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Maxwell's equations in Fourier space and coupling between elementary excitations in solids

Equações de Maxwell no espaço de Fourier e acoplamento entre excitações elementares em sólidos

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Maxwell's equations are fundamental to the understanding of electromagnetic events, as they describe the totality of experimentally verified electromagnetic phenomena from its boundary conditions and constitutive relations. Although, they are normally presented in the time and space domain, many physical effects and their associated mathematical manipulation are easier to understand when we use Maxwell's equations in Fourier space. In this work we give a general introduction about Maxwell's equations in Fourier domain in material media. The simplicity of the obtained equations in comparison with the ones in space-time domain is emphasized, and the link between them and the elementary excitations in solids is presented and explored. In particular, the coupling between various types of quasiparticles in solids is explained.

Keywords: Maxwell equations, Fourier space, elementary excitations, plasmon, phonon-polariton.

As equações de Maxwell são fundamentais para a compreensão dos fenômenos eletromagnéticos, pois descrevem a totalidade dos eventos eletromagnéticos verificados experimentalmente a partir de suas condições de contorno e das relações constitutivas. Embora sejam normalmente apresentados no domínio do espaço e do tempo, muitos efeitos físicos e suas manipulações matemáticas são mais fáceis de entender quando usamos as equações de Maxwell no espaço de Fourier. Neste trabalho é apresentada uma introdução geral sobre as equações de Maxwell no domínio de Fourier em meios materiais. É enfatizada a simplicidade das equações obtidas em comparação com as do domínio espaço-tempo, bem como explorada a ligação entre elas e as excitações elementares em sólidos. Em particular, é explicado o acoplamento entre vários tipos de quasipartículas em sólidos.

Palavras-chave: Equações de Maxwell, espaço de Fourier, excitações elementares, plásmon, fônon-polariton.

1. Introduction

The starting point to study the interaction of electromagnetic fields with matter is Maxwell's equations which describe how electric charges and electric currents create electric and magnetic fields, how those fields change in time and how an electric field can generate a magnetic field, (and vice versa). Furthermore, from Maxwell's equations it was possible to develop the theory of electromagnetic waves, including visible light.

Maxwell's equations, together with Lorentz force law (which describes how electric and magnetic fields act on charges and currents) form the theoretical foundation of classical electrodynamics and is one of the major milestones of theoretical physics, even though its historical genesis took place in a context heavily dominated by mechanical ideas according to which the electromagnetic field did not have an intrinsic reality, but a consequence of the mechanical properties of an ethereal medium [1].

Perhaps the most spectacular prediction of Maxwell's equations is the existence of electromagnetic waves and that light is a form of an electromagnetic wave. From a practical point of view, electromagnetic waves are widely used in devices such as radio, cell phones, television, radars, medical imaging and many others. As a fundamental theory, Maxwell's equations can be appreciated from an aesthetic point of view [2]. Additionally, these equations are capable of providing a solid basis for understanding the basic principles of new research areas such as plasmonics [3], as we will see in this work.

Optical property describes a material's response when electromagnetic radiation (in particular visible light) is incident on the material and are consequences how it reflect, transmit, and absorb or scatters the incident radiation [4, 5]. Detailed knowledge of the optical properties of matter has important implications for both to understand the essential principles of radiation-matter interaction and for a wide range of research fields and applications, e.g, photonics and plasmonics [3, 6].

In the study of optical properties of materials, it is more convenient to present Maxwell's equations in Fourier space, as the coupling of the electromagnetic field with elementary excitations of the medium becomes easier to analyze. This aspect of Maxwell's equations is rarely presented in most textbooks, yet it is very useful because of the direct determination of physical

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properties, as well as general expressions for the dispersion relation, it permits. These aspects will be explored in this work.

The outline of the remainder of this paper is as follows. In section 2 we make a summary of Maxwell theory in material media. In section 3 we present the relations that describing the behavior of matter under the influence of electromagnetic fields, which are known as constitutive relations. In section 4 we present Maxwell's equations in Fourier domain and the advantages of this formalism. In sections 5 and 6 the properties of elementary excitations of an electron gas and the vibrations of a lattice are discussed, together with their interaction with electromagnetic fields. Finally, in section 7 we present our conclusions.

2. Maxwell's Equations in Material Media

In differential form and in SI units Maxwell's equations for the fundamental electromagnetic fields **E** (electric field) and **B** (magnetic induction) in the presence of matter are, in standard notation:

$$\nabla \cdot \mathbf{E}(\mathbf{r},t) = \frac{\rho_{total}(\mathbf{r},t)}{\epsilon_0} \tag{1}$$

$$\nabla \cdot \mathbf{B}(\mathbf{r},t) = 0 \tag{2}$$

$$\nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{\partial \mathbf{B}(\mathbf{r},t)}{\partial t} \tag{3}$$

$$\nabla \times \mathbf{B}(\mathbf{r},t) = \mu_0 J_{total}(\mathbf{r},t) + \mu_0\epsilon_0 \frac{\partial \mathbf{E}(\mathbf{r},t)}{\partial t} \tag{4}$$

where ϵ_0 and μ_0 are the electric permittivity and magnetic permeability of vacuum, respectively, and ρ_{total} is the total charge density, namely the sum of the free charge density and the bound charge density:

$$\rho_{total} = \rho_{ext}(\mathbf{r},t) + \rho_{pol}(\mathbf{r},t) \tag{5}$$

where ρ_{ext} is an external charge density added from outside and ρ_{pol} is given by

$$\rho_{pol} = -\nabla \cdot \mathbf{P}(\mathbf{r},t) \tag{6}$$

where **P** is polarization vector (electric dipole moment per unit volume). $\mathbf{J}_{total}$ is the total electric current density given by:

$$\mathbf{J_{total}}(\mathbf{r},t) = \mathbf{J_{cond}}(\mathbf{r},t) + \mathbf{J_{bound}}(\mathbf{r},t) \tag{7}$$

The bound density current is given by:

$$\mathbf{J_{bound}}(\mathbf{r},t) = \frac{\partial \mathbf{P}(\mathbf{r},t)}{\partial t} + \nabla \times \mathbf{M}(\mathbf{r},t) \tag{8}$$

where **M** is the magnetization field (magnetic dipole moment per unit volume) The auxiliary fields **D** and **H** are defined as

$$\mathbf{D}(\mathbf{r},t) = \epsilon_0 \mathbf{E}(\mathbf{r},t) + \mathbf{P}(\mathbf{r},t) \tag{9}$$

$$\mathbf{H}(\mathbf{r},t) = \frac{1}{\mu_0}\mathbf{B}(\mathbf{r},t) - \mathbf{M}(\mathbf{r},t) \tag{10}$$

Using these two new fields Maxwell's equations become

$$\nabla \cdot \mathbf{D}(\mathbf{r},t) = \rho_{ext}(\mathbf{r},t) \tag{11}$$

$$\nabla \cdot \mathbf{B}(\mathbf{r},t) = 0 \tag{12}$$

$$\nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{\partial \mathbf{B}(\mathbf{r},t)}{\partial t} \tag{13}$$

$$\nabla \times \mathbf{H}(\mathbf{r},t) = \mathbf{J_{cond}}(r,t) + \frac{\partial \mathbf{D}(\mathbf{r},t)}{\partial t} \tag{14}$$

which is the most conventional form to write the equations in the presence of matter [7], which do not show an explicit dependence on the density and current of the bound charges whose contributions are hidden within **D** and **H**.

The most impressive prediction of Maxwell's equations are the electromagnetic wave equations, which can be obtained by applying the curl operator on (13) and (14) and using the definitions of auxiliary fields (9) and (10):

$$\begin{aligned}\nabla \times (\nabla \times \mathbf{E}(\mathbf{r},t)) &+ \frac{1}{c^2}\frac{\partial^2 \mathbf{E}(\mathbf{r},t)}{\partial t^2} \\ &= -\mu_0 \frac{\partial}{\partial t}\left[\mathbf{J}_{cond}(\mathbf{r},t) + \frac{\partial \mathbf{P}(\mathbf{r},t)}{\partial t} + \nabla \times \mathbf{M}(\mathbf{r},t)\right]\end{aligned} \tag{15}$$

$$\begin{aligned}\nabla \times (\nabla \times \mathbf{H}(\mathbf{r},t)) &+ \frac{1}{c^2}\frac{\partial^2 \mathbf{H}(\mathbf{r},t)}{\partial t^2} \\ &= \nabla \times \mathbf{J}_{cond}(\mathbf{r},t) + \nabla \times \frac{\partial \mathbf{P}(\mathbf{r},t)}{\partial t} + \frac{1}{c^2}\frac{\partial^2 \mathbf{M}(\mathbf{r},t)}{\partial t}\end{aligned} \tag{16}$$

where $c = 1/\sqrt{\mu_0\epsilon_0}$ is the speed of light in the free space. Note that the expression in the brackets of equation (15) is the total current density given by equation (7). Equations (15) and (16) represent inhomogeneous wave equations for the fields **E** and **H**, respectively, and the right hand sides are the wave sources. In practice, these equations are so complicated that analytical solutions cannot be obtained. For this reason, there are different methods to approach the wave equation, depending on the physical problem under analysis. In reference [8], for example, the paraxial approximation used in the study of electromagnetic waves is presented, while in reference [9] the Fresnel-Kirchhoff scalar theory is used to study the diffraction pattern in slits in the Fresnel regime.

3. Constitutive Relations

The equations (11–14) are not complete. To find a self-consistent solution for the electromagnetic field, these equations must be supplemented by additional relations between fields **E** and **D** and also **H** and **B**. These equations are known as constitutive relations. In the simplest case of linear, isotropic[1], homogeneous and

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[1] A **linear medium** is one in which the polarization produced by an applied electric or magnetic field is proportional to that field. An **isotropic medium** is one in which all directions in space are equivalent

non-dispersive medium we have

$$\mathbf{P}(\mathbf{r},t) = \epsilon_0 \chi_e \mathbf{E}(\mathbf{r},t) \tag{17}$$

$$\mathbf{M}(\mathbf{r},t) = \chi_m \mathbf{H}(\mathbf{r},t) \tag{18}$$

where χ_e and χ_m denote the electric and magnetic susceptibility, respectively. Using equations (17) and (18) in (9) and (10) we obtain

$$\mathbf{D}(\mathbf{r},t) = \epsilon_0 \epsilon \mathbf{E}(\mathbf{r},t) \tag{19}$$

$$\mathbf{B}(\mathbf{r},t) = \mu_0 \mu \mathbf{H}(\mathbf{r},t) \tag{20}$$

where $\epsilon = 1 + \chi_e$ and $\mu = 1 + \chi_m$ are the dielectric constant (or relative permittivity) and the magnetic permeability, respectively. In the study of the optical phenomena of solids, the relative permittivity is a most important parameter.

Another important constitutive relation is found between the conduction current density $\mathbf{J}_{cond}$ and the electric field $\mathbf{E}$, defined via the conductivity σ by

$$\mathbf{J}_{cond}(\mathbf{r},t) = \sigma \mathbf{E}(\mathbf{r},\mathbf{t}) \tag{21}$$

In this work we shall be concerned only with non-magnetic media, hence $\mathbf{M}$ is zero. For this situation and using constitutive relations (19–21), the general wave equations (15) and (16) are reduced to

$$\nabla \times (\nabla \times \mathbf{E}(\mathbf{r},t)) + \frac{\epsilon}{c^2}\frac{\partial^2 \mathbf{E}(\mathbf{r},t)}{\partial t^2} + \mu_0 \sigma \frac{\partial \mathbf{E}(\mathbf{r},t)}{\partial t} = 0 \tag{22}$$

$$\nabla \times (\nabla \times \mathbf{H}(\mathbf{r},t)) + \frac{\epsilon}{c^2}\frac{\partial^2 \mathbf{H}(\mathbf{r},t)}{\partial t^2} + \mu_0 \sigma \frac{\partial \mathbf{H}(\mathbf{r},t)}{\partial t} = 0 \tag{23}$$

The equations (19), (20) and (21) are only correct for linear media that do not have temporal or spatial dispersion.

For *nonlinear* media we must consider higher power terms in the constitutive relationship equations. For *anisotropic* media ϵ, μ and σ are tensors.

If the quantities ϵ, μ and σ are functions of the position, the medium is called spatially dispersive, and temporally dispersive in the case they are functions of time.

The most general linear response of a medium at position $\mathbf{r}$ and time t to an electric field $\mathbf{E}(\mathbf{r'}$,t') at position $\mathbf{r'}$ and time t' is given by [10]

$$\mathbf{D}(\mathbf{r},t) = \epsilon_0 \int\int_{-\infty}^{\infty} \epsilon(\mathbf{r}-\mathbf{r}', t-t')\mathbf{E}(\mathbf{r}',t')d^3\mathbf{r}'dt' \tag{24}$$

where we assume that the system is translation invariant in both time and space. In a similar way we have

$$\mathbf{J}(\mathbf{r},t) = \int\int_{-\infty}^{\infty} \sigma(\mathbf{r}-\mathbf{r}', t-t')\mathbf{E}(\mathbf{r}',t')d^3\mathbf{r}'dt' \tag{25}$$

Now we will show that equations (24) and (25) are enormously simplified if we consider their Fourier transforms. We will assume that all fields and sources appearing in Maxwell's equations can be decomposed into a complete set of plane waves. Thus, we can write for the electric field

$$\mathbf{E}(\mathbf{r},t) = \frac{1}{(2\pi)^4}\int\int_{-\infty}^{\infty} \mathbf{E}(\mathbf{k},w) exp\left\{i(\mathbf{k}\cdot\mathbf{r} - \omega t)\right\} d\omega d^3\mathbf{k} \tag{26}$$

where the Fourier transform of $\mathbf{E}$(r,t) is given by

$$\mathbf{E}(\mathbf{k},w) = \int\int_{-\infty}^{\infty} \mathbf{E}(\mathbf{r},t) exp\left\{-i(\mathbf{k}\cdot\mathbf{r} - \omega t)\right\} dt d^3\mathbf{r} \tag{27}$$

With similar equations for the $\mathbf{D}$ field. Substituting (27) into (24)

$$\begin{aligned}\int\int_{-\infty}^{\infty} &\mathbf{D}(\mathbf{k},\omega) exp\left\{i(\mathbf{k}\cdot\mathbf{r} - \omega t)\right\} d\omega d\mathbf{k} \\ &= \epsilon_0 \int\int_{-\infty}^{\infty} \epsilon(\mathbf{r}-\mathbf{r'}, t-t') \\ &\quad \cdot \left[\int\int_{-\infty}^{\infty} \mathbf{E}(\mathbf{k},\omega) exp\left\{i(k\mathbf{r'} - \omega t')\right\} d\omega d^3\mathbf{k}\right] d^3\mathbf{r'}dt'\end{aligned} \tag{28}$$

Making the variable change

$$\begin{gathered}\mathbf{r} - \mathbf{r}' = \mathbf{r}'' \\ t - t' = t''\end{gathered}$$

$$\begin{aligned}\int\int_{-\infty}^{\infty} &\mathbf{D}(\mathbf{k},\omega) exp\left\{i(\mathbf{k}\cdot\mathbf{r} - \omega t)\right\} d\omega d\mathbf{k} \\ &= \epsilon_0 \int\int_{-\infty}^{\infty} \mathbf{E}(\mathbf{k},\omega) exp\left\{i(k\mathbf{r} - \omega t)\right\} d\omega d^3\mathbf{k} \\ &\quad \mathbf{X}\left[\int\int_{-\infty}^{\infty} \epsilon(\mathbf{r}'',t'') exp\left\{i(k\mathbf{r}'' - \omega t'')\right\} d\mathbf{r}''dt''\right]\end{aligned} \tag{29}$$

or even

$$\begin{aligned}\int\int_{-\infty}^{\infty} &\mathbf{D}(\mathbf{k},\omega) exp\left\{i(\mathbf{k}\cdot\mathbf{r} - \omega t)\right\} d\omega d\mathbf{k} \\ &= \epsilon_0 \int\int_{-\infty}^{\infty} \epsilon(\mathbf{k},\omega)\mathbf{E}(\mathbf{k},\omega) exp\left\{i(\mathbf{kr} - \omega t)\right\} d\omega d\mathbf{k}\end{aligned} \tag{30}$$

Finally we obtain

$$\mathbf{D}(\mathbf{k},\omega) = \epsilon_0 \epsilon(\mathbf{k},\omega)\mathbf{E}(\mathbf{k},\omega) \tag{31}$$

which is the constitutive relation in the Fourier domain. Comparing equations (24) and (31) we see that a nonlocal relationship in space and time becomes a local relationship in Fourier space, which is much easier to work on. In a similar way we obtain for equation (25)

$$\mathbf{J}(\mathbf{k},\omega) = \sigma(\mathbf{k},\omega)\mathbf{E}(\mathbf{k},\omega) \tag{32}$$

which is a remarkably simple relationship between $\mathbf{J}$ and $\mathbf{E}$ compared to equation (25).

4. Maxwell's Equations in Fourier Domain

Likewise, Maxwell's equations in Fourier space can be written as (details are given in the Appendix)

$$i\mathbf{k}\cdot\mathbf{D}(\mathbf{k},\omega)=\rho_{ext}(\mathbf{k},\omega) \tag{33}$$

$$\mathbf{k}\cdot\mathbf{B}(\mathbf{k},\omega)=0 \tag{34}$$

$$\mathbf{k}\times\mathbf{E}(\mathbf{k},\omega)=\omega\mathbf{B}(\mathbf{k},\omega) \tag{35}$$

$$i\mathbf{k}\times\mathbf{H}(\mathbf{k},\omega)=-i\omega\mathbf{D}(\mathbf{k},\omega)+\mathbf{J}(\mathbf{k},\omega) \tag{36}$$

Comparing equations (11–14) with equations (33–36) we can see a great simplification in Maxwell's equations when written in terms of Fourier components. Time derivatives are replaced by a simple multiplication by scalar and the operators divergent and curl (spacial derivatives) become dot product and cross product, respectively.

It is also useful to obtain the wave equation in the Fourier domain. Multiplying vectorially the equation (35) by $\mathbf{k}$ we obtain after some calculations

$$\begin{aligned}\mathbf{k}\times(\mathbf{k}\times\mathbf{E}(\mathbf{k},\omega))+\frac{\omega^2}{c^2}\mathbf{E}(\mathbf{k},\omega)\\ =-i\mu_0\omega[\mathbf{J}(\mathbf{k},\omega)-i\omega\mathbf{P}(\mathbf{k},\omega)-i\mathbf{k}\times\mathbf{M}(\mathbf{k},\omega)]\end{aligned} \tag{37}$$

In a similar way we obtain for $\mathbf{H}$

$$\begin{aligned}\mathbf{k}\times(\mathbf{k}\times\mathbf{H}(\mathbf{k},\omega))+\frac{\omega^2}{c^2}\mathbf{H}(\mathbf{k},\omega)\\ =-i\mathbf{k}\times\mathbf{J}_c(\mathbf{k},\omega)-\omega\mathbf{k}\times\mathbf{P}(\mathbf{k},\omega)-\frac{\omega^2}{c^2}\mathbf{M}(\mathbf{k},\omega)\end{aligned} \tag{38}$$

Equations (37) and (38) are equivalent to equations (15) and (16) written in Fourier space. In the special case of absence of external charge and free current we have

$$\mathbf{k}\cdot\mathbf{D}(\mathbf{k},\omega)=0 \tag{39}$$

$$\mathbf{k}\cdot\mathbf{B}(\mathbf{k},\omega)=0 \tag{40}$$

$$\mathbf{k}\times\mathbf{E}(\mathbf{k},\omega)=\omega\mathbf{B}(\mathbf{k},\omega) \tag{41}$$

$$\mathbf{k}\times\mathbf{H}(\mathbf{k},\omega)=-\omega\mathbf{D}(\mathbf{k},\omega) \tag{42}$$

Multiplying vectorially the equation (41) by $\mathbf{k}$ and considering non-magnetic media

$$\mathbf{k}\times(\mathbf{k}\times\mathbf{E}(\mathbf{k},\omega))=\omega\mathbf{k}\times\mathbf{B}(\mathbf{k},\omega)=\mu_0\omega\mathbf{k}\times\mathbf{H}(\mathbf{k},\omega) \tag{43}$$

Using equation (42) and the constitutive relation (31), we obtain

$$\mathbf{k}\times(\mathbf{k}\times\mathbf{E}(\mathbf{k},\omega))=-\frac{\omega^2}{c^2}\epsilon(\mathbf{k},\omega)\mathbf{E}(\mathbf{k},\omega) \tag{44}$$

which could be obtained directly from equation (37). Using the identity

$$\mathbf{a}\times(\mathbf{b}\times\mathbf{c})=\mathbf{b}(\mathbf{a}\cdot\mathbf{c})-\mathbf{c}(\mathbf{a}\cdot\mathbf{b})$$

we obtain

$$\mathbf{k}(\mathbf{k}\cdot\mathbf{E}(\mathbf{k},\omega))-\mathbf{k}^2\mathbf{E}(\mathbf{k},\omega)=-\frac{\omega^2}{c^2}\epsilon(\mathbf{k},\omega)\mathbf{E}(\mathbf{k},\omega) \tag{45}$$

which is the wave equation in the Fourier domain. Although equation (45) is very general and difficult to solve analytically, we can obtain relevant information about elementary excitations of the medium which are valid for all materials. Initially we can consider two cases representing the longitudinal and transverse modes that can occur in a solid.

Case 1 – Longitudinal oscillations

If $\mathbf{k}$ is parallel to $\mathbf{E}$ the left side of equation (45) is zero and $\epsilon(\mathbf{k},\omega)$ has to vanish for equation (45) to be satisfied. Thereby, the condition

$$\epsilon(\mathbf{k},\omega)=0 \tag{46}$$

determines the longitudinal oscillations of the system which occur at frequencies corresponding to zeros of $\epsilon(\mathbf{k},\omega)$.

Case 2 – Transverse oscillations

Using the transverse mode condition ($\mathbf{k}$ perpendicular to $\mathbf{E}$) in equation (45), we get

$$\mathbf{k}^2=\frac{\omega^2}{c^2}\epsilon(\mathbf{k},\omega) \tag{47}$$

Expression (47) is a generic dispersion relation in a material medium whose behavior depends on the form of $\epsilon(\mathbf{k},\omega)$. The knowledge of $\epsilon(\mathbf{k},\omega)$ allow us to study the propagation of transverse wave inside the medium.

In the next sections we will apply the formalism developed here to analyze the properties of an electron gas and the vibration modes of a crystal lattice.

5. Transverse and Longitudinal Oscillations in a Free Electron Gas

Over a wide frequency range, the optical properties of some solids, namely noble metals and doped semiconductors, can be understood based on the free electron gas model [11]. For metals we consider the valence electrons of the constituent atoms of the crystal as conduction electrons free to wander through a lattice of positive ions which maintain the charge neutrality of the system. Within this model the interactions of conduction electrons with themselves and with the ions are ignored. The motion of electrons is damped via collisions with unspecified collision centers (e.g, lattice ions, other electrons, etc.) which occur with a characteristic collision frequency $\gamma=1/\tau$ where τ is the relaxation time of the free electron gas (for metals τ is typically in the order of $10^{-14}s$). Band-structure corrections can be incorporated into an effective mass m_e which is in general different from the free-electron mass m_o.

The fundamental physical quantity that describes the optical and dispersive properties of a system is the dielectric function. In the long-wavelength limit ($\mathbf{k} \to 0$) the dielectric response $\epsilon(\omega, \mathbf{k})$ can be simplified to $\epsilon(\omega, \mathbf{k} = 0) = \epsilon(\omega)$. In this limit, using the Drude–Sommerfeld model for the free-electron gas, the dielectric function is given by [6]

$$\epsilon_{Drude}(\omega) = \epsilon(\infty)\left[1 - \frac{\omega_p^2}{\omega^2 + i\omega\gamma}\right] \tag{48}$$

where $\epsilon(\infty)$ is the relative dielectric constant arisen from the bound charges of the lattice background, γ is the damping coefficient and ω_p given by

$$\omega_p = \sqrt{\frac{ne^2}{m_e\epsilon_0\epsilon(\infty)}} \tag{49}$$

is the bulk plasma frequency of the free electron gas screened by the dielectric constant $\epsilon(\infty)$, where n is the density of charge carriers, m_e is the electron effective mass that incorporates the band structure of the material and $-e$ is the electronic charge. Typical values for plasma frequency for metals are on the order of 10 eV. The significance of plasma frequency will be explored in Subsection 5.1.

The real and imaginary parts of this complex dielectric function $\epsilon_{Drude}(\omega) = \epsilon'(\omega) + i\epsilon''(\omega)$ are expressed as

$$\epsilon'_{Drude}(\omega) = \epsilon(\infty)\left[1 - \frac{\omega_p^2}{\omega^2 + \gamma^2}\right] \tag{50}$$

$$\epsilon''_{Drude}(\omega) = \epsilon(\infty)\frac{\gamma\omega_p^2}{\omega(\omega^2 + \gamma^2)} \tag{51}$$

Despite its simplicity, the Drude–Sommerfeld model gives accurate results for the optical properties of metals in the infrared and visible regimes, although, in the latter case, it is necessary to take into account the bound electrons and transitions between electronic bands.

Parameters $\epsilon(\infty), \gamma$ and ω_p are chosen in order to reproduce the experimental results. For gold, for example, these parameters are: $\epsilon(\infty) = 9.84$, $\hbar\omega_p = 9$ eV and $\hbar\gamma = 0.072$ eV [12]. As in the visible range ω is smaller than ω_p the real part of ϵ_{Dru} becomes negative. As a result, electromagnetic waves are totally reflected in the region with $\epsilon'(\omega) < 0$.

5.1. Longitudinal oscillations of the free electron gas. Plasmon excitation

Equation (46) states that the zeros of the dielectric function determine the frequencies of the longitudinal electromagnetic modes. We can see from equations (31) and (46) that for longitudinal ressonance frequency $\mathbf{E}$ is not necessarily null even when $\mathbf{D}$=0. In this case the electric field $\mathbf{E}$ is a pure depolarization field given by $\mathbf{E} = -\mathbf{P}/\epsilon_0$. This means that no external charges are needed to generate an electric field when the system oscillates at the frequency determined by the condition $\epsilon(\omega) = 0$.

In the small damping limit ($\gamma \to 0$) we can see from equation (50) that $\epsilon_L(\omega) = 0$ when (assuming $\epsilon(\infty)$=1)

$$\omega = \omega_{pl}$$

We thus see the significance of the plasma frequency: ω_{pl} corresponds to a collective longitudinal mode, in other words, ω_{pl} is a collective longitudinal oscillation frequency of the conduction electron gas with respect to the background of positive ions cores.

The quanta of this charge oscillation are called bulk plasmons whose energy can be calculated as $E = \hbar\omega_p$ where $\hbar$ is the reduced Planck constant. It is important to emphasize that due to its longitudinal nature, bulk plasmons can not be excited by a transverse wave like an electromagnetic wave.

The method most frequently used for plasmon observation is Electron Energy Loss Spectroscopy (EELS) which is a technique based on inelastic scattering of fast electrons by a sample. Electrons with an energy of several keV are reflected from or transmitted to an electron gas, showing an energy loss equal to integer multiples of the plasmon energy $\hbar\omega_p$. (See, for example, Figure 14.8 of [13]).

Plasma oscillations can also exist on interface between a metallic and a dielectric surface. In the presence of a planar boundary they are called surface plasmons (SPs), which corresponds to an oscillattions in the direction normal to the surface plane and thus acquiring a transversal character. Thereby, unlike bulk plasmons, surface plasmons can couple with photons to generate hybrid excitations called surface plasmon polaritons (SPPs), which propagate along the interface between a conductor and a dielectric material, evanescently confined in the perpendicular direction. The physical properties of SPPs can be obtained solving Maxwell's equations and using the appropriate boundary conditions as shown in detail in reference [14].

The frequency of a surface plasma oscilattion is given by $\omega_S = \omega_p/\sqrt{2}$. Thus, the energy of SPPs is lower than those of bulk plasmons.

5.2. Transverse electromagnetic waves in a free electron gas

Let us now obtain the dispersion relation for transverse electromagnetic waves in a free electron gas. Using (50) in (47) we obtain for dispersion relation

$$\omega_\pm^2 = \frac{1}{2}\left[\omega_p^2 + \frac{k^2c^2}{\epsilon(\infty)} - \gamma^2 \pm \omega_p^2\sqrt{\left(1 + \frac{k^2c^2}{\epsilon(\infty)\omega_p^2} - \frac{\gamma^2}{\omega_p^2}\right)^2 + \frac{4\gamma^2k^2c^2}{\epsilon(\infty)\omega_p^4}}\right] \tag{52}$$

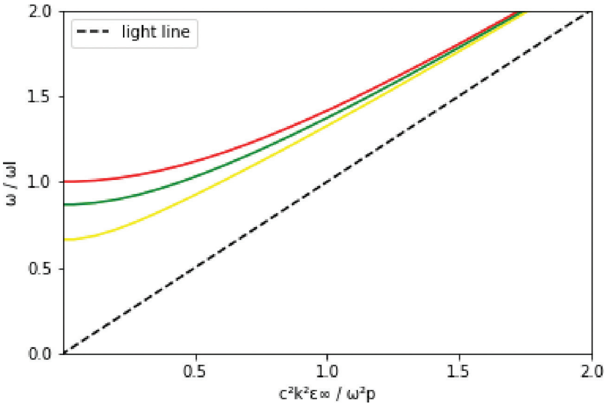

Figure 1: Dispersion relation for transverse electromagnetic waves in a free electron gas with damping.

The resulting dispersion is shown for a generic material in Figure 1 for three different values of γ : $\gamma = 0$ (red curve), $\gamma = 0.1\omega_p$ (green curve) and $\gamma = 0.5\omega_p$ (yellow curve). For $\gamma = 0$ we can see that for $\omega < \omega_p$ the propagation of transverse electromagnetic waves is forbidden inside the material. On the other hand, for $\omega > \omega_p$ the electron gas supports transverse waves propagating with group velocity $vg = d\omega/d\mathbf{K} < c$. Thus, we see that ω_p also represents the low frequency cutoff for the transverse electromagnetic waves in a free electron gas. With damping ($\gamma > 0$) we can see that the cutoff frequency is lower than the plasma frequency, i.e., the wave can propagate at a frequency lower than the plasma frequency.

6. Phonon Contribution to Dielectric Function

In the previous section we considered only the contribution of free conduction electrons to the dielectric function. However, there is a large number of physical properties of solids for which the consideration of lattice is fundamental.

Let us now consider the contribution of the crystal lattice to the dielectric function, in particular the contribution of the vibrational modes of crystalline lattices.

For a diatomic linear lattice the resulting dispersion relation $\omega(\mathbf{k})$ presents two branches: the lower part of the dispersion relation is called the acoustic branch and the upper part is called optical branch [13]. The acoustic branch show a linear relationship between frequency and phonon wave-vector in long wavelength limit. This is the reason why this branch is called acoustic. The branches that have a non-zero frequency in the limit $k \to 0$ are called optical branches. When we have two different atoms in the unit cell, vibrating out of phase, the optical modes create a time-varying electric dipole moment which can be excited by electromagnetic radiation (these vibrations can emit or absorb light); thus these modes are responsible for most optical behavior of a crystal.

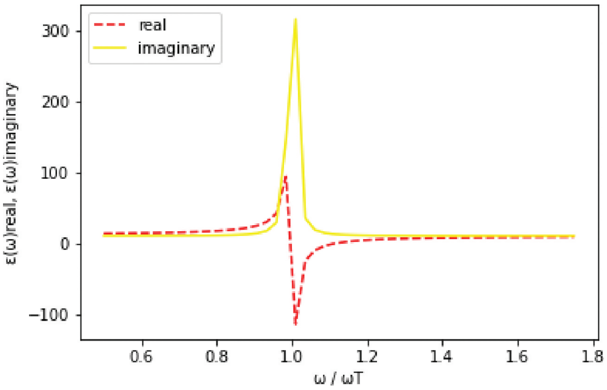

Figure 2: Phonon contribuition to the dieletric function.

The quanta of these normal modes of vibration are called phonons. Thus, a phonon is a quantum of crystal vibrational energy. In the acoustic and optical branches we have longitudinal LA and transverse TA acoustic and longitudinal LO and transverse TO optical modes.

Initially we must write the expression for the dielectric function. For a collection of classical charged simple harmonic oscillators of charge Q, mass M and natural vibrational frequency ω_T the classical expression [2] for the dielectric function is given by [16]

$$\epsilon_{lattice}\left(\omega\right) = \epsilon(\infty) + \frac{NQ^2}{\epsilon_0 M(\omega_T^2 - \omega^2 - i\Gamma\omega)} \tag{53}$$

where N is the number of oscillators per unit volume, $\epsilon(\infty)$ is the high frequency dielectric constant and Γ is a damping constant. The real and imaginary parts of ϵ_{latt} can be written as

$$\epsilon\prime_{latt}(\omega) = \epsilon(\infty)\left[1 + \frac{\left(\omega_L^2 - \omega_T^2\right)\left(\omega_T^2 - \omega^2\right)}{\left(\omega_T^2 - \omega^2\right)^2 + \left(\Gamma\omega\right)^2}\right] \tag{54}$$

$$\epsilon\prime\prime_{latt}(\omega) = \epsilon(\infty)\frac{\left(\omega_L^2 - \omega_T^2\right)\Gamma\omega}{\left(\omega_T^2 - \omega^2\right)^2 + \left(\Gamma\omega\right)^2} \tag{55}$$

where ω_L is given by equation (56). A plot of the real and imaginary parts of $\epsilon_{lattice}(\omega)$ for $\Gamma/\omega_T = 0.05$, $\omega_L/\omega_T = 1.12$ and $\epsilon(\infty) = 10$ (which are typical values for semiconductors) is shown in Figure 2. A resonant behavior is observed for the imaginary part and dispersionlike behavior is observed for the real part. Also we can see that the real part is negative between the TO and LO phonon frequencies.

6.1. Plasmon-optical phonon coupling

The excitation frequency that corresponds to a longitudinal mode must obey condition (46). Neglecting

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[2] A quantum mechanical expression for dielectric function of the lattice can be found in [15].

damping, we see from equation (53) that ω_L is given by

$$\omega_L^2 = \omega_T^2 + \frac{NQ^2}{\epsilon_0 \epsilon(\infty) M} \tag{56}$$

Thus, ω_L is the frequency that characterizes the longitudinal resonance frequency of the phonon subsystem. Likewise, the plasma frequency ω_P represents the longitudinal resonance frequency of the free electron gas subsystem. From equation (56) we can see that ω_L (the longitudinal resonance frequency) is always greater than ω_T (the transverse resonance frequency). Longitudinal optical phonons and photons cannot couple. However, LO phonons can couple with plasmon since both are longitudinal. The expression for the coupled plasmon-phonon LO modes is obtained considering the contribution of plasmons and phonons to the dielectric function of the system. The total dielectric function is given by

$$\epsilon_{total}(\omega) = \epsilon(\infty) + \chi_{Drude} + \chi_{latt} \tag{57}$$

Calculating χ_{Drude} and χ_{latt} from equations (50) and (54) we obtain in the limit of zero damping

$$\epsilon_{total}(\omega) = \epsilon(\infty)\left[1 + \frac{\omega_L^2 - \omega_T^2}{\omega_T^2 - \omega^2} - \frac{\omega_{pl}^2}{\omega^2}\right] \tag{58}$$

Thus, if the equation (58) is set equal to zero we obtain the biquadratic equation

$$\omega_\pm^2 = \frac{1}{2}\left[\left(\omega_L^2 + \omega_p^2\right) \pm \sqrt{\left(\omega_L^2 + \omega_p^2\right)^2 - 4\omega_p^2\omega_T^2}\right] \tag{59}$$

Figure 3 shows a plot of equation (59) against ω_p. We can see two branches: one upper (ω_+) and one lower (ω_-) which are mixtures of longitudinal phonon and plasmon. For small values of ω_p (lower free carrier concentration n) the lower branch has a plasmon-like behavior and when ω_p increases this branch becomes phononlike. Conversely, at low ω_p the upper branch is mainly an LO phonon and approaches to plasmon as ω_p increases.

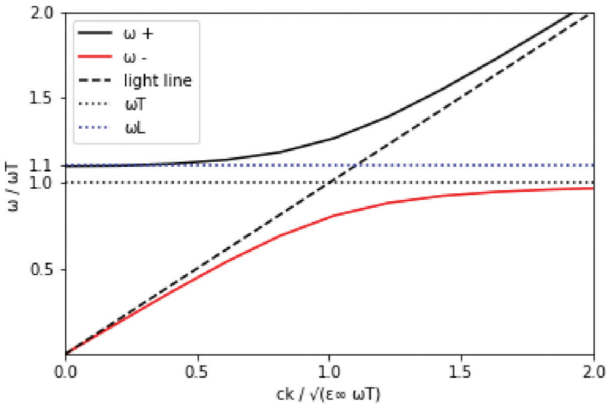

Figure 3: Plasmon-Longitudinal Optical Phonon coupled modes.

6.2. Phonon polariton. Dispersion relation

As already noted, due to its longitudinal nature, bulk plasmon cannot interact with electromagnetic waves. However, electromagnetic waves can couple to transverse excitations like TO phonons. The resultant transverse wave is known as a phonon-polariton. In a quantum mechanical picture phonon-polariton are quasiparticles resulting from the coupling between photon and transverse optical phonons.

Generally speaking, polaritons can be defined as quasiparticles that result from the interaction between photons and another quasiparticle. So we can have different types of polariton: phonon polariton, exciton polariton and plasmon polariton. Here we will only discuss phonon-polariton, which are admixtures of electromagnetic waves and lattice vibrations. The determination of the dispersion relation of the coupled phonon-photon transverse wave proceeds in a similar way as in the plasmon case. We obtain the dispersion relation for the phonon-polariton using (53) in (47). Neglecting damping and using equation (56) we get

$$\omega_\pm^2 = \frac{1}{2}\left[\omega_L^2 + \frac{c^2k^2}{\epsilon(\infty)} \pm \sqrt{\left(\omega_L^2 + \frac{c^2k^2}{\epsilon(\infty)}\right)^2 - 4\omega_T^2\frac{c^2k^2}{\epsilon(\infty)}}\right] \tag{60}$$

The dispersion relation given by equation (60) represents the coupling between photon and transverse optical phonon.

Figure 4 shows a plot of equation (60) for $\omega_L = 1.097\omega_T$. The dotted lines represent the dispersion curves in the absence of coupling for phonons and photons. The curves represented by solid lines show the dispersion relation for the bulk phonon polariton. We can see two branches: one upper (ω_+) and one lower (ω_-). When $\mathbf{k} \to 0$ the upper branch approaches to the longitudinal resonant frequency ω_L and shows phonon-like behavior while the lower branch approaches to $\omega = ck/\sqrt{\epsilon(\infty)}$ and exhibits a phonon-like behavior. In the opposite limiting case, $\mathbf{k} \to \infty$, the upper branch approaches to $\omega = ck/\sqrt{\epsilon(\infty)}$ while the lower branch

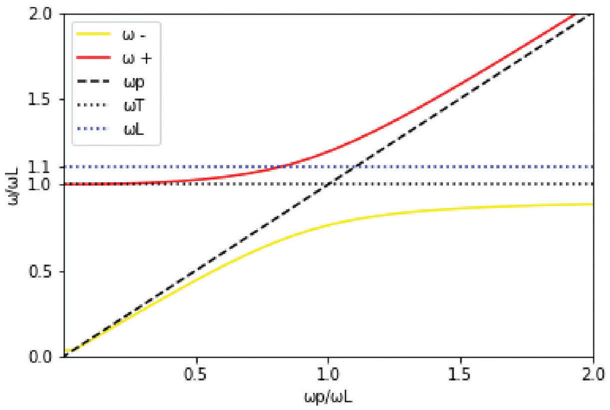

Figure 4: Dispersion relation for the phonon-polariton.

approaches asymptotically the transverse resonance frequency ω_T, represented by the horizontal straight line. We can also observe that there are no polariton modes in the range frequency $\omega_T < \omega < \omega_L$ (called gap polariton); within this frequency range the wavevector is purely imaginary and the wave is attenuated.

7. Conclusion

Maxwell's equations are normally presented in the time and space domain. However, Maxwell's equations in Fourier domain are much more suitable for investigating the optical properties of materials. In this work Maxwell's equations' Fourier transforms are presented and their benefits are emphasized. To clarify and show the scope of this formalism, we presented how elementary excitations in solids arise.

From equation (45), which is the wave equation in the Fourier domain, we can obtain the very general conditions for collective longitudinal oscillations to occur in the medium, given by equation (46), and the condition of propagation of transverse waves, given by equation (47). From these equations and knowing the dielectric function of the system, it is possible to describe elementary excitations in solids and the coupling between them that gives rise to new quasiparticles. In this case, the dispersion curve has two branches – the upper and the lower – and exhibit an anticrossing behavior, as seen in Figures 3 and 4.

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Supplementary Material

The following online material is available for this article:
Appendix A

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