}$  in this thesis. The second integral is over waves with  $k_{\rho} > k_0$ . Hence, these waves are evanescent in separation gap.

These modes, which evanescently decay perpendicular to the surface in a distance approximately equal to the dominant wavelength of thermal radiation  $\lambda$ , can contribute to heat transfer if the separation gap is less than  $\lambda$  (i.e., when  $D \leq \lambda$ ). The flux of heat transfer from medium 1 to medium 3 due to the evanescent waves is shown by  $q_{\omega}^{\prime\prime^{evan}}$  in this thesis [101, 102, 99]. Hence the spectral flux of NFRHT from medium 1 to medium 3 can be written as:

$$q_{\omega,13}'' = q_{\omega,13}''^{\text{prop}} + q_{\omega,13}''^{\text{evan}}$$
(2.11)

When the appropriate form of Weyl components of DGF [98, 99, 103] are substituted into Eq. 2.10,  $q''_{\omega,13}$  can be written as:

$$q_{\omega,13}^{\prime\prime^{\text{prop}}} = \frac{\Theta(\omega,T_1)}{4\pi^2} \int_0^{k_0} \sum_{\gamma=\text{TE,TM}} k_\rho Z_{13}^{\text{prop}} dk_\rho$$

$$q_{\omega,13}^{\prime\prime^{\text{evan}}} = \frac{\Theta(\omega,T_1)}{\pi^2} \int_{k_0}^{\infty} \sum_{\gamma=\text{TE,TM}} k_\rho Z_{13}^{\text{evan}} dk_\rho$$
(2.12)

where

$$Z_{13}^{\text{prop}} = \frac{\left(1 - |r_{21}^{\gamma}|^2\right) \left(1 - |r_{23}^{\gamma}|^2\right)}{\left|1 - r_{21}^{\gamma} r_{23}^{\gamma} e^{2ik'_{22}2d}\right|^2}$$

$$Z_{13}^{\text{evan}} = \frac{\text{Im}(r_{21}^{\gamma}) \text{Im}(r_{23}^{\gamma})}{\left|1 - r_{21}^{\gamma} r_{23}^{\gamma} e^{-2k''_{22}d}\right|^2}$$
(2.13)

The heat flux transferred from medium 3 to medium 1  $(q''_{\omega,31})$  can be found similarly as:

$$q_{\omega,31}^{\prime\prime^{\text{prop}}} = \frac{\Theta(\omega,T_3)}{4\pi^2} \int_0^{k_0} \sum_{\gamma=\text{TE,TM}} k_\rho Z_{31}^{\text{prop}} dk_\rho$$

$$q_{\omega,31}^{\prime\prime^{\text{evan}}} = \frac{\Theta(\omega,T_3)}{\pi^2} \int_{k_0}^{\infty} \sum_{\gamma=\text{TE,TM}} k_\rho Z_{31}^{\text{evan}} dk_\rho$$
(2.14)

The net heat flux from medium 1 to medium 3,  $q''_{\omega}$ , can then be obtained as:

$$q''_{\omega} = q''_{\omega,13} - q''_{\omega,31} \tag{2.15}$$

Substituting  $q''_{\omega,13}$  and  $q''_{\omega,31}$  from Eqs. 2.12 and 2.14,  $q''_{\omega}$  is found as:

$$q_{\omega}^{\prime\prime^{\text{prop}}} = \frac{\Theta(\omega, T_1) - \Theta(\omega, T_3)}{4\pi^2} \int_0^{k_0} \sum_{\gamma = \text{TE,TM}} k_{\rho} Z_{13}^{\text{prop}} dk_{\rho}$$

$$q_{\omega}^{\prime\prime^{\text{evan}}} = \frac{\Theta(\omega, T_1) - \Theta(\omega, T_3)}{\pi^2} \int_{k_0}^{\infty} \sum_{\gamma = \text{TE,TM}} k_{\rho} Z_{13}^{\text{evan}} dk_{\rho}$$
(2.16)

where  $\Theta$  is the mean energy of a Planck oscillator, D is the distance between the two media,  $k''_{z2}$  is the imaginary part of the z-component of the wavevector in medium 2,  $\gamma$ shows the polarization of waves (TE for the transverse electric and TM for transverse magnetic polarization) and  $r_{ij}$  is the Fresnel reflection coefficient at the interface of media *i* and *j* (refer to Fig. 2.4). The Fresnel reflection coefficients for the TE and TM polarizations can be expressed as [104, 105]:

$$r_{ij}^{TE} = \frac{k_{zi} - k_{zj} - \mu_0 \sigma \left(\omega, k_\rho, T\right) \omega}{k_{zi} + k_{zj} + \mu_0 \sigma \left(\omega, k_\rho, T\right) \omega}$$

$$r_{ij}^{TM} = \frac{\varepsilon_j k_{zi} - \varepsilon_i k_{zj} + \frac{\sigma(\omega, k_\rho, T) k_{zi} k_{zj}}{\varepsilon_0 \omega}}{\varepsilon_j k_{zi} + \varepsilon_i k_{zj} + \frac{\sigma(\omega, k_\rho, T) k_{zi} k_{zj}}{\varepsilon_0 \omega}}$$
(2.17)

In Eq. 2.17,  $\varepsilon_i$  and  $\varepsilon_j$  are the dielectric functions of media *i* and *j*, respectively, and  $\sigma$  is the electrical conductivity of graphene.

Equation 2.16 is obtained by assuming that media 1 and 3 are optically thick. In other words, it is assumed that thermal radiation incident on these media cannot escape the backside of these media as they are thick enough such that they will absorb thermal radiation before it exits from the other end. In the case of suspended graphene sheets (with no substrate), thermal radiation can be transmitted through the graphene. In this case, the Weyl component of the DGFs also include Fresnel transmission coefficient. In this case:

$$Z_{13}^{\text{prop}} = \frac{\left(1 - \left|r_{21}^{\gamma}\right|^{2} - \left|t_{21}^{\gamma}\right|^{2}\right) \left(1 - \left|r_{23}^{\gamma}\right|^{2} - \left|t_{23}^{\gamma}\right|^{2}\right)}{\left|1 - r_{21}^{\gamma} r_{23}^{\gamma} e^{2ik_{2}D}\right|^{2}}$$

$$Z_{13}^{\text{evan}} = \frac{\text{Im}(r_{21}^{\gamma}) \text{Im}(r_{23}^{\gamma})}{\left|1 - r_{21}^{\gamma} r_{23}^{\gamma} e^{2ik_{2}D}\right|^{2}}$$
(2.18)



Figure 2.4. The Fresnel reflection  $(r_{ij})$  and transmission coefficients  $(t_{ij})$  describe the reflection or transmission of EM waves incident on the interface between medium i and j.

In Eq. 2.18,  $t_{ij}^{\gamma}$  is the Fresnel transmission coefficient (refer to Fig. 2.4). The transmission coefficient is given by [104, 105]:

$$t_{ij}^{\text{TE}} = \frac{2k_{zi}}{k_{zi} + k_{zj} + \mu_0 \sigma \left(k_{\rho}, \omega, T\right) \omega}$$

$$t_{ij}^{\text{TM}} = \sqrt{\frac{\varepsilon_i}{\varepsilon_j} \operatorname{Re}\left[\frac{k_{zj}}{k_{zi}}\right]} \frac{2\varepsilon_j k_{zi}}{\varepsilon_j k_{zi} + \varepsilon_i k_{zj} + \frac{\sigma(k_{\rho}, \omega, T)k_{zi}k_{zj}}{\varepsilon_0 \omega}}$$

$$(2.19)$$

The radiative conductance between media 1 and 3 is defined as :

$$G_{\omega} = \lim_{\delta T \to 0} \frac{q_{\omega}''}{\delta T} \tag{2.20}$$

where  $q''_{\omega}$  is the heat flux between the two media and  $\delta T$  is their temperature difference. Substituting for  $q''_{\omega}$  from Eq. 2.16, the radiative conductance is found as:

$$\begin{aligned}
G_{\omega}^{\text{prop}} &= \frac{1}{4\pi^2} \frac{\partial \Theta}{\partial T} \int_0^{k_0} \sum_{\gamma = \text{TE,TM}} Z_{13}^{\text{prop}} k_{\rho} dk_{\rho} \\
G_{\omega}^{\text{evan}} &= \frac{1}{4\pi^2} \frac{\partial \Theta}{\partial T} \int_{k_0}^{\infty} \sum_{\gamma = \text{TE,TM}} Z_{13}^{\text{evan}} k_{\rho} dk_{\rho}
\end{aligned} \tag{2.21}$$

In Eq. 2.21,  $G_{\omega}^{\text{prop}}$  and  $G_{\omega}^{\text{evan}}$  are the propagating and evanescent part of the radiative conductance.

#### 2.3 Graphene Electrical Conductivity Models

As seen from Eqs. 2.17 and 2.19, the reflection and transmission coefficients and thus radiative heat flux strongly depend on the graphene electrical conductivity. So far, NFRHT in graphene-based media is calculated using the Kubo formula for the electrical conductivity. The Kubo formula is obtained by assuming that  $k_{\rho} = 0$ . Since this expression does not account for the variation of  $\sigma$  with  $k_{\rho}$ , it is referred to as a local model. As discussed previously, radiative heat transfer can be mediated by all electromagnetic waves having a  $k_{\rho}$  between 0 and infinity. Therefore, using the Kubo formula for near-field radiative heat transfer calculations can be questionable.

There is another model for electrical conductivity of graphene, referred to as the Lindhard formula [106, 61], which accounts for the variation of  $\sigma$  with  $k_{\rho}$  as well. These two formulas for the electrical conductivity of graphene are discussed in the following subsections.

#### 2.3.1 Kubo Formula

Ignoring the impact of magnetic field, the Kubo formulation is [39, 107, 50, 104, 108]:

$$\sigma(\omega,\mu_c,T) = -\frac{ie^2(\omega+i\gamma)}{\pi\hbar^2} \left(\frac{1}{(\omega+i\gamma)^2} \int_0^\infty E\left(\frac{\partial f(E)}{\partial E} - \frac{\partial f(-E)}{\partial E}\right) dE - \int_0^\infty \frac{f(-E) - f(E)}{(\omega+i\gamma)^2 - 4(E/\hbar)^2} dE\right)$$
(2.22)

where  $f(E) = \{1 + \exp[(E - \mu_c)/k_{\rm B}T]\}^{-1}$  is the Fermi distribution function, e is the elementary charge,  $\gamma = \tau^{-1}$  is the electron scattering rate,  $\tau = \mu_m \mu_c / e\nu_F^2$  is the electron relaxation time in graphene where  $\mu_m$  is the carrier mobility,  $\nu_F = 9.5 \times 10^5 m/s$  is the Fermi velocity, and  $\mu_c$  is the chemical potential of graphene in Joules (J). The first and second terms in Eq. 2.22 correspond to the intraband and interband electron transitions, respectively [109]. When the integrations in Eq. 2.22 are performed, the Kubo electrical conductivity can be written as:

$$\sigma = \sigma^{\text{intra}} + \sigma^{\text{inter}} \tag{2.23}$$

In Eq. 2.23,  $\sigma^{\text{intra}}$  and  $\sigma^{\text{inter}}$  refer to electrical conductivity due to intraband and interband transitions, respectively, and they are given by:

$$\sigma^{\text{intra}}(\omega,\mu_c,T) = \frac{\sigma_0}{\pi} \frac{4}{\hbar\gamma - i\hbar\omega} \left[ \mu_c + 2k_B T \ln\left(1 + e^{-\mu_c/k_B T}\right) \right]$$
  
$$\sigma^{\text{inter}}(\omega,\mu_c,T) = \sigma_0 \left[ G(\hbar\omega/2) + i\frac{4\hbar\omega}{\pi} \int_0^\infty \frac{G(E) - G(\hbar\omega/2)}{(\hbar\omega)^2 - 4E^2} dE \right]$$
(2.24)

where

$$G(x) = \frac{\sinh\left(\frac{x}{k_BT}\right)}{\cosh\left(\frac{\mu_c}{k_BT}\right) + \cosh\left(\frac{x}{k_BT}\right)}$$
(2.25)

and  $\sigma_0 = e^2/(4\hbar)$ . It is shown that the intraband contribution is dominant in the THz and far-infrared regions, while the interband plays a significant role in the near-infrared and visible regions [110]. contribution from both interband ad intraband transitions are accounted for in this study.

#### 2.3.2 Lindhard Formula

The Lindhard formula provides a wavevector-dependent conductivity for graphene as [111]:

$$\sigma\left(k_{\rho},\omega,\mu_{c}T\right) = ie^{2}\frac{\omega}{k_{\rho}^{2}}\chi\left(k_{\rho},\omega,\mu_{c},T\right)$$
(2.26)

where  $\chi(k_{\rho}, \omega, \mu_c, T)$  is the susceptibility of graphene. The susceptibility of graphene is a complex number and is expressed as:

$$\chi(k_{\rho},\omega,\mu_{c},T) = \operatorname{Re}\left[\chi(k_{\rho},\omega,\mu_{c},T)\right] + i\operatorname{Im}\left[\chi(k_{\rho},\omega,\mu_{c},T)\right]$$
(2.27)

The real and imaginary parts in Eq. 2.27 are given using the Lindhard formula as [61]:

$$\operatorname{Re}\left[\chi\left(k_{\rho},\omega,\mu_{c},T\right)\right] = \frac{1}{\pi} \sum_{\alpha=\pm} \left(\frac{-2k_{B}T\ln\left(1+e^{\alpha\mu_{c}/k_{B}T}\right)}{\left(\hbar v_{F}\right)^{2}} + H(\hbar\omega - \hbar v_{F}k_{\rho})\right)$$
$$\times k_{\rho}^{2} f\left(\hbar\omega,\hbar v_{F}k_{\rho}\right) \left[G_{-}^{(\alpha)}\left(k_{\rho},\omega,T\right) - G_{+}^{(\alpha)}\left(k_{\rho},\omega,T\right)\right] + H(\hbar v_{F}k_{\rho} - \hbar\omega)$$
$$\times k_{\rho}^{2} f\left(\hbar v_{F}k_{\rho},\hbar\omega\right) \left[-\frac{\pi}{2}\delta_{\alpha,-} + D_{-}^{(\alpha)}\left(k_{\rho},\omega,T\right)\right]\right)$$
(2.28)

$$\operatorname{Im}\left[\chi\left(k_{\rho},\omega,\mu_{c},T\right)\right] = \frac{1}{\pi} \sum_{\alpha=\pm} \left(H\left(\hbar v_{F}k_{\rho}-\hbar\omega\right)k_{\rho}^{2}f\left(\hbar v_{F}k_{\rho},\hbar\omega\right)\right)$$
$$\times \left[G_{+}^{(\alpha)}\left(k_{\rho},\omega,\mu_{c},T\right)-G_{-}^{(\alpha)}\left(k_{\rho},\omega,T\right)\right] + H\left(\hbar\omega-\hbar v_{F}k_{\rho}\right)k_{\rho}^{2}f\left(\hbar\omega,\hbar v_{F}k_{\rho}\right)$$
$$\times \left[-\frac{\pi}{2}\delta_{\alpha,-}+D_{+}^{(\alpha)}\left(k_{\rho},\omega,T\right)\right]\right)$$
(2.29)

In Eqs. 2.28 and 2.29, H(x) is the Heaviside step function, and,

$$f(x,y) = \frac{1}{2\sqrt{x^2 - y^2}}$$

$$G_{\pm}^{(\alpha)}(k_{\rho},\omega,\mu_c,T) = \int_1^{\infty} \frac{\sqrt{u^2 - 1}}{\exp\left(\frac{|\hbar\nu_F k_{\rho} u \pm \hbar\omega| - 2\alpha\mu_c}{2k_B T}\right) + 1} du$$

$$D_{\pm}^{(\alpha)}(k_{\rho},\omega,\mu_c,T) = \int_{-1}^{1} \frac{\sqrt{1 - u^2}}{\exp\left(\frac{|\hbar\nu_F k_{\rho} u \pm \hbar\omega| - 2\alpha\mu_c}{2k_B T}\right) + 1} du$$
(2.30)

The electrical conductivity calculated using Eq. 2.26 through 2.30 is referred to as the Lindhard formula for graphene's electrical conductivity. The Lindhard formula has not been used in NFRHT calculations. Hence, the effect of wavevector dependency on NFRHT problems involving graphene has not been investigated yet.



Figure 2.5. The SPPs appear in the interface of metal and dielectric with permittivities of  $\varepsilon_1$  and  $\varepsilon_2$ , respectively and decay exponentially away from the surface.

#### 2.4 Surface Plasmon Polaritons

When the real part of the dielectric function changes sign at the interface of two materials, the coherent oscillations of delocalized electrons result in thermal emission of a type of surface modes called surface plasmon polaritons. The existence of these modes, which usually have a significant amount of energy, causes a peak in NFRHT. The existence of this peak is highly demanded for NFRHT applications such as nano-gap thermophotovoltaic devices.

The field generated by surface plasmons is confined near the surface and its amplitude decays exponentially by moving away from the interface [9, 112, 113, 114] (refer to Fig. 2.5). SPPs are non-propagating surface waves because the wavevector is larger than the vacuum wavevector. These surface waves also do not couple to propagating electromagnetic waves in a vacuum [115]. The magnitude of the wavevector of the SPPs excited at a metal-dielectric interface (semi-infinite metallic and dielectric media) is expressed as:

$$|k_{sp}| = k_0 \sqrt{\frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2}} \tag{2.31}$$

where  $\varepsilon_1$  and  $\varepsilon_2$  are the dielectric functions of the metallic and dielectric media (refer to Fig. 2.5).

SPPs in metals are not tunable and have high energy loss [116, 117]. They also get excited in the visible range. Thermal excitation of metal SPPs requires high temperatures, which limits their application in NFRHT [118]. The search for a material with better SPP characteristics has unveiled graphene as a potential candidate.

#### 2.5 Graphene Surface Plasmons

In this section, the dispersion relation of graphene plasmons, which relate the wavevector and the frequency of these modes, is derived.

As mentioned before, the frequency of graphene SPPs, unlike metal SPPs, can be tuned by controlling graphene's charge densities via electrical gating or chemical doping [107, 119, 120, 121]. Graphene SPPs get excited in near-infrared to terahertz regions [121, 122] depending on the chemical potential of graphene which is highly demanded for NFRHT applications.

Here, we consider the structure shown in Fig. 2.6, where two graphene covered dielectric media with permittivity  $\varepsilon_1$  and  $\varepsilon_2$  are separated by a vacuum gap of size D. We derive the dispersion relation for the bottom graphene sheet. The electric and magnetic fields propagate along the z-direction. Graphene supports both TE and TM modes, but TE SPPs in graphene are not appropriately confined, and hence are not of interest for high-confinement applications such as NFRHT [123].

For TM-polarized SPPs with the parallel wavevector of  $k_{\rho}$ , the magnetic field can be written as:

$$H_y = A e^{-\kappa_3 x} e^{ik_\rho z} \qquad x > 0$$
  
$$H_y = B e^{\kappa_1 x} e^{ik_\rho z} \qquad x < 0$$
  
(2.32)



Figure 2.6. The graphene sheet structure which can support SPP modes sandwiched between two surrounding media.

where A and B are undetermined coefficients and  $\kappa_j = \sqrt{k_{\rho}^2 - \varepsilon_j k_0^2}$ . The electric field component in the z direction for 0 < x < D can be found from Maxwell's equations as:

$$E_z = -i \frac{1}{\omega \varepsilon_0 \varepsilon_2} \frac{\partial H_y}{\partial x}$$
(2.33)

The boundary conditions at x = 0 and x = D are:

$$E_{x1}(0) = E_{x2}(0) \quad \text{and} \quad H_{y1}(0) - H_{y2}(0) = \sigma_1 E_{x1}(0) \quad \text{at } z = 0$$
  

$$E_{x2}(d) = E_{x3}(d) \quad \text{and} \quad H_{y2}(d) - H_{y3}(d) = \sigma_2 E_{x2}(d) \quad \text{at } z = d$$
(2.34)

where the numeric subscripts show the region of interest (refer to Fig. 2.6). By solving Eqs. 2.32 and 2.33 and imposing the boundary conditions in Eq. 2.34, the following expressions for the dispersion relation of graphene's SPPs can be obtained.

$$\frac{\varepsilon_2}{\kappa_2} \tanh(\kappa_2 D/2) + \frac{\varepsilon_1}{\kappa_1} + i\frac{\sigma}{\omega\varepsilon_0} = 0$$

$$\frac{\varepsilon_2}{\kappa_2} \coth(\kappa_2 D/2) + \frac{\varepsilon_1}{\kappa_1} + i\frac{\sigma}{\omega\varepsilon_0} = 0$$
(2.35)

## CHAPTER 3 RESEARCH METHOD AND RESULTS

In this chapter, we discuss the implementation of the Kubo and Lindhard models for electrical conductivity of graphene in MATLAB in Section 3.1. In Section 3.2 the Kubo, Lindhard, and the NFRHT codes are verified against data available in literature. Finally, in Section 3.3 a thorough comparison of the radiative conductance between two graphene sheets as obtained using the Kubo and Lindhard models is conducted. Since the the Lindhard model captures the wavevector-dependence of the electrical conductivity of graphene, the effect of the temperature and gap size on the radiative conductance of the problem under consideration is studied using this model. Copies of the developed codes are provided in the appendix.

#### 3.1 Research Method

In this thesis, the Kubo (Eq. 2.22) and Lindhard (Eqs. 2.28 and 2.29) models for electrical conductivity of graphene, the model for near-field radiative conductance between graphene sheets (Eq. 2.21), as well as the dispersion relation of graphene (Eq. 2.35) are implemented in MATLAB. A diagram for the developed code structures is shown in Fig. 3.1 and 3.2.


Figure 3.1. The structure of the codes developed for calculation of NFRHT and near-field radiative conductance.

The radiative conductance (G) and the NFRHT are implemented using the code structure in Fig. 3.1 (refer to Eq. 2.16 and 2.21). Z\_P and Z\_E are the propagating and evanescent exchange functions shown in Eq. 2.18. The calculation of the Fresnel reflection and transmission coefficients requires the calculation of the electrical conductivity of graphene (refer to Eqs. 2.17 and 2.19). Hence the Z\_P and Z\_E functions call the Kubo and Lindhard functions in which graphene's electrical conductivity is implemented. The Kubo formula (Eq. 2.24) has an integral part, and the integral in  $\sigma^{inter}$  is calculated using the I function in the code. On the other hand, the Lindhard formula (refer to Eqs. 2.28 and 2.29) involves H, G, and D functions (refer to Eq. 2.30) that are implemented in functions with the same name (Fig. 3.1).



Figure 3.2. The structure of the codes developed for calculation of the dispersion relation.

The structure of the codes developed for the dispersion relation is a function of the graphene's electrical conductivity, wavevector, gap size, frequency, and the permittivity of the surrounding media (refer to Eq. 2.35). Therefore, the only functions needed for dispersion relation are the Kubo and the Lindhard functions. To solve Eq. 2.35, which is as implicit function, an optimization technique of MATLAB named *fminbnd* is used. *fminbnd* is a one-dimensional minimization technique that minimizes the function in a specified range. The functions are minimized with respect to the parallel component of wavevector.

# 3.2 Verification

In this section, the developed codes for calculating the Kubo and Lindhard formulas for the electrical conductivity of graphene as well as the code developed for NFRHT are verified against the data available in the literature.

## 3.2.1 Kubo Formula

For verification of the developed Kubo code, a graphene sheet was assumed at T = 300K,  $\mu_c = 0.3eV$  and scattering rate  $(\gamma) = 5.62 \times 10^{12} s^{-1}$ . The electrical conductivity of graphene has been computed using the developed MATLAB code for the Kubo formula (refer to appendix A). The result of the MATLAB code for the electrical conductivity using the Kubo formula is compared with the electrical conductivity of graphene reported in Ref. [124] for the same T and  $\mu_c$  in Fig. 3.3. The conductivity is normalized by  $\sigma_0$  (refer to Eq. 2.24). As it is seen from Fig. 3.3, the result of the Kubo code in the present study is in great agreement with the data in Ref. [124].



Figure 3.3. Verification of the Kubo code against the data available in Ref. [68] for  $\mu_c = 0.3$  eV, T = 300 K and  $\gamma = 5.62 \times 10^{12} s^{-1}$ .

#### 3.2.2 Lindhard Formula

For verification of the developed Lindhard code, a free-standing graphene sheet at T = 0 K and  $\omega = 0$  rad/s was considered. Graphene's susceptibility is computed using the developed MATLAB code for the Lindhard formula (refer to appendix A), which can then be converted to electrical conductivity by Eq. 2.26.

The result of the MATLAB code for the susceptibility using the Lindhard formula is compared with the susceptibility of graphene reported in Ref. [61] for the same T and  $\omega$  in Fig. 3.4. The susceptibility is normalized by  $\nu(E_f) = 2E_f/\pi n u_F^2$ , where  $E_f$  is the Fermi energy. The x-axis is normalized using the Fermi wave number,  $(k_F = \sqrt{n\pi})$  with n being the electron density. The electron density is related to the chemical potential (for more information refer to Ref. [61]). Fig. 3.4 shows a great agreement between the data in Ref .[61] and the result obtained using the Lindhard code developed in the present study.

#### 3.2.3 NFRHT

In order to ensure that the exchange functions Z\_E.m and Z\_P.m (refer to Fig. 3.1) and the NFRHT codes are implemented correctly, another verification is necessary. The results obtained using these two functions are compared with the data presented in Messina et al. [65] to ensure the accuracy of these MATLAB functions. The data presented in Messina et al. [65] is concerned with the total near-field heat flux between a zinc sulfide (ZnS) slab, kept at a temperature of 290 K, and a gallium arsenide (GaAs) slab that is kept at a temperature of 310 K (refer to Fig.3.5). A 10 nanometers vacuum gap separates the two slabs. Heat transfer in this system is studied for two cases. In the first case the GaAs slab is not covered with a graphene sheet while in the second case it is covered with a graphene sheet. In the study by Messina et al., the calculated electrical conductivity of graphene is modeled using the Kubo formulation.

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Figure 3.4. Verification of the Lindhard code against the data presented in Ref. [70] for T = 0 K and  $\omega = 0$  rad/s.

To determine the frequency range in which thermal radiation is non-negligible, first the total heat flux is computed in the frequency range of  $1.88 \times 10^{12} rad/s$  to  $1.88 \times 10^{17}$  rad/s. Then we reduced the upper limit to  $1.88 \times 10^{16}$  rad/s and increased the lower limit to  $1.88 \times 10^{14}$  rad/s until no change in the radiative heat flux was observed. The total (spectrally integrated) heat transfer is integrated numerically over the frequency. To ensure the convergence of the numerical integral, the number of frequencies used for discretizing a given frequency range was increased until no change in the total heat flux is observed. The convergence analysis data are summarized in Table 3.1.



Figure 3.5. Near-field radiative heat transfer between a GaAs slab at 310 K and a ZnS slab at 290 K. The GaAs slab is covered with a graphene sheet

Table 3.1. Frequency range and frequency count dependency analysis on near-field heat flux between graphene covered GaAs at T = 310K and ZnS at T = 290K.

$\omega_{max}  [rad/s]$	$\omega_{min} \; [rad/s]$	Frequency count	$q_{total}''[W/m^2]$
$1.88 \times 10^{16}$	$1.88 \times 10^{15}$	500	$3.95 \times 10^{3}$
$1.88 \times 10^{16}$	$1.88 \times 10^{15}$	1000	$3.95 \times 10^3$
$1.88 \times 10^{16}$	$1.88 \times 10^{15}$	2000	$3.95 \times 10^3$
$1.88 \times 10^{16}$	$1.88 \times 10^{14}$	500	$4.39 \times 10^3$
$1.88 \times 10^{16}$	$1.88 \times 10^{14}$	1000	$4.27 \times 10^3$
$1.88 \times 10^{16}$	$1.88 \times 10^{14}$	4000	$4.24 \times 10^3$
$1.88 \times 10^{16}$	$1.88 \times 10^{14}$	10000	$4.24 \times 10^3$
$1.88 \times 10^{16}$	$1.88 \times 10^{13}$	1000	$4.56 \times 10^3$
$1.88 \times 10^{16}$	$1.88 \times 10^{13}$	10000	$4.27 \times 10^3$
$1.88 \times 10^{16}$	$1.88 \times 10^{13}$	20000	$4.25 \times 10^3$
$1.88 \times 10^{17}$	$1.88 \times 10^{12}$	1000	$6.25 \times 10^2$
$1.88 \times 10^{17}$	$1.88 \times 10^{12}$	10000	$6.09 \times 10^{3}$
$1.88 \times 10^{17}$	$1.88 \times 10^{12}$	100000	$4.27 \times 10^3$

It is seen from Table 3.1 that radiative heat transfer between the slabs is only non-negligible in the frequency range of  $1.88 \times 10^{14} rad/s$  to  $1.88 \times 10^{16} rad/s$ . Additionally, Table 3.1 shows that dividing the frequency range into 4000 sub-intervals is sufficient. The total heat transfer versus the chemical potential is presented in Messina et al. [65] is shown in Fig. 3.6.

As it is seen from Fig. 3.6, the results obtained using the implemented codes match the ones presented in Messina et al. [65]. Therefore, developed codes are verified. Now the focus shall be shifted toward presenting the results.



Figure 3.6. Total radiative heat flux between graphene covered GaAs-ZnS and bare GaAs-ZnS separated by a 10 nm vacuum gap, as a function of chemical potential using Kubo formula separated.

# 3.3 Results

In this section, the electrical conductivity of graphene is calculated using both the Kubo and Lindhard formulas, and the Kubo and Lindhard electrical conductivities are compared. Then the radiative conductance obtained by these models are compared for various conditions and finally, the effect of gap size and temperature on radiative conductance is discussed.

#### 3.3.1 Comparison of Kubo and Lindhard methods: Electrical Conductivity

The conductivity of graphene is calculated using the Kubo (Eq. 2.24) and Lindhard (Eqs. 2.28 and 2.29) formulas. In order to compare the two methods, the conductivity of a single graphene sheet at T = 300 K is calculated using both methods in the frequency range of  $5 \times 10^{11}$  rad/s to  $5 \times 10^{14}$  rad/s. The frequency and wavevector dependant colorplots of graphene's conductivity at  $\mu_c = 0.1$  eV and 0.3 eV are shown in Fig. 3.7 and 3.8, respectively. In Fig. 3.7 and 3.8, panels (a) and (c) are calculated using the Lindhard formula, while panels (b) and (d) are found by using the Kubo formula. Panels (a) and (b) show the imaginary part of the electrical conductivity of graphene, while panels (c) and (d) show the real part of it.

Figures 3.7 and 3.8 show that graphene's conductivity obtained using the Lindhard formula is a function of wavevector  $(k_{\rho})$ , while the Kubo electrical conductivity doesn't depend on the wavevector. As the wavevector increases, the imaginary part of Lindhard electrical conductivity at higher frequencies increases. However, this variation is not captured by the Kubo formula. Similar trend is observed from the comparison of the imaginary part of graphene's Kubo and Lindhard conductivities at T = 300 K and  $\mu_c = 0.3$ eV (refer to Fig. 3.8.a and 3.8.b).



Figure 3.7. Graphene's electrical conductivity at  $\mu_c = 0.1$  eV in frequency range  $5 \times 10^{11}$  rad/s to  $5 \times 10^{14}$  rad/s at T = 300 K. Panels (c), (a), (d) and (b) show the real and imaginary parts of the Kubo electrical conductivity and the real and imaginary parts of the Lindhard electrical conductivity, respectively.

Comparison of the real part of the Kubo and Lindhard electrical conductivity at T = 300 K and  $\mu_c = 0.1$  eV (refer to Fig. 3.7.c and 3.7.d) presented in Figs. 3.7.c and 3.7.d also show that graphene's conductivity by the Lindhard formula is a function of wavevector whereas the Kubo one is not. Another observation from these figures is that graphene's electrical conductivity calculated using the Kubo formula at small frequencies  $(\omega < 6 \times 10^{13} \text{ rad/s})$  is almost 6 folds that calculated by the Lindhard formula. Similar observation are made from Fig. 3.8.c and 3.8.d for  $\mu_c = 0.3$  eV at T = 300 K, where at  $\omega < 4 \times 10^{13} \text{ rad/s}$  there is almost an order of magnitude difference in the electrical conductivity calculated using the Kubo and Lindhard formulas. Both methods agree at zero to small wavevectors for  $\omega < 6 \times 10^{13} \text{ rad/s}$ .



Figure 3.8. Graphene's electrical conductivity at  $\mu_c = 0.3$  eV in frequency range  $5 \times 10^{11}$  rad/s to  $5 \times 10^{14}$  rad/s at T = 300 K. Panels (c), (a), (d) and (b) show the real and imaginary parts of the Kubo electrical conductivity and the real and imaginary parts of the Lindhard electrical conductivity, respectively.

## 3.3.2 Comparison of Kubo and Lindhard methods: Radiative conductance

In this section, the radiative conductance (refer to Eq. 2.21) between two free-standing graphene sheets at T = 300 K separated by a vacuum gap of size D = 50 nm is calculated using both the Kubo and Lindhard formulas. The schematic of the problem is shown in Fig. 3.9. The radiative conductance per unit frequency and wavevector is plotted versus  $\omega$  and  $k_{\rho}/k_0$  in Fig. 3.10 for various chemical potential values ( $\mu_c$ ). The spatial dispersion of graphene plasmons are also shown in this figure as well. In Fig. 3.10, panels (a), (b), (c) and (d) are found using the Lindhard function while panels (e), (f), (g) and (h) are found using the Kubo formula. Fig. 3.10.a and e are for  $\mu_c = 0.05$  eV, Fig. 3.10.b and f are for  $\mu_c = 0.1$  eV, Fig. 3.10.c and g are for  $\mu_c = 0.3$  eV and Fig. 3.10.d and h are for  $\mu_c = 0.5$  eV.



Figure 3.9. Schematic of the problem under study. Two graphene sheets at T = 300 K are separated by a 50 nm vacuum gap.



Figure 3.10. Radiative conductance versus  $\omega$  and  $k_{\rho}/k_0$  at T = 300 K and D = 50 nm. Panels a ( $\mu_c = 0.05$  eV), b (0.1 eV), c (0.3 eV) and d (0.5 eV) are calculated using Lindhard formula while panels e ( $\mu_c = 0.05$  eV), f (0.1 eV), g (0.3 )eV and h (0.5 eV) are found using the Kubo formula.

It can be seen from Fig. 3.10 that there is non-negligible differences between the radiative conductance and dispersion relation as obtained using the Kubo and Lindhard electrical conductivities. The difference between the Kubo and Lindhard radiative Conductance is particularly significant around the dispersion relation of graphene's surface plasmons.

The difference between radiative conductance obtained using the Lindhard formula and the one found using the Kubo formula is smaller at smaller values of chemical potential. As the chemical potential increases, the bright bands (corresponds to higher radiative conductance) obtained using the Lindhard formula fade. At the same time, the Kubo formula still exhibits sharp detectable bright bands at  $\mu_c = 0.3$  eV and 0.5 eV. The quantity of interest in NFRHT is the spectral radiative conductance that is found by integrating the radiative conductance over  $k_{\rho}$ . The spectral radiative conductance between two graphene sheets at T = 300 K separated by a gap of size D = 50 nm is plotted in Fig. 3.11. Figure 3.11.a is obtained by using the Kubo formula, and Fig. 3.11.b is obtained by using the Lindhard formula. It can be seen that as the chemical potential increases, the peak frequency, which corresponds to thermal excitation of graphene's SPPs shifts toward higher frequencies.



Figure 3.11. Spectral radiative conductance between two graphene sheets at T = 300 K separated by a gap of D = 50 nm for different chemical potentials calculated using (a) Kubo formula and (b) Lindhard formula.

The spectral radiative conductance ontained using the Kubo and Lindhard formula are compared in Fig. 3.12 for T = 300 K, D = 50 nm and at different chemical potentials. Fig. 3.12.a is for  $\mu_c = 0.05$  eV, Fig. 3.12.b is for  $\mu_c = 0.1$  eV, Fig. 3.12.c is for  $\mu_c = 0.3$  eV and Fig. 3.12.d is for  $\mu_c = 0.5$  eV.



Figure 3.12. Spectral radiative conductance between two graphene sheets at T = 300 K separated by a gap size of D = 50 nm for different chemical potentials of (a)  $\mu_c = 0.05$ , (b) 0.1, (c) 0.3 and (d) 0.5 eV.

It can be seen from Fig. 3.12 that the peak of radiative conductance experiences a blueshift as the chemical potential of the graphene increases. The radiative conductance calculated using the Kubo and Lindhard methods shows great agreement at  $\mu_c = 0.05$  eV and 0.1 eV for high frequencies (for  $\mu_c = 0.05$  eV the agreement region is  $\omega > 10^{14}$  rad/s and it is  $\omega > 1.5 \times 10^{14}$  rad/s for  $\mu_c = 0.1$  eV). Another observation is that at chemical potentials of 0.3 eV and 0.5 eV, the Kubo formula estimates a broadband radiative conductance while there is a well-defined plasmon resonance in the conductance curve using the Lindhard formula. It is also seen that at large values of graphene's chemical potential, the Kubo formula overestimates the radiative conductance. This shows that the non-local effects of electrical conductivity cannot be ignored for large values of chemical potential.

A quantitative comparison between the total radiative heat flux using the Kubo and Lindhard formulas for two graphene sheets at  $T_1 = 300$  K and  $T_2 = 290$  K, separated by a 50 nm vacuum gap, is provided in Fig. 3.13.



Figure 3.13. Total radiative heat flux between graphene sheets at  $T_1 = 300$  K and  $T_2 = 290$  K separated by a vacuum gap of D = 50 nm as a function of chemical potential.

The total heat flux presented in Fig. 3.13 shows the effects of chemical potential on the agreement of Kubo formula and Lindhard formulas. It can be seen that both methods agree for chemical potentials less than 0.05 eV. For  $\mu_c = 0.1$  eV, there is a 25% difference, and the difference grows to an order of magnitude for  $\mu_c = 0.5$  eV. Fig. 3.13 shows that at large chemical potentials, the Kubo formula overestimates NFRHT significantly.



Figure 3.14. Peak frequency of radiative conductance between two graphene sheets at T = 300 K, separated by a gap of D = 50 nm versus  $\mu_c$ .

The effect of changing chemical potential of graphene sheets on peak frequency of radiative conductance in the problem shown in Fig. 3.9 is studied in Fig. 3.14. Fig. 3.14 shows that at chemical potential smaller than 0.15 eV, the difference is less than 15%. This difference increases by increasing the chemical potential up to  $\mu_c = 0.42$  eV, where the difference is two orders of magnitude. Fig. 3.14 shows a reduction in the difference of the peak frequency of radiative conductance found using the Kubo and Lindhard formulas above  $\mu_c = 0.42$  eV. It can be concluded that the Kubo formula can be used for predicting the peak frequency for chemical potentials up to  $\mu_c = 0.15$  eV under the studied conditions, and the Kubo results above  $\mu_c = 0.15$  eV deviate too much from the Lindhard ones.

# 3.3.3 Effect of temperature and gap size on radiative conductance and peak frequency

In this subsection, the effect of temperature and gap size on radiative conductance and the peak or resonant frequency of the radiative conductance are studied. First the effect of gap size on the radiative conductance is studied for  $\mu_c = 0.2$  eV and T = 300 K. Figure 3.15.a shows the radiative conductance for the Kubo formula while Fig. 3.15.b shows the same for the Lindhard formula. It can be seen that both methods predict that by increasing the gap size, the spectral radiative conductance decreases and the peak frequency of the spectral radiative conductance shifts toward smaller frequencies.



Figure 3.15. Spectral radiative conductance between two graphene sheets at T = 300 K and  $\mu_c = 0.2$  eV at different gap sizes as calculated using (a) the Kubo formula and (b) the Lindhard formula.

In order to understand the effect of gap size on the agreement of the Kubo and Lindhard formulas for predicting the resonant frequency of radiative conductance, the resonant frequency of radiative conductance versus gap size is plotted in Fig. 3.16. It is shown in Fig. 3.16 that at  $D < 10^{-8}$  m, the resonant frequency obtained using both Kubo and Lindhard are very close (less than 3% difference), and by increasing the gap size, the resonant frequency estimated by Kubo and Lindhard formulas diverge to a point that at  $D = 10^{-6}$  m and  $D = 4.6 \times 10^{-7}$  m, the relative difference is about 49% and 42%, respectively. Hence increasing the gap size deteriorates Kubo formula's ability to predict the resonant frequency correctly. Another observation from Fig. 3.16 is that by increasing the gap size, both methods predict that the resonant frequency shifts to lower frequencies.



Figure 3.16. Resonant frequency of the radiative conductance of two graphene sheets at T = 300 K and  $\mu_c = 0.2$  eV versus gap size, D.

Total radiative conductance between graphene sheets at T = 300 K and  $\mu_c = 0.2$  eV is plotted versus gap size, D, in Fig. 3.17. Figure 3.17 shows that there is a 90% difference in the total radiative conductance calculated using the Kubo and Lindhard formulas at gap sizes  $(D > 10^{-7} \text{ m})$ , and this difference reduces to 60% as the gap size reduces to  $D = 10^{-8}$ m and about 30% for  $D = 10^{-9}$ . This shows that the overestimation of total radiative conductance using the Kubo formula increases as the gap size increase.



Figure 3.17. Total radiative conductance between two graphene sheets at T = 300 K and  $\mu_c = 0.2$  eV versus gap size, D.

The effect of temperature on radiative conductance between two graphene sheets with  $\mu_c = 0.2$  eV that are placed 50 nm apart is studied using the Kubo formula in Fig. 3.18.a and the Lindhard formula in Fig. 3.18.b. It can be seen that increasing the temperature from 100 K to 1000 K shifts the resonant frequency of radiative conductance to lower frequencies and increases the radiative conductance significantly.



Figure 3.18. Spectral radiative conductance between two graphene sheets at D = 50 nm and  $\mu_c = 0.2$  eV at different temperatures as calculated (a) using the Kubo formula and (b) Lindhard formula.

The resonant frequency of the radiative conductance versus temperature is plotted in Fig. 3.19. It can be seen that the resonant frequency obtained using the Kubo formula is  $4.1 \times 10^{13}$  rad/s for T = 100 K, and it increases to  $2.43 \times 10^{14}$  rad/s for T = 380 K. As the temperature increases further, the resonant frequency slightly decrease, such that it is equal to  $2.22 \times 10^{14}$  rad/s at T = 1000 K. On the other hand, the Lindhard formula predicts a decrease in the resonant frequency as temperature increases from 100 K to 1000 K.



Figure 3.19. Resonant frequency of radiative conductance of two graphene sheets at  $\mu_c = 0.2$ eV separated by a vacuum gap of size D = 50 nm versus temperature, T.

The total radiative conductance between graphene sheets versus the temperature is plotted in Fig. 3.20. Figure 3.20 shows that when T < 200 K, there is two orders of magnitude difference between the results obtained using the Kubo and Lindhard formulas. This difference reduces to almost 20% when 600 K < T < 800 K and finally reaches 6% at T = 1000 K. Hence, Fig. 3.20 shows that as the temperature of graphene sheets grows, the result of the Kubo and Lindhard formulas converge. Figure 3.20 and 3.19 show that the Kubo formula does not provide a suitable representation for graphene sheets in NFRHT applications at temperatures less than 400 K.



Figure 3.20. Total radiative conductance between two graphene sheets at  $\mu_c = 0.2$  eV separated by a vacuum gap of size D = 50 nm versus temperature, T.

The results presented in this chapter shows that graphene is a non-local material whose properties can be tuned significantly by changing its chemical potential. The Kubo formula, which is a local model for graphene's electrical conductivity, cannot capture the non-local behavior of graphene at low temperatures and high chemical potentials, and applying the Kubo formula under these conditions causes significant errors. To avoid this error, the Lindhard formula should be used for modeling graphene's electrical conductivity in NFRHT calculations.

#### CHAPTER 4

## CONCLUSIONS, FUTURE WORK AND RECOMMENDATIONS

#### 4.1 Conclusions

This thesis investigates the non-locality of graphene's electrical conductivity and the non-local effects of electrical conductivity on near-field radiative heat transfer (NFRHT). In NFRHT studies found in literature, graphene electrical conductivity has been modeled using a local model (Kubo formula). To study the effect of non-local electrical conductivity of graphene on NFRHT, the near-field radiative conductance between two suspended graphene sheets separated by a vacuum gap has been modeled using the Kubo formula and a non-local model, namely, the Lindhard formula. For this system of two graphene sheets, the electrical conductivity of graphene for various wavevectors and frequencies, the wavevector dependent spectral radiative conductance, spectral and total radiative conductance, resonant frequency as well as dispersion relation have been studied. The effect of temperature and gap size on applicability of the local model of graphene's electrical conductivity has also been studied.

Comparing the spectral radiative conductance (Fig. 3.11 and 3.12) and total heat flux versus chemical potential (Fig. 3.13) as obtained using the Kubo and Lindhard formulas showed that as the chemical potential ( $\mu_c$ ) of graphene increases, the disagreement of the two models increases. It was shown that for  $\mu_c < 0.1$  eV, there is less than 25% difference in the total heat flux of the two models. the difference grows to an order of magnitude as chemical potential increases to  $\mu_c = 0.5$  eV. The same observation was made for the resonant frequency versus chemical potential (Fig. 3.14), where it was found that at  $\mu_c < 0.15$  eV, the resonant frequency predicted by the local and non-local models is only 15% and the difference increases significantly by increasing the chemical potential of the graphene sheets. These findings show that the non-local effects of graphene's electrical conductivity play a significant role when  $\mu_c > 0.1$  eV, and hence using the Kubo formula can result in non-negligible errors.

The difference between the resonant frequency and the total radiative conductance of the two graphene sheets was also been studied for various gap sizes (Fig. 3.16 and refgtotgap). It was seen that as the gap size grows, the Kubo formula fails more to predict a resonant frequency of radiative conductance which is reasonably close to the one obtained by using the Lindhard formula. For example, at  $D < 10^{-8}$  m, the difference is only 3%. However, the difference increases to 49% at  $D = 10^{-6}$  m. It was also shown that decreasing the gap size from  $10^{-7}$  m to  $10^{-9}$  m, at  $\mu_c = 0.2$  eV and T = 300 K, reduces the difference of the total radiative conductance obtained using the two methods. The difference between the two models is 60% at  $D = 10^{-8}$ . Therefore, the Kubo formula is invalid at large separation gaps.

Comparison of resonant frequency (Fig. 3.19) and the total radiative conductance (Fig. 3.20) for various temperatures showed that as the temperature increases, the difference between the two models decreases. It was seen that when T > 400 K, the resonant frequency obtained using both models are less than 7% apart. The difference between the total radiative conductance for T < 200 K is about two orders of magnitude different, and this difference reduces to 20% for T > 600 K. Therefore, the Kubo model cannot fully capture the non-local behavior of graphene's electrical conductivity at low temperatures and hence the Kubo formula is not suggested for NFRHT applications in this temperature range.

Based on the fact that the Kubo formula is not applicable at large values of chemical potential and separations gaps as well as at low temperatures, it is recommended that the non-local behavior of graphene's electrical conductivity be considered in NFRHT application. The Lindhard formula can capture the non-local effects on the electrical

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conductivity of graphene. It should be mentioned that the computational cost of the Lindhard formula is only slightly higher than the Kubo formula.

## 4.2 Future Work and Recommendations

Graphene is a very promising material for NFRHT applications as if support tunable surface plasmon polaritons in the infrared. In this thesis we showed that the effect of non-local electrical conductivity on graphene's NFRHT is non-negligible and should be taken into account. Some recommendations for future work are presented hereafter.

1. Experimentally demonstrate that non-local effects affect NFRHT in graphene-based materials. Total heat transfer can be measured and compared with the theoretical predictions using the Kubo and Lindhard formulas.

2. It is shown that if graphene substrate supports surface phonon polaritons (such as  $SiO_2$  and SiC), the graphene SPPs can be coupled to the SPhPs of the substrate. This coupling can result in enhancement and tunability of NFRHT. It is recommended to study if such coupling, enhancement and tuning are observed when non-local effects of the electrical conductivity are considered.

3. Graphene has been proposed as a base material for designing metamaterials such as hyperbolic metamaterials and magneto-dielectric metamaterials. It is recommended to study how the non-local electrical conductivity of graphene can affect thermal radiation of the proposed metamaterial.

5. It is recommended that the effect of non-local electrical conductivity on NFRHT in other two-dimensional materials, such as black phosphorene, that have been proposed for near-field applications be analyzed.

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## APPENDIX A

# MATLAB CODES

# A.1 MATLAB code for NFRHT

```
1 clear all
  clc
2
3
  global eps1 eps2 eps3 w D iw T1 T3 muc Sigma1 Sigma3
4
\mathbf{5}
6 %Constants
_{7} hbar = 1.05457173e-34;
 {}_{8} {\rm Kb} = 1.3806488 {\rm e}{-23}; 
  ev = 1.60217646e - 19;
9
10
11
  %Problem geometry
12
13
_{14} D = 10e-9; % equal to dc which is the gap between media 1 and 3
  T1 = 300;
15
  T3 = 290;
16
  muc = 0.5 * ev; %chemical potential of graphene in eV
17
^{18}
  ww = linspace(5e11, 5e14, 200);
19
  Nw = length(ww);
20
^{21}
_{22} QP = 0;
_{23} QE = 0;
```
```
_{24} Q(1:Nw) = 0;
25
26
  for iw = 1:Nw
27
       iw
^{28}
       w = ww(iw);
29
30
       Sigma1 = Kubo(muc, T1);
31
       Sigma3 = Kubo(muc, T3);
32
33
       eps1 = 1.0;
34
       eps2 = 1.0;
35
       eps3 = 1.0;
36
37
       %Theta
38
       theta1 = hbar*w/(exp((hbar*w)/(Kb*T1))-1);
39
       theta 3 = hbar * w/(exp((hbar * w)/(Kb*T3))-1);
40
       theta = theta1-theta3;
^{41}
42
       %Wavevectors
43
       k2 = w/2.998e8; \%kv
44
45
       %Integraton of the propagating waves
46
       Integ = quadgk (@Z_P_v2, 0, k2 - 1e - 6);
47
       QP = theta/(4*pi^2)*Integ;
48
49
       % defining a waypoint
50
```

```
cc = logspace(8, 15, 10);
51
       co = cc.*k2;
52
53
       %Integraton of the evaneent waves
54
       Integ = quadgk (@Z_E_v2, k2+1e-4, inf, 'waypoint', co, 'RelTol', 1e-6);
55
       QE = theta/(4*pi^2)*Integ;
56
57
       Q(iw) = QP + QE;
58
  end
59
60
  Q_total = trapz(ww,Q);
61
```

## A.2 MATLAB code for radiative conductance

```
1 clear all
  clc
2
3
  global eps1 eps2 eps3 w D iw T muc Sigma
4
\mathbf{5}
6 %Constants
_{7} hbar = 1.05457173e-34;
  Kb = 1.3806488e - 23;
8
  ev = 1.60217646e - 19;
9
10
11
  %Problem geometry
12
13
_{14} D = 50e-9; % equal to dc which is the gap between media 1 and 3
```

```
15
  T = 800;
16
  muc = 0.2 * ev;
17
  ww = linspace(5e11, 5e14, 200);
18
19
  Nw = length(ww);
20
  eps1 = 1.0;
^{21}
  eps2 = 1.0;
22
  eps3 = eps1;
^{23}
24
  QP = 0;
25
  QE = 0;
26
27
^{28}
   for iw = 1:Nw
29
        iw
30
^{31}
       w = ww(iw);
32
33
        Sigma = Kubo(muc,T);
34
35
       %Differentiation of Theta
36
        theta = hbar *w/(exp((hbar *w)/(Kb*T))-1);
37
        theta = theta.^2.*\exp(hbar*w./Kb./T)./(Kb*T^2);
38
39
       %Wavevectors
40
       {
m k2}~=~{
m w}/2.998\,{
m e8}\,;~~\%{
m kv}
41
```

```
42
      %Integraton of the propagating waves
43
       Integ = quadgk (@Z_P_v2, 0, k2-1e-6);
44
      QP = theta/(4*pi^2)*Integ;
45
46
      %Defining a waypoint
47
       cc = logspace(1, 10, 10);
48
       co = cc.*k2;
49
50
      %Integraton of the evaneent waves
51
       Integ = quadgk (@Z_E_v2, k2+1e-4, inf, 'waypoint', co, 'RelTol', 1e-6);
52
      QE = theta/(4*pi^2)*Integ;
53
54
      Q(iw) = QP + QE;
55
56
  end
57
        MATLAB code for Dispersion Relation
  A.3
```

```
1 clear all
2 clc
3
4 global w D iw T1 muc k0 eps1 eps3 S3
5
6 %Constants
7 hbar = 1.05457173e-34;
8 Kb = 1.3806488e-23;
9 ev = 1.60217646e-19;
```

```
% Vacuum permittivity
  e0 = 8.8542 e - 12;
10
  eps1 = 1;
11
  eps3 = 1;
12
13
  %Problem geometry
14
15
  D = 50e-9; % equal to dc which is the gap between media 1 and 3
16
  T1 = 300;
               %temperatue
17
  c0 = 299792458; %Speed of light in vacuum (m/s)
18
  muc = 0.0 * ev; %chemical potential of graphene in eV
19
  nuf =c0/300;
                    %Fermi velocity
20
21
  ww = linspace(5e11, 5e14, 20);
22
  Nw = length(ww);
23
^{24}
  for iw = 1:Nw
25
       iw
26
      w = ww(iw);
27
       k0 = w/2.998e8; \%kv
^{28}
       k00(iw) = k0;
29
30
       S3 = Kubo(muc, T1);
^{31}
32
      %first solution
33
       f1 = @(x) func(x);
34
      %second solution
35
       f2 = @(x) func2(x);
36
```

```
% Solution from the general formula
37
       f = @(x) func3(x);
38
39
       x1 = fminbnd(f1, 0, 400 * k0);
40
       x2 = fminbnd(f2, 0, 400 * k0);
^{41}
       x3 = fminbnd(f, 0, 400 * k0);
42
43
       answer1(iw) = x1/k0;
44
       answer2(iw) = x2/k0;
45
       answer3(iw) = x3/k0;
46
  end
47
```

## A.4 MATLAB code for propagating exchange function

```
function [ZP] = Z_P_v2(krho)
1
  global w D T muc Sigma1
2
3
                                   % Vacuum permittivity
  e0 = 8.8542e - 12;
4
  m0 = 1.25663706143592D-06; \% Vacuum permeability
\mathbf{5}
6
  Sigma1 = RPA(muc, krho, T);
\overline{7}
8
  %Wavevectors
9
       k2 = w/2.998e8;
10
11
  %Calculating kzs
12
       kz2 = sqrt(k2^2-krho.^2);
13
14
```

```
15 %Fresnel reflection coefficients
```

```
_{16} % In TE polarization
```

```
{}_{17} \ \ r21TE \ = \ -(2*kz2\,.\,/\,(\,Sigma1\,.*m0\,.*w)\,{+}1)\,.\,\hat{}\,(\,{-}1)\,;
```

```
{}_{18} \ \ {\rm t21TE} \ = \ (1{+}{\rm m0.*w.*Sigma1./2./kz2})\,.\,\hat{}\,(-1)\,;
```

```
19
```

```
_{\rm 20} % IN TM polarization
```

```
<sup>21</sup> r21TM = (2*e0*w./(Sigma1.*kz2)+1).^{(-1)};
```

```
{}_{^{22}} \ t21TM \ = \ (1 + Sigma1. * kz2. / w. / 2. / e0) . \ (-1);
```

23

```
_{24} %Exchange factors
```

```
\begin{array}{ll} {}_{25} & {\rm ZP\_TE} = \ \left(1 - {\rm abs} \left( {\rm r21TE} \right).^2 - {\rm abs} \left( {\rm t21TE} \right).^2 2 \right).^2 2. / \\ {}_{26} & \left( {\rm abs} \left(1 - {\rm r21TE}.^2 .* \exp \left( 2\,{\rm i}.*\,{\rm kz2}*{\rm D} \right) \right).^2 2 \right); \\ {}_{27} & {\rm ZP\_TM} = \ \left(1 - {\rm abs} \left( {\rm r21TM} \right).^2 - {\rm abs} \left( {\rm t21TM} \right).^2 2 \right).^2 2. / \\ {}_{28} & \left( {\rm abs} \left( 1 - {\rm r21TM}.^2 2.* \exp \left( 2\,{\rm i}.*\,{\rm kz2}*{\rm D} \right) \right).^2 2 \right); \\ {}_{29} & {\rm ZP} = \left( {\rm ZP\_TE+ZP\_TM} \right).*\,{\rm krho}; \end{array}
```

30

31 end

# A.5 MATLAB code for evanescent exchange function

```
1 function [ ZE ] = Z_E_v2( krho )
2 global w D T muc Sigma1
3
4 e0 = 8.8542e-12; % Vacuum permittivity
5 m0 = 1.25663706143592D-06; % Vacuum permeability
6
7 Sigma1 = RPA( muc, krho, T );
8
```

```
%Wavevectors
9
       k2 = w/2.998e8;
10
  %Calculating kzs
11
       kz2 = sqrt(k2.^2-krho.^2);
12
13
14
  %Fresnel reflection coefficients
15
  \% In TE polarization
16
  r21TE = -(2*kz2./(Sigma1.*m0.*w)+1).^(-1);
17
18
  % IN TM polarization
19
  r21TM = (2*e0*w./(Sigma1.*kz2)+1).^{(-1)};
20
21
  %Exchange factors
22
  ZE TE = 4.*imag(r21TE).^{2}.*exp(-2.*imag(kz2)*D)./
23
                     (abs(1-r21TE.^{2}.*exp(-2.*imag(kz2)*D)).^{2});
^{24}
  ZE_TM = 4.*imag(r21TM).^2.*exp(-2.*imag(kz2)*D)./
^{25}
                     (abs(1-r21TM.^{2}.*exp(-2.*imag(kz2)*D)).^{2});
26
  ZE = (ZE_TE + ZE_TM) . * krho;
27
  end
^{28}
```

# A.6 MATLAB code for RPA

```
1 function [ Sigma_RPA ] = RPA( muc, krho,T )
2
3 global w
4
5 % constant
```

```
_{6} hbar = 1.054571817e-34;
                                % Planck's constant in J.s
_{7} KB = 1.380649e-23;
                                 \% Boltzmann constant (J/K)
 c0 = 299792458; 
                                 \% Speed of light in vacuum (m/s)
  e charge = 1.602176634e - 19; % electron charge (C)
9
10
                                 %Fermi velocity (m/s) from "An Introduction
  nuf = c0/300;
11
                                 %to graphene plasmonics", Page 32
12
  alpha = [1, -1];
                                 % Alpha
13
14
       [Chi\_re, Chi\_im] = deal(0,0);
15
16
  for i = 1: length (alpha)
17
18
       C1 = heaviside (hbar.*nuf.*krho-hbar.*w).*krho.^2./
19
                                      (2*hbar*sqrt((nuf.*krho).^2-(w).^2));
20
       C2 = heaviside(hbar.*w-hbar.*nuf.*krho).*krho.^2./
^{21}
                                      (2*hbar*sqrt((w).^2-(nuf.*krho).^2));
22
       if (T = 0)
23
           if (alpha(i) = 1)
^{24}
                C3 = -2.*alpha(2).*muc./(hbar.*nuf).^2;
25
           else
26
                C3 = 0;
27
           end
^{28}
       else
29
           C3 = -2.*KB.*T.*log(1+exp(alpha(i).*muc./KB./T))
30
                                      ./(hbar.*nuf).^{2};
31
32
       end
```

33 delta = (abs(alpha(i))-alpha(i))./2;3435GP func = @(x) G(alpha(i), krho, x, 1, w, T, muc, nuf); 36  $GM_func = @(x) G(alpha(i), krho, x, -1, w, T, muc, nuf);$ 37HP func = @(x) D(alpha(i), krho, x, 1, w, T, muc, nuf);38  $HM_func = @(x) D(alpha(i), krho, x, -1, w, T, muc, nuf);$ 39 40Chi im = Chi im +(C1.\*(integral(GP func, 1, inf, 'ArrayValued', true))41 -integral (GM\_func, 1, inf, 'ArrayValued', true)) 42+C2.\*(-pi./2.\*delta +integral(HP\_func, -1, 1, 'ArrayValued', true))) 4344Chi\_re = Chi\_re + (C2.\*(integral(GM\_func,1,inf,'ArrayValued', true) 45-integral(GP func, 1, inf, 'ArrayValued', true)) 46+C1.\*(-pi./2.\*delta +integral(HM\_func, -1, 1, 'ArrayValued', true))) 47 $Chi_re = Chi_re + (C3./pi);$  $^{48}$ end 49Sigma RPA =  $1i * e charge^{2*w*}$ 50 $(Chi_re + 1i.*Chi_i)./krho.^2;$ 51end 52A.7MATLAB code for functions used in RPA

1 function [ f ] = H(alpha,x,krho,fsign,w,T,muc)
2
3 hbar = 1.054571817e-34; % plancks contant in J.s
4 KB = 1.380649e-23; % Boltzmann constant (J/K)
5 nuf = 1e6; % fermi velocity (m/s)

```
_{7} f = sqrt (1 - x.^{2})./(exp((hbar*abs(nuf.*krho.*x+fsign.*w)
                                    -2.* alpha .* muc) ./2./ KB./T) +1);
8
9 end
<sup>1</sup> function [ f ] = G(alpha, krho, x, fsign, w, T, muc, nuf)
\mathbf{2}
                               % plancks contant in J.s
 hbar = 1.054571817e - 34;
3
                                    % Boltzmann constant (J/K)
_{4} KB = 1.380649e-23;
\mathbf{5}
_{6} f = sqrt (x. 2 -1)./(exp((abs(hbar.*nuf.*krho.*x+fsign.*hbar.*w)
                                         -2.*alpha.*muc)./(2*KB*T))+1);
\overline{7}
 end
8
 function [f] = D(alpha, krho, x, fsign, w, T, muc, nuf)
1
\mathbf{2}
  hbar = 1.054571817e-34; % plancks contant in J.s
3
                              % Boltzmann constant (J/K)
_{4} KB = 1.380649e-23;
\mathbf{5}
_{6} f = sqrt (1 - x.^{2})./(exp((abs(hbar.*nuf.*krho.*x+fsign.*hbar.*w))))
                                         -2.* alpha .* muc) ./(2*KB*T))+1);
\overline{7}
<sup>8</sup> end
  A.8
        MATLAB code for Kubo
```

```
1 function [ Sigma_Kubo ] = Kubo( EF,T )
2
3 global w
4
```

6

5 % constant  $_{6}$  hbar = 1.054571817e-34; % plancks contant in J.s  $_{7}$  KB = 1.380649e-23; % Boltzmann constant J/K eV = 1.60218e - 19;% eV to J, and electron charge in C % Add reference tau = 1e - 13;9 10gamma = 1/tau; % 3.7 e - 3 \* eV/hbar;11sigma  $0 = eV^2/(4*hbar);$ 1213intra = 4/(pi\*(hbar\*gamma-1i\*hbar\*w))\*14  $(EF+2*KB*T*\log(1+\exp(-EF/(KB*T))));$ 15func = @(x) (G2(x,T,EF)-G2(hbar.\*w./2,T,EF))./ 16  $((hbar.*w).^2 - 4.*x.^2);$ 17 inter1 = G2(hbar.\*w./2,T,EF); 18 integ = integral (func , 0, Inf , 'RelTol', 1e-6, 'ArrayValued', true); 19 inter 2 = 4i.\*hbar.\*w./pi.\*integ; $^{20}$ inter = inter1 + inter2; $^{21}$ 22 Sigma Kubo = sigma 0\*(intra + inter); $^{23}$ end  $^{24}$ 

## A.9 MATLAB code for function used in Kubo

```
1 function [ f ] = G2(x,T,muc)
2 KB = 1.380649e-23; % Boltzmann constant (J/K)
3
4 f = 1./(cosh(muc./KB./T)./sinh(x./KB./T)+coth(x./KB./T));
5 end
```

#### A.10 MATLAB code for functions used in Dispersion Relation

```
function f1 = func(krho)
1
2
  global w D T1 muc S1 k0 eps1 eps3
3
4
                                      % Vacuum permittivity
       e0 = 8.8542e - 12;
5
       S1 = RPA(muc, krho, T1);
6
       kz = sqrt(krho.^2-k0^2);
7
8
       f1 = abs(eps3./kz.*coth(kz*D./2)+eps1./kz+1i.*S1./w./e0);
9
  end
10
  function f2 = func2(krho)
1
2
  global w D T1 muc S1 k0 eps1 eps3
3
4
                                      % Vacuum permittivity
       e0 = 8.8542 e - 12;
5
       S1 = RPA(muc, krho, T1);
6
       kz = sqrt(krho.^{2}-k0^{2});
7
8
       f2 = abs(eps3./kz.*tanh(kz*D./2)+eps1./kz+1i.*S1./w./e0);
9
  end
10
  function f1 = func3(krho)
1
2
  global w D S3 k0 eps1 eps3
3
                                      % Vacuum permittivity
       e0 = 8.8542e - 12;
4
       kz = sqrt (krho.^{2}-k0^{2});
\mathbf{5}
```

 ${}_{6} \qquad \qquad f1 \; = \; abs \left(\,eps3\,.\,/\,kz\,.\,*\,coth \left(\,kz\,*D.\,/\,2\,\right) + eps1\,.\,/\,kz + 1\,i\,.\,*\,S3\,.\,/\,w.\,/\,e0\,\right)\,;$ 

7 end

#### **BIOGRAPHY OF THE AUTHOR**

Born in Gilan Province of Iran. At early age, diagnosed with X-Linked Retinoschisis and meningioma which caused lost most of eyesight and many other problems. In 2008, attended the Gilan University as a BSc mechanical engineering student majoring in heat and fluids while working as a programmer and web developer to find the money for brain surgery. In spite of all these, managed to get my MSc in mechanical engineering from University of Zanjan. By overcoming these hardships, found a much more explicit purpose for life: to pull as many people alike out of the misery I, myself was stuck in.

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