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Shedding light on and comparing three different mathematical models of the optical conductivity concept

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ABSTRACT

The optical response in materials offers valuable insights into their properties, especially regarding interband transitions, distinct from direct current responses. By adjusting the frequency of electromagnetic radiation, interband transitions and energy band mappings can be explored, even in materials like graphene. Optical conductivity, which measures a material's ability to conduct electricity under the influence of light, is pivotal across physics, materials science, and engineering. It quantifies a material's efficiency in absorbing and transporting electromagnetic energy as photons. Typically described by Drude's model, optical conductivity has applications in diverse fields, from designing specific optical properties in materials to optimizing solar cells and developing photonic devices. Plasmonics, meta-materials, and renewable energy research also benefit from understanding and controlling optical conductivity. The optical conductivity problem centers on comprehending materials' electrical interactions with light across the optical spectrum, which is vital for various technologies. Theoretical models, simulations, and experiments address this problem, aiming to develop tunable materials and enhance theoretical models for accurate prediction of optical properties. Mathematical models, such as Maxwell's equations, the Lorentz-Drude model, and the Hosam-Heba model, elucidate optical conductivity, aiding in understanding light-material interactions and predicting material behavior under electromagnetic radiation. Each model offers a unique perspective on optical conductivity, with different theoretical foundations and mathematical formulations that can be applied depending on the specific properties of the material being studied. Understanding and manipulating optical conductivity is foundational to utilizing light across various technological applications.

1. Introduction

The term optical conductivity/response is a physical parameter relates the polarization-current density to the incident light at various frequencies, is attributed to the direct interband optical transitions of electrons, also known as light-induced density fluctuations. The optical conductivity is frequently used to describe material optical properties such as absorptions, transmissions, and reactions [1]. In other words, the term optical conductivity refers to the ability of a material to conduct electricity under the influence of light, typically in the visible or infrared spectrum. It's a key property in understanding how materials interact with light, which has implications across various fields including physics, materials science, and engineering. In other words, the Optical conductivity is a measure of how efficiently a material conducts electric current in response to light of a specific frequency. It quantifies the ability of a material to absorb and transport electromagnetic energy in the form of photons. The optical conductivity of a material is determined by

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its electron band structure, specifically the possible transitions from an initial occupied to an empty state of electrons [2].

In general the optical response is a strong tool for extracting information about a variety of material properties. The sensitivity to interband transitions distinguishes the optical or alternating current response from the direct current equivalent [3–6]. Tuning the frequency of electromagnetic radiation allows one to investigate alternative interband transitions, identify selection rules, and map the energy bands of diverse materials, including those with unique spectra like graphene and Dirac semimetals [7–10]. Mathematically, the Optical conductivity is often described by Drudge's model, using some of the parameters such as the electronic charge, relaxation time, and effective mass of the charge carriers, in addition to the angular frequency of light. Optical conductivity has a variety of applications in different fields. For example in material sciencethe Understanding of optical conductivity is crucial for designing materials with specific optical properties. By the way, in semiconductor devices, the optical conductivity determines the material's ability to absorb and emit light, which is fundamental to their operation [11].

In the field of Photonics and Optoelectronics studies, the Optical conductivity is essential in the design of photonic devices such as lasers, LEDs, photodetectors, and optical fibers. It governs the efficiency of light absorption, emission, and propagation in these devices [12,13]. On the other side, in Plasmonics, the interaction of light with free electrons at metallic surfaces or nanoparticles is characterized by their optical conductivity. This field is critical for applications like sensing, imaging, and light manipulation at the Nano scale. At the renewable energy researches such as Solar Cells: Understanding and controlling optical conductivity is vital for improving the performance of solar cells, the optical conductivity influences light absorption and charge carrier generation within the solar cell material [4–6].

Also, the Optical conductivity plays a crucial role in the development of metamaterials with engineered optical properties, such as negative refractive index or perfect absorption, leading to applications in cloaking, imaging, and sensing. Ongoing research focuses on developing materials with tunable optical conductivity, exploring novel materials and nanostructures, and improving theoretical models to accurately predict and manipulate optical properties [14,15]. In essence, optical conductivity is a fundamental property that underpins numerous technologies and scientific endeavors, shaping our ability to control and harness light for various applications. The optical conductivity problem is the study of how materials interact with light in terms of their electric conductivity. It focuses on how materials respond to electromagnetic radiation across the optical spectrum, from ultraviolet to infrared wavelengths. This includes understanding how electrons in a material respond to light's electric field, resulting in phenomena such as light absorption, reflection, and transmission. Researchers study optical conductivity to better understand the underlying features of materials and how they behave under various electromagnetic situations. This understanding is essential for a variety of applications, including the development of optical devices, photonic circuits, sensors, and materials for energy collection and conversion [14–18]. The optical conductivity problem is addressed by theoretical models, computer simulations, and experimental approaches such as spectroscopy, which allow scientists to investigate and understand this phenomenon. Given the relevance of the topic, the purpose of this study is to provide an overview, shed light on, and compare three different mathematical models of the optical conductivity concept.

2. Description of the optics problem

The problem of the optical response of a solid sample can be generalized as shown in Fig. 1, which exhibits a light beam impinges on a dielectric sample of thickness t and length l. Depending on photon energy and layer thickness, the radiation is both transmitted and reflected. A portion of the radiation may be internally absorbed. Where, the structure's total light reflection and transmission are calculated by adding the amplitudes of partially reflected and partially transmitted beams. This feature is fundamental to a wide range of applications. Depending on the situation, the sample may be clear or absorbent [19–22]. Fig. 1 depicts a structure that shows an optical response problem in how the spectrum response of the sample's known parameters is calculated, including its optical constants as a function of photon wavelength, as well as its thickness.

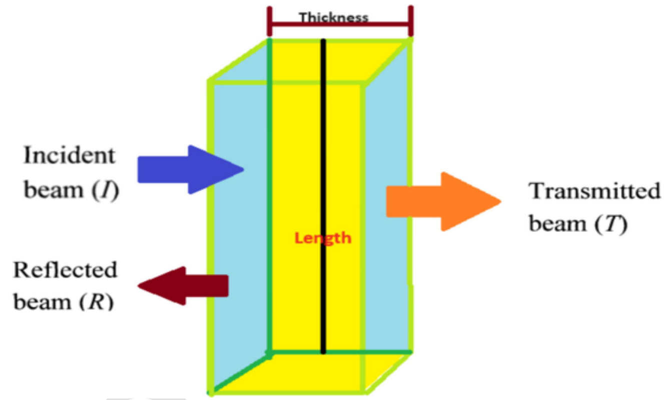

Fig. 1. A light beam impinges on a dielectric sample of thickness t and length l. Depending on photon energy and layer thickness, the radiation is both transmitted and reflected. A portion of the radiation may be internally absorbed.

Mathematically, the optical response problem is direct. The phenomenon is described by a partial differential wave equation (derived from Maxwell equations), with the assumption that the parameters and boundary conditions are known. The direct problem consists of calculating the wave's state. Analytic solutions are possible if it is assumed that the incident wave is pure and that the boundaries of the sample are regular. In more complex circumstances, numerical solutions are required. However, even when analytic calculations are feasible, the practical computation of the response might be quite expensive. This is because pure waves do not exist in most optical experiments, therefore the genuine answer is an average of multiple waves of varying wavelengths. Although the transmitted and reflected energies of pure waves can be expressed in a closed analytic form, analytic integration is not possible, and numerical integration is computationally expensive [23–26]. Generally, the interaction of electromagnetic radiation with either dielectric or semiconductor solids is addressed by adding boundary conditions to Maxwell equation solutions at the interface of distinct media. The wavelength of light is always substantially larger than the interatomic dimensions. Thus, the interaction between light and these types of solid matter is averaged over a large number of structural units. As a result, the optical properties inside the solid can be defined macroscopically in terms of phenomenological parameters, also known as optical constants or optical parameters [27–32].

3. Mathematical modelization of optical conductivity

3.1. Shankar Model

When an electromagnetic wave interacts with dielectric solid sample, with optical loss, the resulting refractive index of such sample should be complicated and dispersive as shown in Eq. (1). In other words, the resulting refractive index n* will consisting of a real component (refractive index n) and an imaginary part (absorption index K). The real and imaginary components of a complex index of refraction (n) [33–35]. The real portion, n, is the ratio of the velocity of light in a vacuum to the velocity of light at a wavelength (λ) in the substance. The imaginary portion, K, is an attenuation coefficient measuring the absorption of light over distance. Using Maxwell equations, the frequency-dependent "constants" can be connected to other optical quantities like the dielectric constant and conductivity.

By considering a plane-polarized wave moving along the positive z-axis with the electric field component, E_x, vibrating in the x-direction, and disregarding any magnetic effects, the electromagnetic wave equation can be stated as shown in Eq. (2), where ε is the dielectric constant/permittivity, and σ is the alternating conductivity. The electric field component in the x-direction, as given in Eq. (3), can be obtained by solving Eq. (2), where E_o is the maximum value of the electric field strength and x is the angular frequency ($\omega = 2\pi f$). Accordingly, Eq. (4) can be found by solving both Eqs. (3) and (2) [35,36].

$$n^* = n + iK \tag{1}$$

$$c^2 \frac{\partial^2 E_x}{\partial t^2} = \varepsilon^* \frac{\partial^2 E_x}{\partial t^2} + \frac{\sigma}{\varepsilon_o}\frac{\partial E_x}{\partial t} \tag{2}$$

$$\varepsilon^* = \varepsilon_1 + i\varepsilon_2$$

$$E_x = E_o e^{\left[i\omega\left(t - z\frac{n}{c}\right)\right]} \tag{3}$$

$$n^{*2} = \varepsilon^* - i\frac{\sigma}{\omega\varepsilon_o} \tag{4}$$

From Eq. (1)

$$n^{*2} = n^2 + K^2 - i2nK \tag{5}$$

By comparing Eqs. (4) and (5), we can derive Eqs. (6) and (7)

$$\frac{\sigma}{\omega\varepsilon_o} = 2nk \tag{6}$$

$$\sigma = 2\omega\varepsilon_o nK \tag{7}$$

Since;

$$K = \frac{\alpha\lambda}{4\pi} = \frac{\alpha C}{4\pi f} = \frac{\alpha C}{2\omega} \tag{8}$$

Therefore;

$$\sigma = 2\omega\varepsilon_o n\frac{\alpha C}{2\omega} = \varepsilon_o n\alpha c(\Omega^{-1}m^{-1}) \tag{9a}$$

$$\sigma = 2\omega\varepsilon_o n\frac{\alpha C}{2\omega} = \frac{n\alpha c}{4\pi}(s^{-1}) \tag{9b}$$

This relation gives the optical conductivity in terms of refractive index, absorption coefficient, and light velocity.

3.2. Hosam–Heba model

Acceding to Eq.1, The refractive index of a solid sample with an optical loss is a complex quantity composed of real part (refractive index n) and an imaginary part (absorption index. This concept can be accepted based on the fact that the electronic polarization, (P_e): the redistribution of electron density within a material in response to an external electric field, throughout a solid sample is proportional to the electric field component E of incident light as well as the average current *i* per unit area of this sample. The interaction between the electromagnetic rays with a dielectric sample can be described by Maxwell's equations, Eqs. (10)–(16), where ρ is the density of the free charge carries, *i* is average current density, D is the electric displacement parameter, c is the space light speed, and ε_o are and space permittivity. The solution of Maxwell's equations resulted in the following plane harmonic waves, Eqs. (17)–(18), their traveling phase velocity v_{phase} is described by Eq. (19), where n is the refractive index [36–38].

$$\rho = -\nabla P \tag{10}$$

$$i = \frac{\partial P}{\partial t} \tag{11}$$

$$\nabla.E = -\frac{\nabla.P}{\varepsilon_o} \tag{12}$$

$$\nabla xE = -\frac{\partial B}{\partial t} \tag{13}$$

$$\nabla.B = 0 \tag{14}$$

$$c^2\nabla xB = \frac{\partial}{\partial t}\left(\frac{P}{\varepsilon_o} + E\right) \tag{15}$$

$$D = \varepsilon_o + P \tag{16}$$

$$E = E_o e^{j(\omega t - kr)} \quad \text{where k is the wave vector} \tag{17}$$

$$H = H_o e^{j(\omega t - kr)} \tag{18}$$

$$v_{phase} = \frac{\omega}{k} = \frac{c}{n} \tag{19}$$

The optical dielectric relaxation ε^* can express the loss of energy parameters (see Eq. (20), which consists of a real and imaginary components ε_1 and ε_2. For unfree damper, the real component ε_1 characterizes the damping of the light propagation through the medium. While the imaginary component is considered as a damping factor describes the amount of energy loss/absorbed within the medium. According to Eq. (21) the complex dielectric constant could be expressed in terms of the complex refractive index n* which can be defined as formulated in Eq. (22).

$$\varepsilon^* = \varepsilon_1 + j\varepsilon_2 \tag{20}$$

$$\varepsilon^* = n^{*2} \tag{21}$$

Where

$$n^* = n + jK \tag{22}$$

Solving of Eqs. 33 and 34 gives Eqs. (35) and (36)

$$\varepsilon_1 = \left(n^2 - K^2\right) \tag{23}$$

$$\varepsilon_2 = 2nK \tag{24}$$

$$\sigma\ \omega\varepsilon_2 \tag{25}$$

$$\sigma = C\omega\varepsilon_2 \tag{26}$$

$$\sigma = 2C\omega nK \tag{27}$$

$$\sigma = \frac{1}{6.25}\omega nK(s^{-1}) \tag{28}$$

The Optical conductivity is known as the relationship between the induced current density and the strength of the generated electric field component of the light. Also, it's well known that the optical conductivity σ is proportional to both the angular frequency of the electromagnetic wave and the dielectric relaxation loss ε_2 of the medium Eq. (25). Mathematically, Eq. (25) can be re-formulated in the form of Eq. (26). Hosam and Heba used numerical methods to estimate the magnitude of the proportional constant C (1/6.25), Accordingly, Eq. (27) took the f form of Eq. (28) which shows that the optical conductivity depends on the values of both the refractive and absorption indices (n and K), which means its dependence on the amount of the energy loss within the optical medium. By a few steps, it can be demonstrated that the last equation is the same as result from the Shankar model, as follows; According to Shankar

$$\sigma = \frac{n\alpha c}{4\pi} \quad \text{where} \quad \alpha = \frac{4\pi K}{\lambda}$$

$$\therefore \sigma = \frac{nc}{4\pi}\frac{4\pi K}{\lambda} = \frac{ncK}{\lambda} = nKf = \left(\frac{1}{2\pi}\right)(2\pi f)\ nK = \left(\frac{1}{6.28}\right)\omega\, nK$$

which is the same as the result of Hosam-Heba equation.

3.3. Lorentz–Drude model

In 1905, Lorentz developed his theory describing the response of dielectric materials. He proposed that when an electron (denoted as e) with a mass (m) moves in an alternating electric field (E) with frequency (ω), it experiences an electric force (eE) [11,38].

$$m(\ddot{x} + \gamma \dot{x} + \omega_e^2 x) = eE \tag{29}$$

$$E(\omega) = E_o e^{-i\omega t} \tag{30}$$

$$x = x_o e^{-i\omega t} \tag{31}$$

$$x_o = \frac{eE_o}{m(\omega_e^2 - \omega^2 - i\gamma\omega)} \tag{32}$$

$$Nex = (\varepsilon - \varepsilon_o) E \tag{33a}$$

$$Nex_o e^{-i\omega t} = (\varepsilon - \varepsilon_o) E_o e^{-i\omega t} \tag{33b}$$

$$Ne \frac{eE_o}{m(\omega_e^2 - \omega^2 - i\gamma\omega)} e^{-i\omega t} = (\varepsilon - \varepsilon_o) E_o e^{-i\omega t} \tag{33c}$$

$$\varepsilon = \varepsilon_o + \frac{Ne^2}{m} \frac{f}{\omega_e^2 - \omega^2 - i\gamma\omega} \tag{34}$$

The equation of motion governing this electron's displacement (x) relative to its equilibrium position (atomic core) is given by Eq. (10). Here, γ represents the bandwidth or damping factor, and ω_o is the resonance frequency. Lorentz postulated that the solution to this equation of motion is described by Eq. (12), from which he derived the maximum electronic displacement (x_o) as expressed in relation (4). Substituting Eqs and 11, 13 into Eq. (14), which defines the electronic polarizability (P): the ability of electrons in an atom, molecule, or material to deform in reaction to an external electric field, enables the estimation of the dielectric function of an oscillator, as shown in Eq. (15). In this equation, ε denotes the dielectric function, ε_o represents the space permittivity, N signifies the electronic density in cm^{-3}, and f denotes the oscillator strength.

Drude postulated that the valence electrons associated with an atom or a group of atoms possess a loose connection to their respective atomic cores, allowing them to exhibit relatively unrestricted (semi-free) motion akin to plasma movements. When subjected to an external electric field (E), these electrons are expected to undergo displacement and collide with one another. Due to their weak bonding to the atoms, there is no significant restoring force acting on them, hence the assumption that the restoring force $f = 1$. Based on Eqs. (29)–(34) Eqs. (35) and (36) can be obtained by substituting $f = 1$, where m* is the electronic reduced mass [12,39–41].

$$m^*(\ddot{x} + \gamma \dot{x}) = eE \tag{35}$$

$$\varepsilon = \varepsilon_o + \frac{Ne^2}{m^8} \frac{1}{\omega_e^2 - \omega^2 - i\gamma\omega} \tag{36}$$

By putting $\omega_{pe} = \sqrt{\frac{Ne^2}{m^*}}$ (plasmon frequency) Eq. (36) becomes as follows Eq. (37). Accordingly, the imaginary component of the Eq. (36) will be in the form Eq.38;

$$\varepsilon = \varepsilon_o + \frac{\omega_{pe}^2}{\omega_e^2 - \omega^2 - i\gamma\omega} \tag{37}$$

$$\varepsilon_{im} = \varepsilon_o + \frac{\omega_{pe}^2 \omega\gamma}{(\omega_e^2 - \omega^2)^2 + (\gamma w)^2} (\text{For N} = 1) \tag{38}$$

For N electronic charges

$$\varepsilon_{im} = \sum_i \frac{\omega_{pei}^2 \omega\gamma}{(\omega_{ei}^2 - \omega^2)^2 + (\gamma_i w)^2} \tag{39}$$

$$\sigma(\omega) = \varepsilon_o \varepsilon \omega \tag{40a}$$

$$\sigma(\omega) = \varepsilon_o \omega \sum_i \frac{\omega_{pei}^2 \omega\gamma}{(\omega_{ei}^2 - \omega^2)^2 + (\gamma_i w)^2} \tag{40b}$$

The last Equation, Eq. (40b), is known as the Drude model for optical conductivity and can be applied to all materials if the frequencies are sufficiently high.

4. Discussion

The three models try to describe optical conductivity but differ in their theoretical basis and mathematical representations. The Shankar and Hosam-Heba models are mainly concerned with the electromagnetic properties of dielectric materials, whereas the Lorentz-Drude model takes into account electron behavior within these materials. Each model provides unique insights and can be used depending on the properties of the substance being studied. After describing the three different models for understanding optical conductivity in materials, a straightforward comparison can be performed between the three models as follows:

a) Shankar Model is an approach which utilizes Maxwell's equations to derive the optical conductivity of a dielectric solid sample based on its optical absorption coefficient as well as its linear refractive index. Such a model provides a mathematical framework for understanding how materials interact with electromagnetic waves. Shankar's optical conductivity model, while less well-known than the Drude model, can be very useful in systems including quantum mechanical effects and interactions. Shankar's model frequently addresses more complex aspects of condensed matter physics, such as strong correlations and collective excitations. Shankar's model could be useful for a lot of materials including High-temperature superconductors and Low-Dimensional Systems (1D conductors, 2D electron gases, transition metal oxides, graphene, and other 2D materials).
b) Hosam–Heba Model is a semi-empirical approach which is Also employs Maxwell's equations to describe the interaction between electromagnetic waves and dielectric samples, resulting in the optical conductivity. Such a model presents the complex dielectric constant in terms of the refractive index, n, and absorption index, K, then derives the optical conductivity (σ) in relation to these parameters. It also offers an alternative perspective on optical conductivity, focusing on the loss of energy parameters within the medium. Because it was published so recently, Hosam and Heba's model for optical conductivity is still not commonly accepted in mainstream condensed matter physics. However, it was effectively used for amorphous solids such as oxide glass, metal oxide, conductive polymers, and inorganic thin films.
c) Lorentz–Drude Model approach that developed by Lorentz to describe the response of dielectric materials, incorporating the motion of electrons in an alternating electric field. This model derives the dielectric function of an oscillator from the equation of motion governing the displacement of electrons relative to their equilibrium positions. Expresses the optical conductivity using the plasmon frequency and electronic density. Such a model provides insights into the behavior of valence electrons in materials and their response to external electric fields. Drude's optical conductivity model is most suited to materials in which free electron activity dominates the electrical and optical properties. These materials typically have a high density of free charge carriers (electrons or holes) that can be considered classical gases. Drude's model applies to the following sorts of materials: Metals like Cu and Ag, doped semiconductors like Si and Ge, inorganic oxides, and simple alloys like brass and bronze, Conductive polymers, graphene, and other two-dimensional materials. While the Drude model is useful, it has limitations in the case of materials with significant electron–electron interactions, strong correlations, or significant

contributions from bound states (such as excitons), which require models other than Drude, such as the Lorentz model or quantum mechanical treatments. For example, complicated. The Drude model cannot effectively explain many materials, including high-temperature superconductors, heavy fermion systems, and materials with substantial spin–orbit coupling or topological characteristics.

5. Conclusion

Mathematical models like Maxwell equations, the Lorentz-Drude model, and the Hosam-Heba model contribute to elucidating light-material interactions and predicting material behavior under electromagnetic radiation. Overall, the study of optical conductivity not only enriches our understanding of fundamental physical phenomena but also drives technological advancements with real-world applications. The comparison between the Shankar, Hosam–Heba, and Lorentz–Drude models highlights their common goal of understanding optical conductivity in materials. Each model approaches this problem from a distinct theoretical framework, utilizing Maxwell's equations and considerations of electron behavior in response to electromagnetic fields. The Shankar model emphasizes the relationship between refractive index and optical conductivity, providing a straightforward mathematical expression for these properties. On the other hand, the Hosam–Heba model delves into the complex dielectric constant to characterize energy loss within the medium, offering insights into absorption phenomena. Meanwhile, the Lorentz–Drude model focuses on the behavior of valence electrons and their interaction with external electric fields, providing a deeper understanding of dielectric materials' response to electromagnetic radiation. Overall, these models contribute to the broader understanding of optical conductivity, offering valuable insights into the underlying physics of light-matter interactions. They provide essential tools for researchers in various fields, from materials science to photonics, enabling the design and optimization of devices with specific optical properties.

Declarations

Ethical Approval

This article doesn't contain any studies involving animals performed by any authors. Also, this article does not have any studies involving human participants performed by any of the authors

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Authors' contributions

Hosam M. Gomaa suggested the research idea, performed all calculations, and wrote the primary manuscript. H. A. Saudi, Shams A.M. Issa, Hesham M.H. Zakaly review the final manuscript, Dr. Graham AL. Haram replied to the reviewers' comments.

Uncited reference

[18].

CRediT authorship contribution statement

Gharam A. Alharshan: Writing – review & editing. **H.A. Saudi:** Writing – review & editing. **Shams A.M. Issa:** Writing – review & editing. **Hesham M.H. Zakaly:** Writing – review & editing. **Hosam M. Gomaa:** Writing – original draft, Methodology, Investigation, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

All the original measurements and data analysis of this work will be available when required.

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