Chapter 2
Basic Electromagnetic Theory

In this chapter, an introduction to the basic electromagnetic concepts that are needed to understand this dissertation are discussed. A full overview of electromagnetics is beyond the scope of this work, and so only the most relevant concepts are reviewed. The reader interested in a more in-depth analysis is referred to Refs. [1, 2].

2.1 Maxwell's Equations

The interaction of light with matter in the classical continuum limit (many hundreds of atoms or more) is described by Maxwell's equations,

$$\frac{\partial}{\partial t}\mathbf{D}(\mathbf{x},t) + \mathbf{J}(\mathbf{x},t) = \nabla \times \mathbf{H}(\mathbf{x},t) \tag{2.1}$$

$$\frac{\partial}{\partial t}\mathbf{B}(\mathbf{x},t) = -\nabla \times \mathbf{E}(\mathbf{x},t) \tag{2.2}$$

$$\nabla \cdot \mathbf{D}(\mathbf{x},t) = \rho \tag{2.3}$$

$$\nabla \cdot \mathbf{B}(\mathbf{x},t) = 0 \tag{2.4}$$

where $\mathbf{E}(\mathbf{x}, t)$ is the electric field, $\mathbf{D}(\mathbf{x}, t)$ is the electric displacement field, $\mathbf{B}(\mathbf{x}, t)$ is the magnetic field, $\mathbf{H}(\mathbf{x}, t)$ is the auxiliary magnetic field (sometimes referred to as just the magnetic field), and $\mathbf{J}(\mathbf{x}, t)$ and ρ are the external current and charge densities, respectively. (In this work, both $\mathbf{B}(\mathbf{x}, t)$ and $\mathbf{H}(\mathbf{x}, t)$ will be referred to as the magnetic field, with the reference clear from the context. Although, it is worth emphasizing that the former is the fundamental quantity, and the latter is a derived one [2]. While collectively known as Maxwell's equations, Eqs. 2.1–2.4 are individually known as the Maxwell–Ampére law, Faraday's law, Gauss' law, and Gauss' law for magnetism, respectively. Before these equations can be solved,

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relationships between both **D**(**x**, t) and **E**(**x**, t) as well as **B**(**x**, t) and **H**(**x**, t) are needed. In this work, a linear constitutive relationship between **B**(**x**, t) and **H**(**x**, t) is assumed, $\mathbf{B}(\mathbf{x},t) = \mu\mathbf{H}(\mathbf{x},t)$, where μ is the permeability of the medium. Furthermore, in applications only nonmagnetic materials will be considered ($\mu = \mu_0$, where μ_0 is the vacuum permeability). In this case, the interaction of light with matter is completely described by the relationship between **D**(**x**, t) and **E**(**x**, t), which is further discussed below, and then again in Chap. 8.

Another fundamental equation, which is not technically one of Maxwell's, but can derived from Eqs. 2.1 and 2.3, is that of continuity

$$\nabla \cdot \mathbf{J}(\mathbf{x},t) = -\frac{\partial}{\partial t}\rho, \tag{2.5}$$

which is the mathematical form of the law of conservation of charge.

As written, the quantities in Eqs. 2.1–2.4 are functions of **x** and t. However, Maxwell's equations can be written in a variety of other forms, which are often useful for solving particular problems. The additional form of most relevance herein corresponds to when the field quantities have a time-harmonic oscillation, $e^{-i\omega t}$, where ω is the angular frequency (often referred to as simply the frequency). The reason for this is that most materials have an electromagnetic response that depends on ω, such as Au or Ag [3, 4] (which are the focus of this work); see Sect. 2.3. In this case, by Fourier transforming Eqs. 2.1–2.4 (see Appendix A.1), Maxwell's equations become

$$-i\omega\mathbf{D}(\mathbf{x},\omega) + \mathbf{J}(\mathbf{x},\omega) = \nabla \times \mathbf{H}(\mathbf{x},\omega) \tag{2.6}$$

$$-i\omega\mathbf{B}(\mathbf{x},\omega) = -\nabla \times \mathbf{E}(\mathbf{x},\omega) \tag{2.7}$$

$$\nabla \cdot \mathbf{D}(\mathbf{x},\omega) = \rho \tag{2.8}$$

$$\nabla \cdot \mathbf{B}(\mathbf{x},\omega) = 0, \tag{2.9}$$

where the quantities are defined similar to before, but are now functions of ω rather than t. It should be understood herein that any time that time-domain quantities are discussed that the frequency-domain solutions may be obtained by Fourier transformation, and vice-versa; Appendix A.1. In passing, it is noted that electrostatics is the limiting case of Eqs. 2.6–2.9 as $\omega \to 0$.

In some cases, it can be beneficial to work with a single equation in terms of **B** and **H** or **D** and **E** alone. For example, working in the frequency domain, simple manipulations of Eqs. 2.6 and 2.7 gives

$$\nabla \times \left[\frac{1}{\mu}\nabla \times \mathbf{E}(\mathbf{x},\omega)\right] - \omega^2\mathbf{D}(\mathbf{x},\omega) = i\omega\mathbf{J}(\mathbf{x},\omega) \tag{2.10}$$

$$\nabla \times \left[\frac{1}{\varepsilon}\nabla \times \mathbf{H}(\mathbf{x},\omega)\right] - \omega^2\mathbf{B}(\mathbf{x},\omega) = \nabla \times \left[\frac{1}{\varepsilon}\mathbf{J}(\mathbf{x},\omega)\right], \tag{2.11}$$

where ε is the permittivity of the medium (where no specific functional dependence is yet attached to this quantity). [Technically, Eq. 2.11 can only be obtained by assuming a linear constitutive relationship between **D** and **E**, i.e., $\mathbf{D}(\mathbf{x}, \omega) = \varepsilon \mathbf{E}(\mathbf{x}, \omega)$.] Equations 2.10 and 2.11 are known as the (inhomogeneous) vector wave equations, and they automatically satisfy Eqs. 2.8 and 2.9.

If the system is invariant along an axis, which herein will be taken to be the z-axis, Eqs. 2.10 and 2.11 can be simplified to (inhomogeneous) scalar wave equations,

$$\left[\frac{\partial}{\partial x}\left(\frac{1}{\mu}\frac{\partial}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{1}{\mu}\frac{\partial}{\partial y}\right)\right] E_z(\mathbf{x}, \omega) + \omega^2 D_z(\mathbf{x}, \omega) = i\omega J_z(\mathbf{x}, \omega) \tag{2.12}$$

$$\begin{aligned}\left[\frac{\partial}{\partial x}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{1}{\varepsilon}\frac{\partial}{\partial y}\right)\right] H_z(\mathbf{x}, \omega) + \omega^2 B_z(\mathbf{x}, \omega) \\ = -\frac{\partial}{\partial x}\left[\frac{1}{\varepsilon} J_y(\mathbf{x}, \omega)\right] + \frac{\partial}{\partial y}\left[\frac{1}{\varepsilon} J_x(\mathbf{x}, \omega)\right],\end{aligned} \tag{2.13}$$

where the electromagnetic field is completely defined by the z-component. Equations 2.12 and 2.13 correspond to two distinct sets of polarization, one where the x and y-components of $\mathbf{E}(\mathbf{x}, \omega)$ and $\mathbf{D}(\mathbf{x}, \omega)$ are transverse to the z-axis, called TE_z polarization (Transverse Electric to z), Eq. 2.12, and one where the x and y-components of $\mathbf{H}(\mathbf{x}, \omega)$ and $\mathbf{B}(\mathbf{x}, \omega)$ are transverse to the z-axis, called TM_z polarization (Transverse Magnetic to z), Eq. 2.13.

2.2 Boundary Conditions

Many functions satisfy Maxwell's equations. However, the physical solution also satisfies boundary conditions. For example, at the interface between two media, the electromagnetic fields must satisfy four field continuity conditions,

$$\hat{n} \times (\mathbf{E}_1 - \mathbf{E}_2) = 0 \tag{2.14}$$

$$\hat{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_S \tag{2.15}$$

$$\hat{n} \times (\mathbf{H}_1 - \mathbf{H}_2) = \mathbf{J}_S \tag{2.16}$$

$$\hat{n} \cdot (\mathbf{B}_1 - \mathbf{B}_2) = 0 \tag{2.17}$$

where the subscripts 1 and 2 denote different mediums, $\hat{n}$ is a unit vector normal to the interface pointing from medium 2 into 1, and ρ_S and $\mathbf{J}_S$ are the surface charge and electric current densities, respectively. The boundary conditions are greatly simplified when one of the mediums cannot sustain internal fields, known as a perfect electric conductor (PEC),

$$\hat{n} \times \mathbf{E} = 0 \tag{2.18}$$

$$\hat{n} \cdot \mathbf{B} = 0 \tag{2.19}$$

where **E** and **B** are the exterior fields, and $\hat{n}$ points away from the surface. Note that, in this case, the boundary can always support surface charge and current densities,

$$\hat{n} \cdot \mathbf{D} = \rho_S \tag{2.20}$$

$$\hat{n} \times \mathbf{H} = \mathbf{J}_S. \tag{2.21}$$

2.3 The Dielectric Function

As mentioned in Sect. 2.1, before Maxwell's equations (in any form) can be solved, relationships between **B** and **H** as well as **D** and **E** are needed. The former was already given, and thus (herein) the latter describes completely how a system responds to light. In the most general case

$$\mathbf{D}(\mathbf{x}, \omega) = \varepsilon_0 \int d\mathbf{x}' \varepsilon(\mathbf{x}, \mathbf{x}', \omega) \mathbf{E}(\mathbf{x}', \omega), \tag{2.22}$$

where $\varepsilon(\mathbf{x}, \mathbf{x}', \omega)$ is a spatially dependent and frequency dispersive relative dielectric function and ε_0 is the vacuum permittivity. Thus, the optical response of a material is described through $\varepsilon(\mathbf{x}, \mathbf{x}', \omega)$, and $\mathbf{D}(\mathbf{x}, \omega)$ can be considered a generalized $\mathbf{E}(\mathbf{x}, \omega)$ that contains information on both the incident $\mathbf{E}(\mathbf{x}, \omega)$ and that due to polarization of the material.

The approximation $\varepsilon(\mathbf{x}, \mathbf{x}', \omega) \approx \varepsilon(\omega)\delta(\mathbf{x} - \mathbf{x}')$ corresponds to local electrodynamics, where only ω is variable. Such an approximation is valid for large structures (those with features greater than ~ 10 nm), and is made for the first portion of this dissertation. The more rigorous case is the subject of Chap. 8.

For a lot of materials at the nanoscale, the dielectric function depends on ω (i.e., with respect to ω, the material is dispersive). For metals like Au and Ag, $\varepsilon(\omega)$ is well described in the classical continuum limit (i.e., many hundreds of atoms or more) by three separate components,

$$\varepsilon(\omega) = \varepsilon_\infty + \varepsilon_{\text{inter}}(\omega) + \varepsilon_{\text{intra}}(\omega) \tag{2.23}$$

the value as $\omega \rightarrow \infty$, ε_∞, the interband contribution from *d*-band to *sp*-band (conduction band) electron transitions, $\varepsilon_{\text{inter}}(\omega)$, and a contribution due to excitations of the *sp*-band electrons, $\varepsilon_{\text{intra}}(\omega)$.

$\varepsilon_{\text{inter}}(\omega)$ can be physically described using a multipole Lorentz oscillator model [5],

$$\varepsilon_{\text{inter}}(\omega) = \sum_n \frac{\omega_{\text{L}n}^2 \Delta\varepsilon_{\text{L}n}}{\omega(\omega + i2\delta_{\text{L}n}) - \omega_{\text{L}n}^2} \tag{2.24}$$

where n is an index labeling the individual d-band to sp-band electron transitions occurring at $\omega_{\mathrm{L}n}$, $\Delta\varepsilon_{\mathrm{L}n}$ is the shift in relative permittivity at the transition, and $\delta_{\mathrm{L}n}$ is the electron dephasing rate. Because the primary focus in this work is on Ag and Au, n is taken to be two, since there are two interband transitions in Au at optical frequencies (near 3 and 4 eV [3]), and only one in Ag (near 3.8 eV, which both poles thus describe).

$\varepsilon_{\mathrm{intra}}(\omega)$ is responsible for the plasmonic optical response of metals, and can be described by the Drude model [5],

$$\varepsilon_{\mathrm{intra}}(\omega) = -\frac{\omega_{\mathrm{D}}^2}{\omega(\omega + i\gamma)} \tag{2.25}$$

where ω_{D} is the plasma frequency and γ is the collision frequency.

Combined, Eqs. 2.23–2.25 correspond to a Drude plus two Lorentz pole oscillator (D2L) dielectric model. The common method to use the D2L model is to fit it to experimentally determined bulk dielectric data (using simulated annealing, for example). For Ag and Au, two of the most common experimental data sets, and which will be used in this work, are those of Johnson and Christry (JC) [3] and Lynch and Hunter (LH) [4]. The D2L model often describes the empirical data well, with only negligible differences.

The use of models for ε is advantageous for a number of reasons. First of all, it allows separation of the different effects in the optical response of a material. For example, physical insight can be obtained into the conduction band electron motion separate from that of the interband transitions. (This issue will be revisited in Chap. 8.) Furthermore, such models are common with time-domain computational methods, such as FDTD (see Sect. 3.2), since the frequency-domain data cannot be used directly. For frequency-domain methods, however, the empirically determined dielectric data can be used directly. Although, in this work, even these methods rely on the D2L model, primarily to create a cohesiveness throughout the work, but also because of the other advantages discussed.

Throughout this work, various D2L fits are used for Ag and Au (for one reason or another), as well as other materials. The D2L parameters used for all calculations have been tabulated in Appendix B.

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