Quantum theory of light-matter interaction: Fundamentals

Lecture 1
Maxwell equations and wave propagation in a medium

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The macroscopic Maxwell equations in a medium

The phenomenological form of the Maxwell equations is

$$\nabla \times \mathbf{H}(\mathbf{r},t) - \dot{\mathbf{D}} = \mathbf{J}_m, \tag{M1}$$

$$\nabla \times \mathbf{E}(\mathbf{r},t) + \dot{\mathbf{B}} = 0, \tag{M2}$$

$$\nabla \mathbf{D} = \rho_m, \tag{M3}$$

$$\nabla \mathbf{B} = 0. \tag{M4}$$

Here ρ_m and $\mathbf{J}_m$ are the charges and currents available for macroscopic measurements. They can be derived from the Maxwell-Lorentz equations with microscopic (atomic) charges and currents by taking a *spatial* average [1].
The phenomenological quantities $\mathbf{D}$ and $\mathbf{H}$ are those parts of the electric and magnetic fields that are created only by the charges and currents, which are seen macroscopically.

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}, \qquad \mathbf{H} = \frac{1}{\mu_0}\mathbf{B} - \mathbf{M}.$$

The macroscopic Maxwell equations in a medium II

The difference between $\mathbf{D}$ and $\mathbf{E}$ is hidden in the presence of atomic polarization charges $\rho_P = -\nabla\mathbf{P}$; in polarization currents $\mathbf{J}_P = \dot{\mathbf{P}}$; and that between $\mathbf{B}$ and $\mathbf{H}$ in the presence of magnetic currents $\mathbf{J}_{mag} = \nabla \times \mathbf{M}$.

In a little more detail:
The source of $\mathbf{E}$ is the total charge in the medium which is $\rho_m + \rho_P$, therefore the macroscopic electric field obeys

$$\nabla\mathbf{E} = \frac{1}{\epsilon_0}(\rho_m + \rho_P) = \frac{1}{\epsilon_0}(\rho_m - \nabla\mathbf{P}),$$

leading to:

$$\nabla(\epsilon_0\mathbf{E} + \mathbf{P}) = \rho_m, \quad \text{i.e.,} \quad \nabla\mathbf{D} = \rho_m.$$

Similarly the total current in a medium is $\mathbf{J}_m + \mathbf{J}_P + \mathbf{J}_{mag}$, the macroscopic $\mathbf{E}$ and $\mathbf{B}$ obey therefore:

$$\nabla \times \mathbf{B}(\mathbf{r},t) - \epsilon_0\mu_0\dot{\mathbf{E}} = \mu_0(\mathbf{J}_m + \mathbf{J}_P + \mathbf{J}_{mag}) = \mu_0(\mathbf{J}_m + \dot{\mathbf{P}} + \nabla \times \mathbf{M}),$$

$$\text{which is equivalent to} \qquad \nabla \times \mathbf{H} - \dot{\mathbf{D}} = \mathbf{J}_m.$$

The inhomogeneous wave equation

From the viewpoint of *optical fields*

1. The magnetic properties of the medium are inessential: $\mathbf{M}=0$ in most cases. Then magnetic fields are connected like in vacuum, $\mathbf{B}=\mu_0\mathbf{H}$.
2. Macroscopic currents are absent or do not play any role: $\rho_m=0$, but we keep $\mathbf{J}_P=\dot{\mathbf{P}}$.

Field losses can be essential in certain cases, and can be introduced by a term proportional to $\dot{\mathbf{E}}$, the first time derivative of $\mathbf{E}$ which is not invariant with respect to time reversal. This is done usually with a fictitious conductivity, σ which – like in a metal – can represent the losses, even in nonconducting materials by writing

$$\mathbf{J}_m=\sigma\mathbf{E}.$$

The curl of the second Maxwell equation and the time derivative of the first one, yields for $\mathbf{E}$:

$$\nabla\times\nabla\times\mathbf{E}+\mu_0\sigma\,\dot{\mathbf{E}}+\mu_0\epsilon_0\ddot{\mathbf{E}}=-\mu_0\ddot{\mathbf{P}}$$

or $$\nabla(\nabla\mathbf{E})-\Delta\mathbf{E}+\mu_0\sigma\dot{\mathbf{E}}+\frac{1}{c^2}\ddot{\mathbf{E}}=-\mu_0\ddot{\mathbf{P}}$$

The inhomogeneous wave equation

The previous equation is now

$$-\nabla(\nabla\mathbf{E})+\Delta\mathbf{E}-\mu_0\sigma\dot{\mathbf{E}}-\ddot{\mathbf{E}}/c^2=\mu_0\ddot{\mathbf{P}}.$$

$\nabla\mathbf{E}\approx 0$ in optics, since most light field vectors vary little along the directions in which they propagate. For example, a plane wave field is transversal, causing $\nabla\mathbf{E}$ to vanish identically. Further on we shall also neglect the direct field losses so we omit the term with $\dot{\mathbf{E}}$:

$$\Delta\mathbf{E}-\frac{1}{c^2}\ddot{\mathbf{E}}=\mu_0\ddot{\mathbf{P}}. \tag{inhwave}$$

This is the well known inhomogeneous wave equation, the source term on the right hand side is the polarization originating from the atomic dipole moments
In most cases we assume a field propagation in one direction, let it be the z direction, and a linearly polarized electric field, as well as polarization density both in the $\hat{\mathbf{x}}$ direction
$\mathbf{E}=E\hat{\mathbf{x}}$, $\mathbf{P}=P\hat{\mathbf{x}}$.
Equation (inhwave) now becomes:

$$\frac{\partial^2 E}{\partial z^2}-\frac{1}{c^2}\frac{\partial^2 E}{\partial t^2}=\mu_0\frac{\partial^2 P(z,t)}{\partial t^2}. \tag{lpwave}$$

Quasi monochromatic fields, positive and negative frequency parts

We are concerned mostly with the interaction of *quasi-monochromatic* light with matter. Then the field can be written as

$$E(z,t) = E^+(z,t) + E^-(z,t)$$

with

$$E^+(z,t) = \frac{1}{2}E_0(z,t)\exp[i(kz - \omega t - \phi(z,t)], \qquad E^-(z,t) = (E^+(z,t))^*.$$

Here $E_0(z,t)$ and $\phi(z,t)$ are the *real amplitude* and the real *phase* "constant" .
Be aware that in the older literature the factor of 1/2 was usually omitted!
Very often one also uses the complex amplitude

$$\mathcal{E}^+(z,t) = E_0(z,t)e^{-i\phi(z,t)},$$
$$E^+(z,t) = \frac{1}{2}\mathcal{E}^+(z,t)\exp[i(kz - \omega t)].$$

$E^+(z,t)$ is the positive frequency component, $E^-(z,t)$ is the negative frequency component of the field. In the semiclassical description this separation and the introduction of the complex quantities is only a convenient tool but it acquires important physical significance in *quantum optics*, where E^+ and E^- become distinct operators.

Slowly varying envelope approximation SVEA

If $E(z,t)$ is truly monochromatic, then E_0 and ϕ are constants in time and space.
More generally, in the quasi monochromatic case we can suppose that they vary sufficiently slowly in time and space on the time scale $2\pi/\omega$ and spatial distance $2\pi/k = \lambda$, i.e., on the time and spatial period of the phase in the exponent.
Mathematically this means that

$$\left|\frac{\partial}{\partial t}\mathcal{E}^+(z,t)\right| \ll |\omega\mathcal{E}^+(z,t)|, \quad \left|\frac{\partial}{\partial z}\mathcal{E}^+(z,t)\right| \ll k|\mathcal{E}^+(z,t)|. \qquad \text{(SVEA)}$$

Which is equivalent to the inequalities

$$\left|\frac{\partial}{\partial t}E_0(z,t)\right| \ll \omega E_0(z,t), \quad \left|\frac{\partial}{\partial z}E_0(z,t)\right| \ll kE_0(z,t),$$
$$\left|\frac{\partial}{\partial t}\phi(z,t)\right| \ll \omega, \quad \left|\frac{\partial}{\partial z}\phi(z,t)\right| \ll k$$

for the real amplitude and phase.

Slowly varying envelope approximation SVEA

For a quasi-monochromatic field, the polarization induced in the medium $P(z,t)$ is also quasi-monochromatic, for an isotropic medium it is of the same direction as $\mathbf{E}$, but in general *its phase is different from that of the field.* The polarization is also decomposed into positive and negative frequency parts:

$$P(z,t) = P^{+}(z,t) + P^{-}(z,t),$$

$$P^{+}(z,t) = \frac{1}{2}\mathcal{P}^{+}(z,t)\exp[i(kz-\omega t)] = \frac{1}{2}P_0\exp[i(kz-\omega t) - i\phi(z,t)],$$

but we do not assume that P_0 is real. The phase of P_0 will be just be the *phase shift* between $\mathcal{E}^{+}$ and $\mathcal{P}^{+}$.
In order to proceed, we substitute $E^{+}(z,t)$ and $P^{+}(z,t)$ into the wave equation, calculate the necessary time and spatial derivatives and make use of $k = \omega/c$. Additionally, we neglect the second derivatives $\frac{\partial^2}{\partial z^2}\mathcal{E}^{+}(z,t)$, $\frac{\partial^2}{\partial t^2}\mathcal{E}^{+}(z,t)$ when compared with terms $\frac{\partial}{\partial z}\mathcal{E}^{+}(z,t)$, $\frac{\partial}{\partial t}\mathcal{E}^{+}(z,t)$, as well as both the first and the second time derivative of $\mathcal{P}^{+}$ compared with $\omega^2\mathcal{P}^{+}$. This yields

$$\left(\frac{\partial}{\partial z} + \frac{1}{c}\frac{\partial}{\partial t}\right)\mathcal{E}^{+}(z,t) = \frac{ik}{2\epsilon_0}\mathcal{P}^{+}.$$

Amplitude and phase equations

As we have just obtained,

$$\left(\frac{\partial}{\partial z}+\frac{1}{c}\frac{\partial}{\partial t}\right)\mathcal{E}^{+}(z,t)=\frac{ik}{2\epsilon_0}\mathcal{P}^{+}.$$

Put $\mathcal{E}^{+}=E_0 e^{-i\phi(z,t)}$, and $\mathcal{P}^{+}=P_0 e^{-i\phi(z,t)}$, with E_0 *real* but P_0 is *not*. By separating the real and imaginary parts, we find

$$\left(\frac{\partial}{\partial z}+\frac{1}{c}\frac{\partial}{\partial t}\right)E_0(z,t)=-\frac{k}{2\epsilon_0}\,\mathrm{Im}\,P_0, \qquad \text{(Amp)}$$

$$E_0\left(\frac{\partial}{\partial z}+\frac{1}{c}\frac{\partial}{\partial t}\right)\phi(z,t)=-\frac{k}{2\epsilon_0}\,\mathrm{Re}\,P_0. \qquad \text{(Phase)}$$

These two equations play a central role in optical physics and quantum optics.

They tell us how light propagates through a medium and specifically how the real and imaginary parts of the polarization act.

Amplitude and phase equations

$$\left(\frac{\partial}{\partial z}+\frac{1}{c}\frac{\partial}{\partial t}\right)E_0(z,t)=-\frac{k}{2\epsilon_0}\,\mathrm{Im}\,P_0 \qquad \text{(Amp)}$$

$$E_0\left(\frac{\partial}{\partial z}+\frac{1}{c}\frac{\partial}{\partial t}\right)\phi(z,t)=-\frac{k}{2\epsilon_0}\,\mathrm{Re}\,P_0 \qquad \text{(Phase)}$$

Equation (Amp) shows that the field amplitude is driven by the imaginary part of the polarization. This in-quadrature component gives rise to absorption and emission.

Equation (Phase) allows us to compute the phase velocity with which the electromagnetic wave propagates in the medium. It is the real part of the polarization, i.e, the part in-phase with the field, that determines the phase velocity. The effects described by this equation are those associated with the index of refraction of the medium, such as dispersion and self focusing.

In both cases the solution requires the knowledge of the source term on the right hand side.

The polarization as an average of atomic dipole moments

The polarization is P, which is the volume density of the dipole moments in the medium, builds up from the individual dipole moments of the entities (atoms, molecules) of the medium.
Denote the number of atoms/(unit volume) by $\mathcal{N}(z)$ in a small but macroscopic (containing many atoms) slice element of the sample around z, and let the time dependent average dipole moment in this slice be denoted by $D_a(z,t)$. Then the dipole moment density, i.e. the polarization is

$$P = \mathcal{N}(z) D_a(z,t).$$

and according to the SVEA we write D_a as

$$D_a = d\frac{X(z,t)}{2} \exp[i(kz - \omega t - \phi(z,t)] + c.c.$$

where d has the dimension of dipole moment being an intrinsic property of the atom and $X(z,t)$ is a slowly varying *dimensionless* amplitude.

The Amplitude and Phase equations II

With the real quantities U and V we write

$$X(z,t) := U(z,t) - iV(z,t)$$

which characterizes the magnitude of the response of the atomic dipole moments to the external field at the actual macroscopic location around z and time t. The polarization amplitude P_0 is obtained accordingly

$$P_0 = d\mathcal{N}(z)(U(z,t) - iV(z,t))$$

With this separation and assuming that d is real, we obtain:

$$\left(\frac{\partial}{\partial z} + \frac{1}{c}\frac{\partial}{\partial t}\right) E_0(z,t) = \frac{k}{2\epsilon_0}\mathcal{N} dV, \qquad \text{(Amp)}$$

$$E_0 \left(\frac{\partial}{\partial z} + \frac{1}{c}\frac{\partial}{\partial t}\right) \phi(z,t) = -\frac{k}{2\epsilon_0}\mathcal{N} dU. \qquad \text{(Phase)}$$

The principle of a self consistent solution

Equations (Amp) and (Phase) alone are not sufficient to describe physical problems completely, since they only tell us how a plane electromagnetic wave responds to a given polarization of the medium. That polarization must still be determined. Of course, we know that the polarization of a medium is influenced by the field to which it is subjected. In particular, for atoms or molecules without permanent polarization, it is the electromagnetic field itself that induces their polarization! Thus the polarization of the medium drives the field, while the field drives the polarization of the medium. In general this leads to a description of the interaction between the electromagnetic field and matter expressed in terms of coupled, nonlinear, partial differential equations that have to be solved self-consistently.

Models of polarization

The quantities on the right hand sides of (Amp) and (Phase) can be calculated from different models

1. *The polarization of a medium is assumed to be simply proportional to the instantaneous value of the field strength. This case will be discussed below in this lecture*
2. *The polarization of a medium consisting of classical simple harmonic oscillators will be discussed in the next lecture*
3. *Lectures 3 and 4 discuss similar media with anharmonic (nonlinear) oscillators.*
4. *Quantum mechanical models of so called two-level atoms or multi-level systems are discussed in later lectures.*

Solution for the linear steady state in terms of the susceptibility

We come to the simplest possibility to determine P_0 (or U and V) by assuming a linear response from the system when

$$P_0 = \{d\mathcal{N}(U - iV)\} = \epsilon_0 \chi E_0(z) = \epsilon_0(\chi' + i\chi'')E_0(z)$$

is assumed to be valid at each time instant, where χ' and χ'' are the real and imaginary parts of the linear susceptibility. An explicit solution of the system (Amp) and (Phase) is possible then in the steady state limit when $\frac{\partial E_0}{\partial t} = 0$. Substituting into (Amp):

$$\frac{d}{dz}E_0(z) = -\frac{k}{2\epsilon_0}\operatorname{Im} P_0 = -\frac{k}{2}\chi'' E_0,$$

$$E_0(z) = E_0(0)e^{-\frac{k}{2}\chi'' z},$$

showing that the imaginary part of χ describes absorbtion.

Solution for the linear steady state in terms of the susceptibility

The (phase) equation allows us to relate the in-phase component of the susceptibility to the index of refraction n. As for the amplitude, we consider the stationary limit, for which $\frac{\partial}{\partial t}\phi(z,t) = 0$.
This, together with $P_0 = \epsilon_0(\chi' + i\chi'')E_0$, gives

$$\frac{d\phi}{dz} = -\frac{k}{2}\chi'.$$

Expanding the slowly varying phase as $\phi(z) = \phi(0) + z d\phi/dz$, we find that the total phase reads

$$kz - \omega t - \phi = kz - \omega t - \phi(0) - z\frac{d\phi}{dz} = -\omega\left(t - \frac{k}{\omega}\left(1 + \frac{1}{2}\chi'\right)z\right),$$

and read off the phase velocity and the real part of the index of refraction:

$$v = \frac{\omega}{k}\frac{1}{1+\chi'/2} = \frac{c}{1+\chi'/2} \quad \Longrightarrow n = 1 + \chi'/2$$

Questions

1. Recall the main physical assumptions beyond the method of Lorentz leading to the phenomenological Maxwell equations.
2. Is the role of the magnetic effects crucial at optical frequencies?
3. What is the source term in the inhomogeneous wave equation for the electric field?
4. What does the term "positive frequency part of a quasi monochromatic field" mean?
5. What does SVEA mean? What are the main assumptions that lead to this approximation?
6. What are the amplitude and phase equations in SVEA?

Questions (continued)

7. What is the physical significance of the imaginary part of the polarization?
8. What is the physical significance of the real part of the polarization?
9. What are the principles of a self consistent description of matter-field interaction?
10. Recall a few physical models of polarization!
11. What physical effect is described by the imaginary part of χ?
12. In the simplest model, which part (real or imaginary) of χ is related to the phase velocity and the index of refraction?

References

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