УНИВЕРСИТЕТ ИТМО

М.А. Горлач, Р.С. Савельев

КОНСПЕКТ ЛЕКЦИЙ ПО «ЭЛЕКТРОДИНАМИКЕ МЕТАМАТЕРИАЛОВ»

Санкт-Петербург
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МИНИСТЕРСТВО НАУКИ И ВЫСШЕГО ОБРАЗОВАНИЯ
РОССИЙСКОЙ ФЕДЕРАЦИИ

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УЧЕБНОЕ ПОСОБИЕ

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The present course of classical electrodynamics is intended for the first year master students studying the program «Nanophotonics and metamaterials». The aim of this course is to provide understanding of the theoretical methods for describing the propagation of electromagnetic radiation in a continuous medium as well as periodic structures. Special attention is paid to the theoretical methods of nanophotonics as well as approaches to the description of metamaterials electromagnetic properties. The present course is composed of two logically connected parts: (i) electrodynamics of a continuous medium; (ii) introduction to nanophotonics and metamaterials.

УНИВЕРСИТЕТ ИТМО

Университет ИТМО – ведущий вуз России в области информационных и фотонных технологий, один из немногих российских вузов, получивших в 2009 году статус национального исследовательского университета. С 2013 года Университет ИТМО – участник программы повышения конкурентоспособности российских университетов среди ведущих мировых научно-образовательных центров, известной как проект «5 в 100». Цель Университета ИТМО – становление исследовательского университета мирового уровня, предпринимательского по типу, ориентированного на интернационализацию всех направлений деятельности.

Contents

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CHAPTER 1

Electrodynamics of a continuous medium

1.1 Maxwell's equations in a medium, constitutive relations

Useful reading: Landau, Lifshitz, vol. 8, Ref. [1].

Formal derivation of Maxwell's equations in a medium.

Maxwell's equations in vacuum in CGS system of units:

$$\mathrm{rot}\,\mathbf{B} = \frac{4\,\pi}{c}\,\mathbf{j} + \frac{1}{c}\,\frac{\partial \mathbf{E}}{\partial t}\,, \tag{1.1}$$

$$\mathrm{div}\,\mathbf{E} = 4\,\pi\,\rho\,, \tag{1.2}$$

$$\mathrm{rot}\,\mathbf{E} = -\frac{1}{c}\,\frac{\partial \mathbf{B}}{\partial t}\,, \tag{1.3}$$

$$\mathrm{div}\,\mathbf{B} = 0\,. \tag{1.4}$$

A medium can be treated as a collection of charged particles and described with Eqs. (1.1)-(1.4). However, this would be impractical. We separate bound charges/currents associated with the medium polarization or magnetization (ρ^{B}, $\mathbf{j}^{\mathrm{B}}$) from the external charges/currents (ρ^{ext}, $\mathbf{j}^{\mathrm{ext}}$):

$$\rho = \rho^{\mathrm{B}} + \rho^{\mathrm{ext}}\,, \tag{1.5}$$

$$\mathbf{j} = \mathbf{j}^{\mathrm{B}} + \mathbf{j}^{\mathrm{ext}}\,, \tag{1.6}$$

where each of pairs ρ^{B}, $\mathbf{j}^{\mathrm{B}}$ and ρ^{ext}, $\mathbf{j}^{\mathrm{ext}}$ satisfies the continuity equation. We define the bound current as follows:

$$\mathbf{j}^{\mathrm{B}} = \frac{\partial \mathbf{P}}{\partial t} + c\;\mathrm{rot}\,\mathbf{M}\,, \tag{1.7}$$

where $\mathbf{P}$ and $\mathbf{M}$ are called the *polarization* and *magnetization* vectors, respectively. Note that Eq. (1.7) defines $\mathbf{M}$ up to the gradient of arbitrary scalar function. As a result, the bound charge density satisfies the equation

$$\frac{\partial \rho^{\mathrm{B}}}{\partial t} = -\,\mathrm{div}\,\mathbf{j}^{\mathrm{B}} = -\frac{\partial\,\mathrm{div}\,\mathbf{P}}{\partial t}\,, \tag{1.8}$$

i.e. we define

$$\rho^{\mathrm{B}} = -\,\mathrm{div}\,\mathbf{P}\,. \tag{1.9}$$

Next we use Eqs. (1.5), (1.6) and put the definitions Eq. (1.7) and (1.9) into

Maxwell's equations in vacuum. We get

$$\operatorname{rot}\mathbf{H} = \frac{4\pi}{c}\mathbf{j}^{\text{ext}} + \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t}\,, \tag{1.10}$$
$$\operatorname{div}\mathbf{D} = 4\pi\,\rho^{\text{ext}}\,, \tag{1.11}$$
$$\operatorname{rot}\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}\,, \tag{1.12}$$
$$\operatorname{div}\mathbf{B} = 0\,, \tag{1.13}$$

where the auxiliary $\mathbf{D}$ and $\mathbf{H}$ fields are defined as

$$\mathbf{D} = \mathbf{E} + 4\pi\,\mathbf{P}\,, \tag{1.14}$$
$$\mathbf{H} = \mathbf{B} - 4\pi\,\mathbf{M}\,. \tag{1.15}$$

Equations (1.10)-(1.13) are known as *Maxwell's equations in a medium*. Equations (1.14)-(1.15) are the so-called *constitutive relations*.

Explaining the physical meaning of $\mathbf{P}$ *and* $\mathbf{M}$*.*

In the reasoning above, vectors $\mathbf{P}$ and $\mathbf{M}$ were introduced formally. Now we analyze their physical meaning.

The time derivative of the system's dipole moment:

$$\begin{aligned}\dot{\mathbf{d}} &= \frac{\partial}{\partial t}\sum_a q_a\,\mathbf{r}_a = \sum_a q_a\,\mathbf{v}_a = \int \mathbf{j}^{\text{B}}\,dV = \\ &= \int \frac{\partial \mathbf{P}}{\partial t}\,dV + c\int \operatorname{rot}\mathbf{M}\,dV = \frac{\partial}{\partial t}\int \mathbf{P}\,dV + \oint_{\Omega}\,[\mathbf{n}\times\mathbf{M}]\;df\,.\end{aligned} \tag{1.16}$$

The surface term vanishes since polarization is zero outside of the medium. Thus, the dipole moment of the finite medium sample reads:

$$\mathbf{d} = \int \mathbf{P}\,dV\,. \tag{1.17}$$

An alternative derivation based on Gauss theorem states (as a homework?):

$$\begin{aligned} d_i &= \int \rho^{\text{B}}\,x_i\,dV = -\int \operatorname{div}\mathbf{P}\,x_i\,dV = -\int\left(\partial_k\,P_k\right)\,x_i dV = \\ &= -\int \partial_k\left(P_k\,x_i\right)\,dV + \int P_k\,\partial_k\,x_i\,dV = \\ &= -\oint P_k\,x_i\,n_k\,df + \int P_i\,dV = \int P_i\,dV\,. \end{aligned} \tag{1.18}$$

The magnetic moment of the system (we neglect the displacement currents here):

$$\mathbf{m} = \frac{1}{2\,c} \int [\mathbf{r} \times \mathbf{j}]\, dV = \frac{1}{2} \int [\mathbf{r} \times \mathrm{rot}\, \mathbf{M}]\, dV\,. \tag{1.19}$$

$$\begin{aligned} \mathbf{r} \times [\nabla \times \mathbf{M}] &= \nabla\, (\mathbf{r} \cdot \underline{\mathbf{M}}) - (\mathbf{r} \cdot \nabla)\, \mathbf{M} = \mathbf{e}_i\, [x_k\, \partial_i\, M_k - x_k\, \partial_k\, M_i] = \\ &= \mathbf{e}_i\, [\partial_i\, (x_k\, M_k) - \delta_{ik}\, M_k - \partial_k\, (x_k\, M_i) + \delta_{kk}\, M_i] = \\ &= \mathbf{e}_i\, [\partial_i\, (x_k\, M_k) - \partial_k\, (x_k\, M_i)] + 2\, \mathbf{M}\,. \end{aligned} \tag{1.20}$$

Volume integrals of the terms like $\partial_k\, T_{ik}$ vanish, because $\int \partial_k\, T_{ik}\, dV = \oint T_{ik}\, n_k\, df$, and finally we obtain

$$\mathbf{m} = \int \mathbf{M}\, dV\,. \tag{1.21}$$

Hence, we define magnetization as the magnetic moment of a unit volume of a medium. Note that this identification is only valid in the low-frequency limit.

Homework. Calculate the time derivative of the electric dipole moment without resorting to the substitution $\int \rho\, \mathbf{r}\, dV = \sum\limits_a q_a\, \mathbf{r}_a$.

Material parameters.

A wide class of linear media is characterized by the linear scalar relation between polarization and electric field. An analogous relation holds for magnetization and magnetic field:

$$\mathbf{P} = \chi^{\mathrm{e}}\, \mathbf{E}\,, \tag{1.22}$$

$$\mathbf{M} = \chi^{\mathrm{m}}\, \mathbf{H}\,. \tag{1.23}$$

The coefficients χ^{e} and χ^{m} are called the electric and magnetic susceptibilities. Normally, they depend on frequency (the so-called frequency dispersion). Their values can be determined either empirically or theoretically. *See Practice 1*.

However, susceptibilities are not necessarily scalar. In a more general case of an anisotropic medium, polarization and magnetization read:

$$P_i = \chi^{\mathrm{e}}_{ik}\, E_k\,, \tag{1.24}$$

$$M_i = \chi^{\mathrm{m}}_{ik}\, H_k\,, \tag{1.25}$$

where the summation over the repeated indices is implied. The permittivity and permeability tensors are defined as

$$\varepsilon_{ik} = \delta_{ik} + 4\,\pi\, \chi^{\mathrm{e}}_{ik}\,, \tag{1.26}$$

$$\mu_{ik} = \delta_{ik} + 4\,\pi\, \chi^{\mathrm{m}}_{ik}\,. \tag{1.27}$$

The material Eqs. (1.24), (1.25) can be rearranged as

$$D_i = \varepsilon_{ik}\, E_k\,, \tag{1.28}$$

$$B_i = \mu_{ik}\, H_k\,. \tag{1.29}$$

1.2 Wave propagation in anisotropic media: the general theory

We consider propagation of a plane electromagnetic wave

$$\tilde{\mathbf{E}} = \mathbf{E}\, e^{i\mathbf{k}\cdot\mathbf{r}-i\omega\, t}\,, \tag{1.30}$$

$$\tilde{\mathbf{H}} = \mathbf{H}\, e^{i\mathbf{k}\cdot\mathbf{r}-i\omega\, t}\,. \tag{1.31}$$

in a non-magnetic anisotropic transparent medium in the absence of external charges and currents. From Maxwell's equations for $\mathrm{rot}\,\tilde{\mathbf{E}}$ and $\mathrm{rot}\,\tilde{\mathbf{H}}$ we obtain linear equations for the field amplitudes:

$$\mathbf{H} = \mathbf{k}\times\mathbf{E}/q\,, \tag{1.32}$$

$$\mathbf{D} = -\mathbf{k}\times\mathbf{H}/q\,, \tag{1.33}$$

where $q = \omega/c$, ω is the angular frequency of the wave and $\mathbf{k}$ is the wave vector.

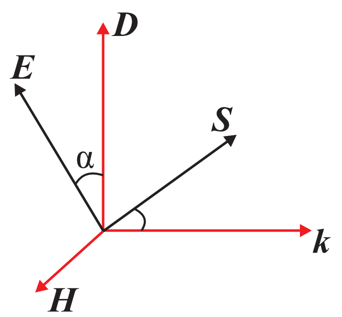

Figure 1.1: Relative alignment of fields in non-magnetic anisotropic medium.

Thus, we notice that the vectors $\mathbf{k}$, $\mathbf{H}$ and $\mathbf{D}$ are mutually orthogonal. Since $\mathbf{H}$ is also orthogonal to $\mathbf{E}$, the vector of electric field lies in the plane defined by the vectors $\mathbf{D}$ and $\mathbf{k}$.

Dispersion equation.

From Eqs. (1.32), (1.33) we obtain:

$$\left[k^2\,\hat{I} - \mathbf{k}\otimes\mathbf{k} - q^2\hat{\varepsilon}\right]\,\mathbf{E} = 0\,. \tag{1.34}$$

Thus, plane wave solutions of Maxwell's equations satisfy the equation

$$\det\left[k^2\,\hat{I} - \mathbf{k}\otimes\mathbf{k} - q^2\hat{\varepsilon}\right] = 0\,. \tag{1.35}$$

For instance, in the system of principal axes of the tensor $\hat{\varepsilon}$ the dispersion equation reads:

$$k^2\,\left[\varepsilon_x\,k_x^2+\varepsilon_y\,k_y^2+\varepsilon_z\,k_z^2\right]-q^2\,\left[k_x^2\,\varepsilon_x\,(\varepsilon_y+\varepsilon_z)+k_y^2\,\varepsilon_y\,(\varepsilon_z+\varepsilon_x)+\right.$$
$$\left.+k_z^2\,\varepsilon_z\,(\varepsilon_x+\varepsilon_y)\right]+q^4\,\varepsilon_x\,\varepsilon_y\,\varepsilon_z=0\,. \quad (1.36)$$

This equation is known in crystal optics as the Fresnel equation. The Fresnel equation is *fourth order* with respect to k. Thus, for the given direction of the wave vector there are *two* refractive indices. Eq. (1.36) determines a surface in k-space known as the *isofrequency surface*.

Note that if the surface is defined by $f(q,\mathbf{k})=0$, $\frac{\partial f}{\partial \mathbf{k}}$ would be the normal to the surface. Since $\frac{\partial f}{\partial q}\frac{\partial q}{\partial \mathbf{k}}+\frac{\partial f}{\partial \mathbf{k}}=0$, the group velocity $\partial\,\omega/\partial\,\mathbf{k}$ is perpendicular to the isofrequency surface. It can be shown that the group velocity and the Poynting vector for an anisotropic medium are parallel. Therefore, *the direction of energy flow is perpendicular to the isofrequency surface*.

Proof that the Poynting vector is normal to the isofrequency surface

We consider the variation of the fields when the direction of propagation is varied (so that $\mathbf{k}$ changes and q stays constant). The variation of equations

$$q\,\mathbf{H}=\mathbf{k}\times\mathbf{E}\,, \quad (1.37)$$
$$q\,\mathbf{D}=-\mathbf{k}\times\mathbf{H} \quad (1.38)$$

yields

$$q\,\delta\mathbf{H}=\delta\mathbf{k}\times\mathbf{E}+\mathbf{k}\times\delta\mathbf{E}\,, \quad (1.39)$$
$$q\,\delta\mathbf{D}=-\delta\mathbf{k}\times\mathbf{H}-\mathbf{k}\times\delta\mathbf{H}\,, \quad (1.40)$$

From these equations we get that

$$\begin{aligned} q\,\mathbf{H}\cdot\delta\mathbf{H}+q\,\mathbf{E}\cdot\delta\mathbf{D}=&\\ &=[\delta\mathbf{k}\times\mathbf{E}]\cdot\mathbf{H}+\mathbf{H}\cdot[\mathbf{k}\times\delta\mathbf{E}]-[\delta\mathbf{k}\times\mathbf{H}]\cdot\mathbf{E}-\mathbf{E}\cdot[\mathbf{k}\times\delta\mathbf{H}]=\\ &=\delta\mathbf{k}\cdot[\mathbf{E}\times\mathbf{H}]+[\mathbf{H}\times\mathbf{k}]\cdot\delta\mathbf{E}-\delta\mathbf{k}\cdot[\mathbf{H}\times\mathbf{E}]-[\mathbf{E}\times\mathbf{k}]\cdot\delta\mathbf{H}=\\ &=2\delta\mathbf{k}\cdot[\mathbf{E}\times\mathbf{H}]+q\,\mathbf{D}\cdot\delta\mathbf{E}+q\,\mathbf{H}\cdot\delta\mathbf{H}\,. \end{aligned} \quad (1.41)$$

Therefore

$$2\delta\mathbf{k}\cdot[\mathbf{E}\times\mathbf{H}]=q\mathbf{E}\cdot\delta\mathbf{D}-q\mathbf{D}\cdot\delta\mathbf{E}=0 \quad (1.42)$$

due to the symmetry of permittivity tensor ($\varepsilon_{ik}=\varepsilon_{ki}$). This means that $\delta\mathbf{k}\cdot\mathbf{S}=0$, i.e. the Poynting vector is orthogonal to the isofrequency surface.

Polarization of the waves propagating in anisotropic medium

We choose the coordinate system with z axis along the $\mathbf{k}$ vector. $\mathbf{D}=-\left[\mathbf{k}\times[\mathbf{k}\times\mathbf{E}]\right]/q^2$. Thus, $\mathbf{D}_\perp=n^2\,\mathbf{E}_\perp$. On the other hand, $E_\alpha=\varepsilon^{-1}_{\alpha\beta}\,D_\beta$, where α, β can take the values 1 or 2, and we take into account that $\mathbf{D}\cdot\mathbf{k}=0$. As a result, we get

$$\left(n^{-2}\,\delta_{\alpha\beta}-\varepsilon^{-1}_{\alpha\beta}\right)\,D_\beta=0\,. \tag{1.43}$$

This is an eigenvalue problem for the symmetric matrix $\varepsilon^{-1}_{\alpha\beta}$. Therefore, the $\mathbf{D}$ vectors for the two eigenmodes are always orthogonal. Each of the eigenmodes is linearly polarized.

1.3 Optical properties of uniaxial crystals

Advanced reading: review on hyperbolic metamaterials by Poddubny et al., Ref. [2]

Dispersion equation for uniaxial crystal

Uniaxial crystals are an important class of anisotropic crystals. They are characterized by the permittivity

$$\hat{\varepsilon}=\varepsilon_\perp\,\hat{I}+(\varepsilon_{||}-\varepsilon_\perp)\,\mathbf{e}_z\otimes\mathbf{e}_z\,. \tag{1.44}$$

In this special case, the dispersion equation can be greatly simplified. We employ several useful formulas:

$$\det\left(a\hat{I}+c\,\mathbf{n}\otimes\mathbf{n}\right)=a^2\,(a+c)\,, \tag{1.45}$$

$$\det\left(a\hat{I}+b\,\mathbf{k}\otimes\mathbf{k}+c\,\mathbf{n}\otimes\mathbf{n}\right)=a\,(a+b\,k^2)\,(a+c)-abc\,(\mathbf{k}\cdot\mathbf{n})^2\,, \tag{1.46}$$

where $\mathbf{n}^2=1$. The dispersion equation Eq. (1.35) reads:

$$\begin{aligned}\det\left[k^2\,\hat{I}-\mathbf{k}\otimes\mathbf{k}-q^2\,\hat{\varepsilon}\right]&=\det\left[(k^2-q^2\,\varepsilon_\perp)\,\hat{I}-\mathbf{k}\otimes\mathbf{k}-q^2\,(\varepsilon_{||}-\varepsilon_\perp)\,\mathbf{e}_z\otimes\mathbf{e}_z\right]=\\&=(k^2-q^2\,\varepsilon_\perp)\,\left[-q^2\,\varepsilon_\perp\,(k^2-q^2\,\varepsilon_{||})-q^2(\varepsilon_{||}-\varepsilon_\perp)\,k_z^2\right]=0\,.\end{aligned} \tag{1.47}$$

Thus, the dispersion equation splits into two independent equations:

$$k^2=q^2\,\varepsilon_\perp\,, \tag{1.48}$$

$$\frac{k_x^2+k_y^2}{\varepsilon_{||}}+\frac{k_z^2}{\varepsilon_\perp}=q^2\,, \tag{1.49}$$

which describe the ordinary and extraordinary waves, respectively. Next, we analyze the polarization of the ordinary and extraordinary waves. For simplicity, we choose x and y axes so that $\mathbf{k}$ lies in the plane Oxz, i.e. $k_y=0$:

$$\begin{pmatrix} k^2 - k_x^2 - q^2\,\varepsilon_\perp & 0 & -k_x\,k_z \\ 0 & k^2 - q^2\,\varepsilon_\perp & 0 \\ -k_x\,k_z & 0 & k^2 - k_z^2 - q^2\,\varepsilon_{||} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix} = 0\,. \tag{1.50}$$

In the case of ordinary waves described by Eq. (1.48), $E_x = E_z = 0$. This means that for the ordinary wave, the electric field is perpendicular both to the wave vector and to the anisotropy axis (i.e. $\mathbf{E}$ is perpendicular to the main plane, TE, or s, polarization).

In the case of an extraordinary wave, $E_y = 0$, i.e. the electric field lies in the plane defined by $\mathbf{k}$ and the axis of anisotropy. Thus, extraordinary waves correspond to TM, or p, polarization.

Isofrequency surfaces for the uniaxial crystal.

Isofrequency surfaces described by the Eqs. (1.48), (1.49) can be easily visualized. They are presented in Fig. 1.2. The dispersion regime when $\varepsilon_\perp$ and $\varepsilon_{||}$ have different signs is called *hyperbolic dispersion regime.*

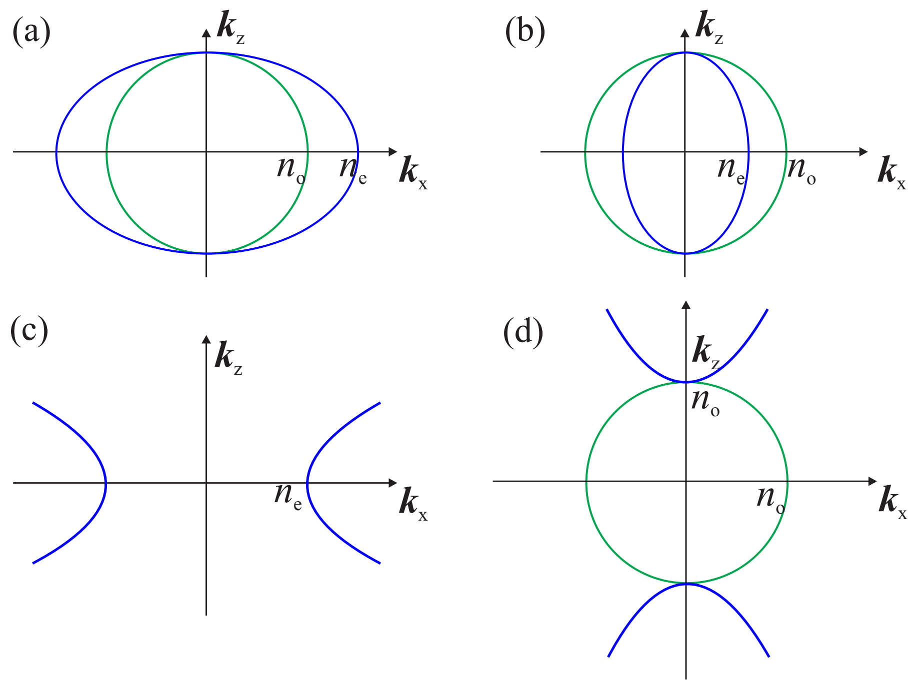

Figure 1.2: Isofrequency contours for the ordinary (green) and extraordinary (blue) waves. (a,b) Elliptic dispersion regime ($\varepsilon_\perp > 0$, $\varepsilon_{||} > 0$). (a) Positive crystal: $n_e > n_o$, $\varepsilon_{||} > \varepsilon_\perp$, e.g., quartz. (b) Negative crystal: $n_e < n_o$, $\varepsilon_{||} < \varepsilon_\perp$, e.g., iceland spar. (c,d) Hyperbolic dispersion regime ($\varepsilon_\perp\,\varepsilon_{||} < 0$). (c) $\varepsilon_{||} > 0$, $\varepsilon_\perp < 0$. (d) $\varepsilon_{||} < 0$, $\varepsilon_\perp > 0$.

Plotting the direction of the refracted wave.

In order to solve boundary problems, we use the continuity of the tangential component of the wave vector at the boundary of the two media. Using the fact that the Poynting vector is normal to the isofrequency surface, one can plot the direction of the refracted wave.

1.4 Systems of units in electrodynamics

Useful reading: book by Jackson Ref. [3] and Ref. [4].

Maxwell's equations in vacuum and the expression for the Lorentz force can be represented in the following general form:

$$\operatorname{div}\mathbf{E} = 4\,\pi\,k_1\,\rho\,, \tag{1.51}$$

$$\operatorname{rot}\,\mathbf{B} = 4\,\pi\,k_2\,\mathbf{j} + k_3\,\frac{\partial \mathbf{E}}{\partial t}\,, \tag{1.52}$$

$$\operatorname{rot}\,\mathbf{E} = -k_4\,\frac{\partial \mathbf{B}}{\partial t}\,, \tag{1.53}$$

$$\operatorname{div}\mathbf{B} = 0\,, \tag{1.54}$$

$$\mathbf{F} = q\,\left[\mathbf{E} + k_5\,[\mathbf{v}\times\mathbf{B}]\right]\,. \tag{1.55}$$

The coefficients k_i depend on the chosen system of units.

Restrictions on the coefficients k_i.

1. Continuity equation [use Eqs. (1.51), (1.52)]:

$$\operatorname{div}\mathbf{j} + \frac{k_1\,k_3}{k_2}\,\frac{\partial\rho}{\partial t} = 0\,. \tag{1.56}$$

   Thus, we require that

$$k_1\,k_3 = k_2\,. \tag{1.57}$$

2. Wave equation [use Eqs. (1.52), (1.53)]:

$$\Delta\,\mathbf{E} - k_3\,k_4\,\frac{\partial^2\mathbf{E}}{\partial t^2} = 0\,. \tag{1.58}$$

   Thus,

$$k_3\,k_4 = 1/c^2\,, \tag{1.59}$$

   where c is the speed of light in a vacuum.

3. Faraday's law [Eqs. (1.53) and (1.55)]. The flux through the closed contour can change due to (a) change in the magnetic field, in which case the electromotive force is given by $\mathfrak{E} = -k_4\,\frac{\partial\Phi}{\partial t}$; (b) change of the contour size and shape, in which case the electromotive force reads $\mathfrak{E} = -k_5\,\frac{\partial\Phi}{\partial t}$. We require that the expression for the electromotive force is the same in both scenarios. Therefore,

$$k_5 = k_4\,. \tag{1.60}$$

4. Coulomb's law [Eq. (1.51)]. The electric field of the point charge

$$E = \frac{k_1\, q}{r^2}\,. \tag{1.61}$$

5. Ampere's law [Eq. (1.52)]. The magnetic field of a constant line current $B = \frac{2\,k_2\,I}{r}$, whereas the force between two parallel currents reads:

$$F = 2\,k_2\,k_5\,\frac{l}{r_{12}}\,I_1\,I_2\,. \tag{1.62}$$

Thus, only two coefficients out of five can be chosen independently.
Examples of the systems of units

- CGS (Gaussian) system of units. $k_1 = 1$ is chosen in order to simplify the Coulomb's law and $k_4 = 1/c$ is chosen in order to to provide that the electric and magnetic fields have the same dimension. Therefore, $k_2 = k_3 = k_5 = 1/c$. Maxwell's equations read:

$$\mathrm{div}\,\mathbf{E} = 4\,\pi\,\rho\,, \tag{1.63}$$

$$\mathrm{rot}\,\mathbf{B} = \frac{4\,\pi}{c}\,\mathbf{j} + \frac{1}{c}\,\frac{\partial \mathbf{E}}{\partial t}\,, \tag{1.64}$$

$$\mathrm{rot}\,\mathbf{E} = -\frac{1}{c}\,\frac{\partial \mathbf{B}}{\partial t}\,, \tag{1.65}$$

$$\mathrm{div}\,\mathbf{B} = 0\,, \tag{1.66}$$

$$\mathbf{F} = q\left[\mathbf{E} + \frac{1}{c}\,[\mathbf{v}\times\mathbf{B}]\right]\,. \tag{1.67}$$

- Heaviside-Lorentz system of units. $k_1 = 1/(4\,\pi)$ (to simplify Maxwell's equations) and $k_4 = 1/c$ (to provide that the electric and magnetic fields have the same dimension). Therefore, $k_2 = 1/(4\,\pi\,c)$, $k_3 = 1/c$, and $k_5 = 1/c$. Maxwell's equations read:

$$\mathrm{div}\,\mathbf{E} = \rho\,, \tag{1.68}$$

$$\mathrm{rot}\,\mathbf{B} = \frac{1}{c}\,\mathbf{j} + \frac{1}{c}\,\frac{\partial \mathbf{E}}{\partial t}\,, \tag{1.69}$$

$$\mathrm{rot}\,\mathbf{E} = -\frac{1}{c}\,\frac{\partial \mathbf{B}}{\partial t}\,, \tag{1.70}$$

$$\mathrm{div}\,\mathbf{B} = 0\,, \tag{1.71}$$

$$\mathbf{F} = q\left[\mathbf{E} + \frac{1}{c}\,[\mathbf{v}\times\mathbf{B}]\right]\,. \tag{1.72}$$

- SI system of units. $k_4 = 1$ (to simplify the Faraday's law), i.e. $k_5 = 1$ and $k_3 = 1/c^2$. The unit of current is introduced. 1 A of current corresponds to the force $2 \cdot 10^{-7}$ N per unit length between the two wires of negligible cross-section placed at the distance of 1 m from each other in vacuum. This yields $k_2 = 10^{-7}\,\mathrm{N/A}^2$.

  Next, we introduce constants $\mu_0 = 4\,\pi\,k_2 = 4\,\pi\,10^{-7}$ H/m and $\varepsilon_0 = 1/(\mu_0\,c^2)$. This yields $k_1 = 1/(4\,\pi\,\varepsilon_0)$. Maxwell's equations in vacuum read:

$$\mathrm{div}\,\mathbf{E} = \rho/\varepsilon_0\,, \tag{1.73}$$

$$\mathrm{rot}\,\mathbf{B} = \mu_0\,\mathbf{j} + \frac{1}{c^2}\frac{\partial\mathbf{E}}{\partial t}\,, \tag{1.74}$$

$$\mathrm{rot}\,\mathbf{E} = -\frac{\partial\mathbf{B}}{\partial t}\,, \tag{1.75}$$

$$\mathrm{div}\,\mathbf{B} = 0\,, \tag{1.76}$$

$$\mathbf{F} = q\,\left[\mathbf{E} + [\mathbf{v}\times\mathbf{B}]\right]\,. \tag{1.77}$$

  The constitutive relations in SI system of units read

$$\mathbf{D} = \varepsilon_0\,\mathbf{E} + \mathbf{P}\,, \tag{1.78}$$

$$\mathbf{B} = \mu_0\,\left(\mathbf{H} + \mathbf{M}\right)\,. \tag{1.79}$$

Note that starting from 2019, the unit of current in SI is defined in terms of elementary electric charge. Magnetic constant μ_0 is no longer exact, but, instead, it is calculated from the measured value of fine structure constant α:

$$\mu_0 = \frac{2\alpha\,h}{c\,e^2}\,. \tag{1.80}$$

The rest of parameters in Eq. (1.80) are exact. Modern value of $\mu_0 = 4\pi \cdot 1.00000000082(20) \cdot 10^{-7}$ H/m. Starting from 2019, the following fundamental constants are considered exact: h, e, k, N_A.

Transformation of expressions between systems of units

Mechanical quantities are not transformed. Electromagnetic quantities are transformed according to the following table:

	CGS	SI
Electric field E (φ, V)	E	$\sqrt{4\pi\,\varepsilon_0}\,E$
Electric induction D	D	$\sqrt{\frac{4\pi}{\varepsilon_0}}\,D$
Charge density ρ (q, I, P)	ρ	$\rho/\sqrt{4\,\pi\,\varepsilon_0}$
Magnetic field H	H	$\sqrt{4\pi\,\mu_0}\,H$
Magnetic induction B	B	$\sqrt{\frac{4\pi}{\mu_0}}\,B$
Magnetization M	M	$\sqrt{\frac{\mu_0}{4\pi}}\,M$
Conductivity σ	σ	$\sigma/(4\,\pi\,\varepsilon_0)$
Polarizability α	α	$\alpha/(4\,\pi)$
Impedance Z	Z	$4\pi\,\varepsilon_0\,Z$

1. Comment on the transformation of units.
E.g. $1\,C = 3\cdot 10^9$ *CGSE,* $1\,V/m = 10^{-4}/3$ *CGSE.*
2. Comment on the analysis of dimensions.

1.5 Analytical properties of dielectric permittivity

Kramers-Kronig relations

We have already discussed that in a wide variety of media, the electric displacement (or polarization) is related to the electric field by linear relation. However, due to retardation effects inherent to medium, the polarization at the moment t can depend on the electric field in the *previous* moments of time:

$$\begin{aligned} D(t) &= E(t) + \int_{-\infty}^{t} f(t-t')\,E(t')\,dt' \\ &= E(t) + \int_{0}^{\infty} f(\tau)\,E(t-\tau)\,d\tau\,, \end{aligned} \tag{1.81}$$

where $f(\tau)$ is some real function decaying with retardation time τ. *The dependence of the displacement/polarization on the retarded electric field is called the time dispersion or the frequency dispersion.* By Fourier transforming Eq. (1.81), we obtain:

$$\begin{aligned} D(\omega) &\equiv \int_{-\infty}^{\infty} D(t)\,e^{i\omega t}\,dt/(2\,\pi) \\ &= E(\omega) + \int_{-\infty}^{\infty} dt\,e^{i\omega t}/(2\pi) \int_{0}^{\infty} f(\tau)\,E(t-\tau)\,d\tau \end{aligned}$$

$$= E(\omega) + \int\limits_0^\infty d\tau\, f(\tau)\, e^{i\omega\,\tau} \int\limits_{-\infty}^\infty E(t-\tau)\, e^{i\omega\,(t-\tau)}\, d(t-\tau)$$

$$= E(\omega) + E(\omega) \int\limits_0^\infty f(\tau)\, e^{i\omega\,\tau}\, d\tau\,. \tag{1.82}$$

As a result, the permittivity of the medium at frequency ω reads:

$$\varepsilon(\omega) = 1 + \int\limits_0^\infty f(\tau)\, e^{i\omega\,\tau}\, d\tau\,. \tag{1.83}$$

Note that the similar reasoning is valid in the case of an anisotropic medium when

$$\varepsilon_{jk}(\omega) = \delta_{jk} + \int\limits_0^\infty f_{jk}(\tau)\, e^{i\omega\tau}\, d\tau\,. \tag{1.84}$$

From this definition it is obvious that $\varepsilon(-\omega) = \varepsilon^*(\omega)$ for real frequencies ω. Therefore,

$$\varepsilon'(-\omega) = \varepsilon'(\omega)\,, \tag{1.85}$$

$$\varepsilon''(-\omega) = -\varepsilon''(\omega)\,. \tag{1.86}$$

By its definition, the function $f(\tau)$ cannot have singularities for $\tau > 0$. Therefore, for complex $\omega = \omega' + i\,\omega''$ with $\omega'' > 0$ (upper half-plane), the function $\varepsilon(\omega)$ defined by Eq. (1.83) is *analytic*. At very high frequencies $\varepsilon(\omega)$ tends to 1 (*give a reference to the calculation of free electron gas permittivity here*).

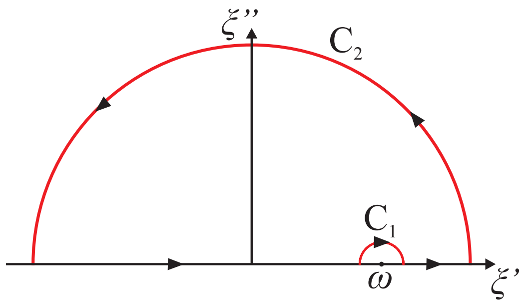

Figure 1.3: Proof of the Kramers-Kronig relations: the integration contour is chosen on the complex plane.

We consider the function $\dfrac{\varepsilon(\xi)-1}{\xi-\omega}$ for a complex frequency ξ and some real frequency ω. We choose the integration contour as indicated in Fig. 1.3. We take into account that the integral over C_2 vanishes and the integral over C_1 yields

$-i\pi\,(\varepsilon(\omega)-1)$. Therefore,

$$\text{v.p.}\int\limits_{-\infty}^{\infty}\frac{\varepsilon(\xi)-1}{\xi-\omega}\,d\xi = i\pi\,\left(\varepsilon(\omega)-1\right)\,. \tag{1.87}$$

By separating the real and imaginary parts in this expression, we deduce the *Kramers-Kronig relations:*

$$\varepsilon'(\omega)-1=\frac{1}{\pi}\,\text{v.p.}\int\limits_{-\infty}^{\infty}\frac{\varepsilon''(\xi)}{\xi-\omega}\,d\xi\,, \tag{1.88}$$

$$\varepsilon''(\omega)=-\frac{1}{\pi}\,\text{v.p.}\int\limits_{-\infty}^{\infty}\frac{\varepsilon'(\xi)-1}{\xi-\omega}\,d\xi\,. \tag{1.89}$$

Physically, equations Eq. (1.88) and (1.89) demonstrate that, for *any* medium, the real and imaginary parts of permittivity are related due to causality. Thus, the medium' dispersion inevitably implies losses and vice versa.

Quite importantly, this reasoning is very general and can be applied to the other types of generalized susceptibilities: polarizability, conductivity, elasticity coefficients, piezoelectric constants, etc.

Now consider harmonic oscillator as an example of the Kramers-Kronig relations application. A harmonic oscillator is a lossless system, and, therefore, the imaginary part of permittivity can be different from zero only at the resonance frequency ω_0. Since the imaginary part of permittivity is an antisymmetric function,

$$\varepsilon''(\omega)=C\,\left[\delta(\omega-\omega_0)-\delta(\omega+\omega_0)\right]\,, \tag{1.90}$$

where C is some constant and ω_0 is the oscillator eigenfrequency (so losses emerge only at resonance). Here, we also take into account that the imaginary part of permittivity is an antisymmetric function of frequency, see Eq. (1.86). Next, we apply the equation (1.88):

$$\varepsilon'(\omega)=1+\frac{2\,C\,\omega_0}{\pi}\,\frac{1}{\omega_0^2-\omega^2}\,. \tag{1.91}$$

Next, we assume that the static permittivity is known and equal to ε_0. Thus, we find that

$$C=\pi\,\omega_0/2\,(\varepsilon_0-1)\,, \tag{1.92}$$

$$\varepsilon'(\omega) - 1 = (\varepsilon_0 - 1)\,\frac{\omega_0^2}{\omega_0^2 - \omega^2}\,, \tag{1.93}$$

$$\varepsilon''(\omega) = \frac{\pi\,\omega_0}{2}\,(\varepsilon_0 - 1)\,\left[\delta(\omega - \omega_0) - \delta(\omega + \omega_0)\right]\,. \tag{1.94}$$

Symmetry of dielectric permittivity

Here, we consider a case of a static field and apply thermodynamic considerations (paragraph 11 vol. 8, LL). Assume that the external field is created by charged conductors and a dielectric object is placed in this field.

To increase the charge on conductors kept at potential φ by δq, external forces have to do the work

$$\delta A = \varphi\,\delta q = -\frac{1}{4\pi}\oint \varphi\,\delta\mathbf{D}\cdot\mathbf{n}\,df = -\frac{1}{4\pi}\int \mathrm{div}(\varphi\,\delta\mathbf{D})\,dV\,. \tag{1.95}$$

Here, we take into account that the charge density on the surface of conductors is equal to $\sigma = -D_n/(4\pi)$, where the *inner normal* to the surface of conductors is chosen.

$$\mathrm{div}\,(\varphi\,\delta\mathbf{D}) = \nabla\varphi\cdot\delta\mathbf{D} + \varphi\;\mathrm{div}\,\delta\mathbf{D} = -\mathbf{E}\cdot\delta\mathbf{D}\,, \tag{1.96}$$

where we take into account that $\mathrm{div}\,\mathbf{D} = 4\pi\,\rho$ and, hence, $\mathrm{div}\,\delta\mathbf{D} = 0$. Thus, the work of external forces is found to be

$$\delta A = \frac{1}{4\pi}\int \mathbf{E}\cdot\delta\mathbf{D}\,dV\,. \tag{1.97}$$

The variation of the internal energy and free energy reads:

$$dU = TdS + \frac{1}{4\pi}\int \mathbf{E}\cdot\delta\mathbf{D}\,dV\,, \tag{1.98}$$

$$dF = -SdT + \frac{1}{4\pi}\int \mathbf{E}\cdot\delta\mathbf{D}\,dV\,. \tag{1.99}$$

Note that in the presence of an external field we can construct the thermodynamic potentials of the two types: F defined above and also $\tilde{F} = F - 1/(4\pi)\int \mathbf{E}\cdot\mathbf{D}\,dV$. It can be shown that the first potential F reaches minimum for fixed temperature and fixed charges of conductors, while the second potential $\tilde{F}$ reaches minimum for fixed temperature and fixed potentials of conductors. *To demonstrate this, we need to write the work in terms of charges and potentials.*

Integration in Eq. (1.99) is done over the entire space. We denote by $\mathbf{E}_0$ the electric field in vacuum which causes the polarization of a dielectric object, whereas the total electric field is $\mathbf{E}$. Next, we construct the quantity $F_d = F - \int \mathbf{E}_0^2/(8\pi)\,dV$

such that

$$
\begin{aligned}
dF &= -S\,dT + \frac{1}{4\pi}\int (\mathbf{E}\cdot\delta\mathbf{D} - \mathbf{E}_0\cdot\delta\mathbf{E}_0)\;dV = \\
&= -S\,dT + \frac{1}{4\pi}\int (\mathbf{D}-\mathbf{E}_0)\cdot\delta\mathbf{E}_0\,dV + \frac{1}{4\pi}\int \mathbf{E}\cdot(\delta\mathbf{D}-\delta\mathbf{E}_0)\;dV \\
&\quad -\frac{1}{4\pi}\int (\mathbf{D}-\mathbf{E})\cdot\delta\mathbf{E}_0\,dV\,. \qquad (1.100)
\end{aligned}
$$

Now we analyze the integrals comprising Eq. (1.100):

$$
\begin{aligned}
I_1 &= \frac{1}{4\pi}\int (\mathbf{D}-\mathbf{E}_0)\cdot\delta\mathbf{E}_0\,dV = -\frac{1}{4\pi}\int (\mathbf{D}-\mathbf{E}_0)\cdot\nabla\delta\varphi_0\,dV = \\
&= -\frac{1}{4\pi}\int \operatorname{div}\left((\mathbf{D}-\mathbf{E}_0)\delta\varphi_0\right)\,dV + \frac{1}{4\pi}\int (\operatorname{div}\mathbf{D} - \operatorname{div}\mathbf{E}_0)\;\delta\varphi_0\,dV = \\
&= -\frac{1}{4\pi}\oint (\mathbf{D}-\mathbf{E}_0)\cdot\mathbf{n}\,\delta\varphi_0\,dV + \frac{1}{4\pi}\int (\operatorname{div}\mathbf{D} - \operatorname{div}\mathbf{E}_0)\;\delta\varphi_0\,dV \quad (1.101)
\end{aligned}
$$

The second integral vanishes since $\operatorname{div}\mathbf{D} = \operatorname{div}\mathbf{E}_0 = 4\pi\,\rho^{\rm ext}$. The first integral vanishes at infinity, whereas at the surface of conductors it yields $\delta\varphi_0/(4\pi)\,\oint\,(\mathbf{D}-\mathbf{E}_0)\cdot\mathbf{n}\,dV$, which also vanishes: the first and second terms yield the surface charge of conductor.

$$
\begin{aligned}
I_2 &= \frac{1}{4\pi}\int \mathbf{E}\cdot(\delta\mathbf{D}-\delta\mathbf{E}_0)\;dV = -\frac{1}{4\pi}\int \nabla\varphi\cdot(\delta\mathbf{D}-\delta\mathbf{E}_0)\;dV = \\
&= -\frac{1}{4\pi}\int \operatorname{div}\left(\varphi\,(\delta\mathbf{D}-\delta\mathbf{E})\right)\,dV + \frac{1}{4\pi}\int \varphi\;(\operatorname{div}\delta\mathbf{D} - \operatorname{div}\delta\mathbf{E}) = \\
&= -\frac{1}{4\pi}\oint \varphi\;(\delta\mathbf{D}-\delta\mathbf{E})\cdot\mathbf{n}\,df = 0\,. \qquad (1.102)
\end{aligned}
$$

Hence, the only nonzero integral is the last one and

$$
\delta F_d = -S\,dT - \int \mathbf{P}\cdot\delta\mathbf{E}_0\,dV\,. \qquad (1.103)
$$

Now we assume that the field is almost homogeneous on the scales of a dielectric object. Hence, polarization of the object can be written as $P_i = \alpha_{ik}\,E_{0k}/V$, where α_{ik} is an object polarizability. Therefore, the free energy reads:

$$
dF_d = -S\,dT - \alpha_{ik}\,E_{0k}\,dE_{0i}\,. \qquad (1.104)
$$

This said,

$$
\alpha_{ik} = \frac{\partial^2 F_d}{\partial E_{0i}\,\partial E_{0k}}\,. \qquad (1.105)
$$

This identity ensures that the polarizability tensor of an object is necessarily symmetric:

$\alpha_{ik} = \alpha_{ki}$. Clearly, by analyzing Eq. (1.103), we can analogously demonstrate that the permittivity tensor is also symmetric: $\varepsilon_{ik} = \varepsilon_{ki}$.

More importantly, the symmetry of the permittivity tensor also holds in the case of time-dependent fields. To prove this, one needs to apply the principle of symmetry of the kinetic coefficients (paragraph 120, vol. 5 LL):

$$\varepsilon_{ik}(\omega) = \varepsilon_{ki}(\omega) \,, \tag{1.106}$$

whereas in the presence of spatial dispersion and external magnetic field/rotation, etc, the following identity holds:

$$\varepsilon_{ik}(\omega, \mathbf{k}, \mathbf{H}, \mathbf{\Omega}) = \varepsilon_{ki}(\omega, -\mathbf{k}, -\mathbf{H}, -\mathbf{\Omega}) \,. \tag{1.107}$$

Reciprocity theorem

We consider some reciprocal medium characterized by the symmetric permittivity and permeability tensors. We assume that the external monochromatic sources $\mathbf{j_1}$ placed in the medium excite the field distribution $(\mathbf{E_1}, \mathbf{H_1})$, whereas external sources $\mathbf{j_2}$ located in the medium excite the field distribution $(\mathbf{E_2}, \mathbf{H_2})$.

Maxwell's equations read:

$$\mathrm{rot}\,\mathbf{E_1} = i\,q\,\mathbf{B_1} \,, \tag{1.108}$$

$$\mathrm{rot}\,\mathbf{H_1} = -i\,q\,\mathbf{D_1} + \frac{4\pi}{c}\,\mathbf{j_1} \,. \tag{1.109}$$

The analogous equations are valid for the fields created by the second source. Therefore,

$$\begin{gathered}(\mathbf{H_2} \cdot \mathrm{rot}\,\mathbf{E_1} - \mathbf{H_1} \cdot \mathrm{rot}\,\mathbf{E_2}) + (\mathbf{E_2} \cdot \mathrm{rot}\,\mathbf{H_1} - \mathbf{E_1} \cdot \mathrm{rot}\,\mathbf{H_2}) \\ = iq\,(\mathbf{H_2} \cdot \mathbf{B_1} - \mathbf{H_1} \cdot \mathbf{B_2}) - iq\,(\mathbf{E_2} \cdot \mathbf{D_1} - \mathbf{E_1} \cdot \mathbf{D_2}) + 4\pi/c\,[\mathbf{E_2} \cdot \mathbf{j_1} - \mathbf{E_1} \cdot \mathbf{j_2}]\end{gathered} \tag{1.110}$$

Due to the presumed symmetry of permittivity and permeability tensors, $\mathbf{H_2} \cdot \mathbf{B_1} = \mathbf{H_1} \cdot \mathbf{B_2}$ and $\mathbf{E_2} \cdot \mathbf{D_1} = \mathbf{E_1} \cdot \mathbf{D_2}$. We also make use of the formula

$$\mathrm{div}\,[\mathbf{a} \times \mathbf{b}] = \mathbf{b} \cdot \mathrm{rot}\,\mathbf{a} - \mathbf{a} \cdot \mathrm{rot}\,\mathbf{b} \,. \tag{1.111}$$

We thus obtain:

$$\mathrm{div}\,(\mathbf{E_1} \times \mathbf{H_2} - \mathbf{E_2} \times \mathbf{H_1}) = \frac{4\pi}{c}\,[\mathbf{E_2} \cdot \mathbf{j_1} - \mathbf{E_1} \cdot j_2] \,. \tag{1.112}$$

By integrating this equation over a sufficiently large volume and transforming the left-hand side with Gauss theorem, we finally prove the *reciprocity theorem*

$$\int \mathbf{j_1} \cdot \mathbf{E_2} \, dV = \int \mathbf{j_2} \cdot \mathbf{E_1} \, dV \, . \tag{1.113}$$

In the case of two dipole sources

$$\mathbf{d_1} \cdot \mathbf{E_2} = \mathbf{d_2} \cdot \mathbf{E_1} \, . \tag{1.114}$$

Now we introduce the dyadic Green's function (see details in Chap. 2) as follows:

$$\mathbf{E_1} = \hat{G}(\mathbf{r_1}, \mathbf{r_2}) \, \mathbf{d_2} \, , \tag{1.115}$$

$$\mathbf{E_2} = \hat{G}(\mathbf{r_2}, \mathbf{r_1}) \, \mathbf{d_1} \, . \tag{1.116}$$

As a consequence,

$$d_{1i} \, G_{ik}(\mathbf{r_1}, \mathbf{r_2}) \, d_{2k} = d_{2k} \, G_{ki}(\mathbf{r_2}, \mathbf{r_1}) \, d_{1i} \, . \tag{1.117}$$

Thus, the following symmetry property of the Green's function holds in an *arbitrary* linear reciprocal medium characterized with symmetric permittivity and permeability tensors:

$$G_{ik}(\mathbf{r_1}, \mathbf{r_2}) = G_{ki}(\mathbf{r_2}, \mathbf{r_1}) \, . \tag{1.118}$$

As a consequence of reciprocity, transmission from the left-hand side of the optical setup to the right is equal to the transmission from right- to the left-hand side. In other words, reciprocity prohibits the construction of optical diode in any linear medium with symmetric permittivity and permeability tensors.

1.6 Dissipation rate, field energy and Poynting vector in the medium with frequency dispersion

In the previous section, we have introduced the phenomenon of the frequency dispersion of dielectric permittivity and deduced some general restrictions on permittivity tensor. Now we turn to the discussion of energy relations in the dispersive medium.

$$\mathrm{rot} \ \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} \, , \tag{1.119}$$

$$\mathrm{rot} \ \mathbf{H} = \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t} \, . \tag{1.120}$$

Equations above yield:

$$\mathrm{div}\ [\mathbf{E}\times\mathbf{H}] \equiv -\mathbf{E}\cdot\mathrm{rot}\,\mathbf{H}+\mathbf{H}\cdot\mathrm{rot}\,\mathbf{E} = -\frac{1}{c}\left[\mathbf{E}\cdot\frac{\partial\mathbf{D}}{\partial t}+\mathbf{H}\cdot\frac{\partial\mathbf{B}}{\partial t}\right] \Rightarrow \tag{1.121}$$

$$-\,\mathrm{div}\,\mathbf{S} = \frac{1}{4\,\pi}\left(\mathbf{E}\cdot\frac{\partial\mathbf{D}}{\partial t}+\mathbf{H}\cdot\frac{\partial\mathbf{B}}{\partial t}\right)\,, \tag{1.122}$$

where the Poynting vector is defined as

$$\boxed{\mathbf{S} = \frac{c}{4\,\pi}\,[\mathbf{E}\times\mathbf{H}]\,,} \tag{1.123}$$

i.e. similarly to the non-dispersive media.

Dissipation rate

We consider a monochromatic wave in a dispersive medium. Since the field energy in monochromatic case does not change in time, the time average $-\langle \mathrm{div}\,\mathbf{S}\rangle$ yields the dissipation rate q: the energy absorbed per unit time in the unit volume of the medium.

$$q = \frac{1}{4\,\pi}\left\langle \mathbf{E}\cdot\frac{\partial\mathbf{D}}{\partial t}+\mathbf{H}\cdot\frac{\partial\mathbf{B}}{\partial t}\right\rangle. \tag{1.124}$$

Since the wave is monochromatic, time dependence of the fields has the form:

$$\mathbf{E} = \mathbf{E}_0\,e^{-i\omega\,t}+\mathbf{E}_0^*\,e^{i\omega\,t}\,, \tag{1.125}$$

$$\mathbf{D} = \mathbf{D}_0\,e^{-i\omega\,t}+\mathbf{D}_0^*\,e^{i\omega\,t}\,, \tag{1.126}$$

$$\frac{\partial\mathbf{D}}{\partial t} = -i\omega\,\mathbf{D}_0\,e^{-i\omega\,t}+i\omega\,\mathbf{D}_0^*\,e^{i\omega\,t}\,. \tag{1.127}$$

Then the averaging yields:

$$\left\langle \mathbf{E}\cdot\frac{\partial\mathbf{D}}{\partial t}\right\rangle = 2\,\omega\,\frac{\mathbf{E}_0^*\cdot\mathbf{D}_0-\mathbf{E}_0\cdot\mathbf{D}_0^*}{2i}\,. \tag{1.128}$$

Assuming the constitutive relations of the form

$$\mathbf{D} = \hat{\varepsilon}\,\mathbf{E}\,, \tag{1.129}$$

$$\mathbf{B} = \hat{\mu}\,\mathbf{H}\,, \tag{1.130}$$

where both $\hat{\varepsilon}$ and $\hat{\mu}$ are frequency-dependent tensors, we finally derive ($\varepsilon' \equiv \mathrm{Re}\,\varepsilon$, $\varepsilon'' \equiv \mathrm{Im}\,\varepsilon$):

$$\boxed{q = \frac{\omega}{2\pi}\left[\frac{\varepsilon_{jk}-\varepsilon_{kj}^*}{2i}\,E_{0j}^*\,E_{0k}+\frac{\mu_{jk}-\mu_{kj}^*}{2i}\,H_{0j}^*\,H_{0k}\right]\,.} \tag{1.131}$$

Thus, a lossless medium is characterized by *Hermitian* permittivity and permeability tensors: $\hat{\varepsilon}^\dagger = \hat{\varepsilon}$, $\hat{\mu}^\dagger = \hat{\mu}$. If the permittivity and permeability tensors are symmetric, losses in the medium are associated with the imaginary parts of these tensors. Since dissipation rate is a positive quantity for a medium in thermodynamic equilibrium, the quadratic form, Eq. (1.131), should be positively defined. This requirement is known as the *passivity condition*. In the isotropic case, for instance, the passivity condition yields

$$\varepsilon'' > 0, \mu'' > 0 \,. \tag{1.132}$$

Frequency intervals where the dissipation rate is small are called *transparency windows*.

Field energy

As we already know, the permittivity of a medium can be negative (e.g. in plasma below plasma frequency). Trying to compute the field energy in such a medium by the conventional formula, we get a negative value of energy, which is an apparent inconsistency. Therefore, we have to revise energy relations in the dispersive medium, restricting the analysis to the transparency window of the medium and an almost monochromatic wave packet with the field given by

$$\mathbf{E}(t) = \mathbf{E_0}(t)\, e^{-i\omega\, t} + \mathbf{E}_0^*(t)\, e^{i\omega\, t}\,, \mathbf{H}(t) = \mathbf{H_0}(t)\, e^{-i\omega\, t} + \mathbf{H}_0^*(t)\, e^{i\omega\, t}\,, \tag{1.133}$$

where the amplitudes $E_0(t)$ and $H_0(t)$ are slowly varying functions of time. *Comment why we can't consider fully monochromatic case here.* For simplicity, we assume that $\mu \equiv 1$ here, i.e. $\mathbf{B} = \mathbf{H}$. Time averaging yields:

$$-\left<\operatorname{div}\mathbf{S}\right> = \frac{1}{4\,\pi}\left\{\left<\mathbf{E}\cdot\frac{\partial\mathbf{D}}{\partial t}\right> + \left<\mathbf{H}\cdot\frac{\partial\mathbf{H}}{\partial t}\right>\right\} \tag{1.134}$$

Averaging for magnetic part is straightforward:

$$\begin{aligned}\left<\mathbf{H}\cdot\frac{\partial\mathbf{H}}{\partial t}\right> &= \frac{1}{2}\frac{\partial}{\partial t}\left<\mathbf{H}^2\right> = \frac{1}{2}\frac{\partial}{\partial t}\left<\left(\mathbf{H}_0\, e^{-i\omega\, t} + \mathbf{H}_0^*\, e^{i\omega\, t}\right)\cdot\left(\mathbf{H}_0\, e^{-i\omega\, t} + \mathbf{H}_0^*\, e^{i\omega\, t}\right)\right> \\ &= \frac{\partial}{\partial t}\left|\mathbf{H}_0\right|^2 .\end{aligned} \tag{1.135}$$

To do averaging for electric part, we represent electric displacement in the form:

$$\mathbf{D}(t) = \mathbf{D}^{(-)}(t) + \mathbf{D}^{(+)}(t)\,, \tag{1.136}$$

where, loosely speaking, $\mathbf{D}^{(-)}(t)$ varies in time as $e^{-i\omega\, t}$ and $\mathbf{D}^{(+)}(t)$ as $e^{i\omega\, t}$. Then

$$\begin{aligned}\left<\mathbf{E}\cdot\frac{\partial\mathbf{D}}{\partial t}\right> &= \left<\left(\mathbf{E}_0\, e^{-i\omega\, t} + \mathbf{E}_0^*\, e^{i\omega\, t}\right)\cdot\left(\dot{\mathbf{D}}^{(-)} + \dot{\mathbf{D}}^{(+)}\right)\right> = \\ &= \mathbf{E}_0\cdot\left<e^{-i\omega\, t}\,\dot{\mathbf{D}}^{(+)}\right> + \mathbf{E}_0^*\cdot\left<e^{i\omega\, t}\,\dot{\mathbf{D}}^{(-)}\right> .\end{aligned} \tag{1.137}$$

In turn, the derivative $\dot{\mathbf{D}}^{(-)}$ can be calculated as:

$$\dot{D}_j^{(-)} = \frac{\partial}{\partial t} \int\limits_{-\infty}^{\infty} D_j^{(-)}(\alpha+\omega)\, e^{-i\,(\omega+\alpha)\,t}\, d\alpha = \frac{\partial}{\partial t} \int\limits_{-\infty}^{\infty} \varepsilon_{jk}(\alpha+\omega)\, E_{0k}(\alpha)\, e^{-i\,(\omega+\alpha)\,t}\, d\alpha \tag{1.138}$$

$$= \int\limits_{-\infty}^{\infty} -i(\alpha+\omega)\,\varepsilon_{jk}(\alpha+\omega)\, E_{0k}(\alpha)\, e^{-i\,(\omega+\alpha)\,t}\, d\alpha\,. \tag{1.139}$$

Since the amplitudes $E_0(\alpha)$ with α close to zero dominate, the following Taylor expansion is applicable:

$$(\alpha+\omega)\,\varepsilon_{jk}(\alpha+\omega) = \omega\,\varepsilon_{jk}(\omega) + \alpha\,\frac{\partial}{\partial\omega}\left(\omega\,\varepsilon_{jk}(\omega)\right)\,. \tag{1.140}$$

As a result,

$$\dot{\mathbf{D}}_j^{(-)}(t) = -i\omega\,\varepsilon_{jk}(\omega)\, E_{0k}(t)\, e^{-i\omega\,t} + \frac{\partial}{\partial\omega}\left(\omega\,\varepsilon_{jk}(\omega)\right)\,\frac{\partial E_{0k}}{\partial t}\, e^{-i\omega\,t}\,. \tag{1.141}$$

At the same time,

$$\dot{\mathbf{D}}_j^{(+)}(t) = \left[\dot{\mathbf{D}}_j^{(-)}(t)\right]^* = i\omega\,\varepsilon_{jk}^*(\omega)\, E_{0k}^*(t)\, e^{i\omega\,t} + \frac{\partial}{\partial\omega}\left(\omega\,\varepsilon_{jk}^*(\omega)\right)\,\frac{\partial E_{0k}^*}{\partial t}\, e^{i\omega\,t}. \tag{1.142}$$

Hence, Eq. (1.137) yields:

$$\begin{aligned}\left\langle \mathbf{E}\cdot\frac{\partial\mathbf{D}}{\partial t}\right\rangle \overset{(1.137)}{=} E_{0k}\left(i\omega\,\varepsilon_{kj}^*(\omega)\, E_{0j}^*(t) + \frac{\partial}{\partial\omega}\left(\omega\,\varepsilon_{kj}^*(\omega)\right)\,\frac{\partial E_{0j}^*}{\partial t}\right) + \\ + E_{0j}^*\left(-i\omega\,\varepsilon_{jk}(\omega)\, E_{0k}(t) + \frac{\partial}{\partial\omega}\left(\omega\,\varepsilon_{jk}(\omega)\right)\,\frac{\partial E_{0k}}{\partial t}\right) = \\ = \frac{\partial}{\partial\omega}\left(\omega\,\varepsilon_{jk}(\omega)\right)\,\frac{\partial}{\partial t}\left(E_{0j}^*\, E_{0k}\right)\,,\end{aligned} \tag{1.143}$$

where we have used the fact that in the transparency window $\varepsilon_{kj}^* = \varepsilon_{jk}$. Finally, combining Eqs. (1.143), (1.135) and (1.134), we obtain that

$$-\left\langle \mathrm{div}\ \mathbf{S}\right\rangle = \frac{1}{4\,\pi}\left[\frac{\partial}{\partial\omega}\left(\omega\,\varepsilon_{jk}(\omega)\right)\,\frac{\partial}{\partial t}\left(E_{0j}^*\, E_{0k}\right) + \frac{\partial}{\partial t}\,\left|\mathbf{H}_0\right|^2\right]\,. \tag{1.144}$$

On the other hand, the energy conservation law reads:

$$\frac{\partial u}{\partial t} = -\left\langle \mathrm{div}\,\mathbf{S}\right\rangle\,, \tag{1.145}$$

where u is the electromagnetic energy density. Comparing the two equations above, we obtain that

$$\boxed{u = \frac{1}{4\,\pi}\,\left[\frac{\partial}{\partial\omega}\,\left(\omega\,\varepsilon_{jk}(\omega)\right)\,E^*_{0j}\,E_{0k} + |\mathbf{H}_0|^2\right]\,.} \tag{1.146}$$

Equation (1.146), known as the Brillouin formula, gives the energy of electromagnetic field in the transparency window of the medium with frequency dispersion. This formula can be readily generalized to the case of dispersive permeability.

1.7 Magneto-optical effects

Electromagnetic properties of a medium can also depend on applied external static electric and magnetic fields. The dependence on static electric field is termed as the Kerr effect, and in the case of an isotropic medium the Kerr effect yields $\varepsilon_{ik} = \varepsilon^{(0)} + \alpha\,E_i\,E_k$. Thus, the external static electric field leads to birefringence, transforming an isotropic medium into the uniaxial one.

Gyrotropic media

Here we will focus on the other possibility: dependence of permittivity on applied static magnetic field. In the absence of dissipation, the permittivity tensor is Hermitian, i.e. $\varepsilon_{ik} = \varepsilon^*_{ki}$. Separating the real and imaginary parts, we get

$$\begin{aligned} \varepsilon'_{ik} &= \varepsilon'_{ki}\,, \\ \varepsilon''_{ik} &= -\varepsilon''_{ki}\,, \end{aligned} \tag{1.147}$$

i.e. the real and imaginary parts of permittivity tensor in a lossless medium are represented by symmetric and antisymmetric tensors, respectively. An antisymmetric tensor ε''_{ik} can be associated with some vector g_n as follows:

$$\varepsilon''_{ik} = e_{ikl}\,g_l\,. \tag{1.148}$$

The constitutive relation then becomes

$$\begin{aligned} D_i = \varepsilon_{ik}\,E_k = \varepsilon'_{ik}\,E_k + i\,\varepsilon''_{ik}\,E_k = \varepsilon'_{ik}\,E_k + i\,e_{ikl}\,g_l\,E_k \Rightarrow \\ \mathbf{D} = \hat{\varepsilon}'\,\mathbf{E} + i\,[\mathbf{E}\times\mathbf{g}]\,. \end{aligned} \tag{1.149}$$

Our derivation of the constitutive relation was based on the fact that $\hat{\varepsilon}$ is Hermitian. The inverse tensor $\hat{\eta} = \hat{\varepsilon}^{-1}$ is obviously also Hermitian. Repeating the similar reasoning for the inverse tensor, we can get the constitutive relation in the equivalent form

$$\mathbf{E} = \hat{\eta}'\,\mathbf{D} + i\,[\mathbf{D}\times\mathbf{G}]\,. \tag{1.150}$$

Vector $\mathbf{g}$ is called the gyration vector, and $\mathbf{G}$ is called the optical activity vector.

To clarify the dependence of the gyration vector on the external magnetic field, we employ the symmetry of the kinetic coefficients which states that

$$\varepsilon_{ik}(\mathbf{H_0}) = \varepsilon_{ki}(-\mathbf{H_0}) \,. \tag{1.151}$$

Using the relations Eq. (1.147), we get

$$\varepsilon'_{ik}(\mathbf{H_0}) = \varepsilon'_{ik}(-\mathbf{H_0}) \,, \tag{1.152}$$
$$\varepsilon''_{ik}(\mathbf{H_0}) = -\varepsilon''_{ik}(-\mathbf{H_0}) \,. \tag{1.153}$$

Thus, the real and imaginary parts of the permittivity tensor are even and odd functions of magnetic field, respectively.

Faraday effect

Now we expand the components of permittivity tensor in series with respect to $\mathbf{H}$ up to the first order and consider a medium which is isotropic in the absence of external field. In this case, $\hat{\varepsilon}'_{ik} = \varepsilon\,\delta_{ik}$ and $\mathbf{g} = f\,\mathbf{H}$, where ε and f are some scalar constants. We also align z axis along the direction of external magnetic field, which yields permittivity tensor in the form

$$\hat{\varepsilon} = \begin{pmatrix} \varepsilon & i f\,H_0 & 0 \\ -i f\,H_0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{pmatrix} \tag{1.154}$$

From Maxwell's equations

$$\mathbf{k} \times \mathbf{H} = -q\,\mathbf{D} \,, \tag{1.155}$$
$$\mathbf{k} \times \mathbf{E} = q\,\mathbf{H} \tag{1.156}$$

we get $\mathbf{D} - n^2\,\mathbf{E}_\perp = 0$, where $\mathbf{E}_\perp$ is the component of electric field perpendicular to the wave vector. The most interesting situation is the propagation along the lines of magnetic field ($\mathbf{k}||\mathbf{H_0}$) when

$$\begin{pmatrix} \varepsilon - n^2 & i f\,H_0 \\ -i f\,H_0 & \varepsilon - n^2 \end{pmatrix} \begin{pmatrix} E_x \\ E_y \end{pmatrix} = 0 \tag{1.157}$$

The dispersion equation reads:

$$n_\pm = \sqrt{\varepsilon \mp f\,H_0} \approx n_0 \mp \frac{f H_0}{2\,n_0} \,, \tag{1.158}$$

where $n_0 = \sqrt{\varepsilon}$. Examining Eq. (1.157), we find that the polarization of the eigenmodes is described by $E_x = \mp i E_y$ so that the polarization vectors are complex: $\mathbf{e}_\pm = \mathbf{e}_x \pm i\,\mathbf{e}_y$. This means that the electric field of the eigenmode reads:

$$\begin{aligned}\mathbf{E}_\pm &= \mathrm{Re}\left[A\ (\mathbf{e}_x \pm i\,\mathbf{e}_y)\ e^{iqn_\pm z - i\omega\, t}\right]\\ &= A\ [\mathbf{e}_x\ \cos\varphi \pm \mathbf{e}_y\ \sin\varphi]\ ,\end{aligned} \tag{1.159}$$

where $\varphi = \omega\, t - q\, n_\pm\, z$ is the phase of the wave. Equation (1.159) describes the vector which rotates counterclockwise/clockwise for $+/-$ sign choice. Thus, we conclude that the eigenmodes in Faraday effect are circularly polarized. Right and left circular polarizations are characterized by the different refractive indices n_+ and n_-, respectively.

To calculate the magnitude of rotation, we assume that the wave entering magneto-optical medium is polarized along x axis, i.e.

$$\mathbf{E}(z=0) = E_0\, \mathbf{e}_x\, e^{-i\omega\, t} = E_0/2\ (\mathbf{e}_+ + \mathbf{e}_-)\ e^{-i\omega\, t}\,. \tag{1.160}$$

At the point with the coordinate z the field is given by

$$\begin{aligned}\mathbf{E}(z) &= E_0\, e^{-i\omega\, t}/2\ \left[e^{iqn_+ z}\, \mathbf{e}_+ + e^{iqn_- z}\, \mathbf{e}_-\right] =\\ &= E_0/2\, e^{iq<n>z - i\,\omega\, t}\ \left[e^{iq\Delta n\, z/2}\, \mathbf{e}_+ + e^{-iq\Delta n\, z/2}\, \mathbf{e}_-\right] =\\ &= E_0\, e^{iq<n>z - i\,\omega\, t}\ [\cos\theta\, \mathbf{e}_x + \sin\theta\, \mathbf{e}_y]\ ,\end{aligned} \tag{1.161}$$

where $\Delta n = n_+ - n_-$, $< n >= (n_+ + n_-)/2$ and $\theta = -q\,\Delta n\, z/2$. Thus, for the linearly polarized wave which passed a distance z in the medium, the polarization plane is rotated by the angle θ proportional to the distance z. Using Eqs. (1.158) for the refractive indices, we get:

$$\theta = V\, H_0\, l\ , \tag{1.162}$$

where $V = q\, f/(2\, n_0)$ is called the Verdet constant. The effect of rotation of the polarization plane in the magneto-optical medium is known as the *Faraday effect.*

Cotton-Mouton effect

Next, we consider another limiting case when the direction of light propagation is orthogonal to the direction of applied static magnetic field. Again, we search for plane wave solutions in such a non-magnetic medium ($\mathbf{B} = \mathbf{H}$), starting from Maxwell's equations

$$\mathbf{k} \times \mathbf{E} = q\, \mathbf{H}\ , \tag{1.163}$$

$$\mathbf{k} \times \mathbf{H} = -q\, \mathbf{D}\ . \tag{1.164}$$

We combine them together and get:

$$k^2\, \mathbf{E} - \mathbf{k}\, (\mathbf{k} \cdot \mathbf{E}) = q^2\, \mathbf{D}\ . \tag{1.165}$$

Due to $\operatorname{div} \mathbf{D} = 0$, the projections of the left- and right-hand sides onto $\mathbf{k}$ are zero, and, therefore, we get:

$$k^2\,\mathbf{E}_\perp = q^2\,\mathbf{D}\,, \tag{1.166}$$

where $\mathbf{E}_\perp$ is a component of the electric field orthogonal to the direction of wave propagation. Note that in the magneto-optical case

$$\mathbf{E} = \varepsilon^{-1}\,\mathbf{D} + iF\,\left[\mathbf{D}\times\mathbf{H}_0\right]\,. \tag{1.167}$$

In the chosen geometry, $\mathbf{D}$ and $\mathbf{H}_0$ are orthogonal to $\mathbf{k}$. Hence, their vector product is parallel to $\mathbf{k}$ and, therefore, is not included in the Eq. (1.166). In the other words, the effect linear in $\mathbf{H_0}$ vanishes.

As a result, in this geometry the corrections to the permittivity tensor, which are second order in $\mathbf{H}_0$, should be taken into account. We consider the equation $\left(\hat{\eta} - \hat{I}/n^2\right)\,\mathbf{D} = 0$, direct x axis along the wave vector (so that $\mathbf{D}$ has y and z components only), and z axis along static magnetic field. The principal components of $\hat{\eta}$ tensor become $\eta_{||}$ for the direction along the magnetic field and $\eta_\perp$ for the direction perpendicular to the magnetic field.

Therefore, the eigenmodes of the medium are linearly polarized and have different refractive indices $\eta_{||}^{-1/2}$ and $\eta_\perp^{-1/2}$. Therefore, after passing magneto-optical medium perpendicularly to the applied magnetic field, the linearly polarized light will become elliptically polarized (*Cotton-Mouton effect*), and *the whole magnetized medium acts similarly to the birefringent crystal*.

Faraday effect for free electron gas

The physics of the Faraday effect can be understood on a simple example of a medium considered as free electron gas. Actually, this approximation is valid for any medium at frequencies much higher than the medium resonance frequencies. Additionally, we assume that the frequency of the driving field is much higher than the cyclotron frequency

$$\omega_c = e\,H_0/(m\,c)\,. \tag{1.168}$$

Electron equation of motion reads

$$m\,\frac{d\mathbf{v}}{dt} = -e\,\mathbf{E}e^{-i\omega\,t} - \frac{e}{c}\left[\mathbf{v}\times\mathbf{H_0}\right]\,, \tag{1.169}$$

where $e > 0$ is an elementary charge. Since $\omega \gg \omega_c$, the last term in Eq. (1.169) representing Lorentz force is considered as a perturbation (i.e. $\mathbf{H_0}$ is considered as small parameter). By solving Eq. (1.169) iteratively, we get:

$$\mathbf{v} = -\frac{ie\,\mathbf{E}}{m\omega}\,e^{-i\omega\,t} - \frac{e^2}{m^2\,\omega^2\,c}\,\left[\mathbf{E}\times\mathbf{H_0}\right]\,e^{-i\omega\,t}\,. \tag{1.170}$$

If concentration of free electrons is n, then $\mathbf{j} = -ne\,\mathbf{v}$. On the other hand, the current density is related to the polarization as $\mathbf{j} = -i\omega\,\mathbf{P}$, i.e. $\mathbf{P} = -ien\,\mathbf{v}/\omega$.

Finally, we obtain the following expression for the effective permittivity:

$$\hat{\varepsilon} = \left[1 - \frac{4\pi\, n\, e^2}{m\,\omega^2}\right] - i\,\frac{4\pi\, n\, e^3}{m^2\,\omega^3\, c}\,\mathbf{H}_0^{\times}\,, \tag{1.171}$$

($\mathbf{H}_0^{\times}$ is tensor dual to vector $\mathbf{H}_0$) which coincides exactly with Eq. (1.149) where the gyration vector $\mathrm{g} = f\mathbf{H}_0$ and

$$\varepsilon'(\omega) = 1 - \frac{4\pi\, n\, e^2}{m\,\omega^2}\,, \tag{1.172}$$

$$f(\omega) = \frac{4\pi\, n\, e^3}{m^2\,\omega^3\, c} = \frac{e}{2mc}\,\frac{d\varepsilon'}{d\omega}\,. \tag{1.173}$$

The Verdet constant can be estimated as

$$V = \frac{4\pi\, n\, e^3}{m^2\, c^2\,\omega^2} = \frac{e}{mc^2}\,(1-\varepsilon')\,. \tag{1.174}$$

1.8 Bi-anisotropic materials and optical activity

Definition of a bi-anisotropic medium

Previously, we supposed that the properties of a medium are fully described by the permittivity and permeability tensors. However, if such simplified description is adopted, a number of physical phenomena cannot be explained properly. The simplest example is the rotation of polarization plane for the light propagating in the water solution of sugar.

We consider the class of materials described by the constitutive relations

$$\mathbf{D} = \hat{\varepsilon}\,\mathbf{E} + \hat{\alpha}\,\mathbf{H}\,, \tag{1.175}$$

$$\mathbf{B} = \hat{\beta}\,\mathbf{E} + \hat{\mu}\,\mathbf{H}\,. \tag{1.176}$$

It can be shown that in the absence of dissipation $\hat{\beta} = \hat{\alpha}^{\dagger}$. The material described by the material equations Eqs. (1.175)-(1.176) is called *bi-anisotropic*. If all the tensors $\hat{\varepsilon}$, $\hat{\mu}$, $\hat{\alpha}$ and $\hat{\beta}$ reduce to scalars, the medium is called *bi-isotropic*.

Discuss the origin of magneto-electric coupling on the example of omega-particle.

Symmetry restrictions

Now we establish the symmetry requirements necessary for nonzero bianisotropy. We note that the magnetic fields $\mathbf{H}$ and $\mathbf{B}$ are even under mirror reflection, whereas the electric fields $\mathbf{E}$ and $\mathbf{D}$ are odd under mirror reflection.

If the medium unit cell has a center of inversion, its material parametrs should be invariant under the inversion. Thus, if we apply inversion to Eqs. (1.175), (1.176), we obtain:

$$-\mathbf{D} = -\hat{\varepsilon}\,\mathbf{E} + \hat{\alpha}\,\mathbf{H}\,, \tag{1.177}$$

$$\mathbf{B} = -\hat{\beta}\,\mathbf{E} + \hat{\mu}\,\mathbf{H}\,. \tag{1.178}$$

This means that bianisotropy tensors $\hat{\alpha}$ and $\hat{\beta}$ should necessarily vanish for the inversion-symmetric medium. Thus, bianisotropy is only possible in the media without inversion symmetry. *Note about chiral sugar molecule*.

Rotation of polarization plane

As an illustrative example, we consider light propagation in bi-isotropic medium with $\alpha = \chi + i\,\varkappa$, $\beta = \chi - i\,\varkappa$. Maxwell's equations for monochromatic field yield:

$$\mathbf{k} \times \mathbf{H} = -q\,\varepsilon\,\mathbf{E} - q\,\left(\chi + i\,\varkappa\right)\,\mathbf{H}\,, \tag{1.179}$$

$$\mathbf{k} \times \mathbf{E} = q\,\left(\chi - i\,\varkappa\right)\,\mathbf{E} + q\,\mu\,\mathbf{H}\,. \tag{1.180}$$

We rewrite Eqs. (1.179), (1.180) in terms of vectors $\mathbf{e}_{\pm} = \left(\mathbf{e}_x \pm i\,\mathbf{e}_y\right)$ assuming that the wave vector $\mathbf{k}$ is directed along z axis. We use the property $\mathbf{e}_z \times \mathbf{e}_{\pm} = \mp i\mathbf{e}_{\pm}$. As a result,

$$\varepsilon\,E_{\pm} + \left[\chi + i\,\varkappa \mp i\,n_{\pm}\right]\,H_{\pm} = 0\,, \tag{1.181}$$

$$\left[\chi - i\,\varkappa \pm i\,n_{\pm}\right]\,E_{\pm} + \mu\,H_{\pm} = 0\,. \tag{1.182}$$

Finally, we obtain that

$$n_{\pm} = \sqrt{\varepsilon\,\mu - \chi^2} \pm \varkappa\,. \tag{1.183}$$

The sign of the square root in Eq. (1.183) is chosen on the basis of passivity condition.

The analysis above shows that the eigenmodes are polarized along complex vectors $\mathbf{e}_{\pm}$. This means that the electric field of the eigenmode reads:

$$\begin{aligned} \mathbf{E}_{\pm} &= \mathrm{Re}\left[A\,\left(\mathbf{e}_x \pm i\,\mathbf{e}_y\right)\,e^{iqn_{\pm}\,z - i\omega\,t}\right] \\ &= A\,\left[\mathbf{e}_x\,\cos\varphi \pm \mathbf{e}_y\,\sin\varphi\right]\,, \end{aligned} \tag{1.184}$$

where $\varphi = \omega\,t - q\,n_{\pm}\,z$ is the phase of the wave. Equation (1.184) describes the vector which rotates counterclockwise/clockwise for $+/-$ sign choice. Thus, we conclude that the eigenmodes of a bi-isotropic medium are circularly polarized. Right and left circular polarizations are characterized by the different refractive indices n_+ and n_-, respectively.

Assume that the wave entering bi-isotropic medium is polarized along x axis, i.e.

$$\mathbf{E}(z = 0) = E_0\,\mathbf{e}_x\,e^{-i\omega\,t} = E_0/2\,\left(\mathbf{e}_+ + \mathbf{e}_-\right)\,e^{-i\omega\,t}\,. \tag{1.185}$$

At the point with the coordinate z, the field is given by

$$\begin{aligned}\mathbf{E}(z) =&E_0\, e^{-i\omega\, t}/2\, \left[e^{iqn_+\, z}\, \mathbf{e}_+ + e^{iqn_-\, z}\, \mathbf{e}_-\right]\\ =&E_0/2\, e^{iq<n>z-i\,\omega\, t}\, \left[e^{iq\Delta n\, z/2}\, \mathbf{e}_+ + e^{-iq\Delta n\, z/2}\, \mathbf{e}_-\right]\\ =&E_0\, e^{iq<n>z-i\,\omega\, t}\, \left[\cos\theta\, \mathbf{e}_x + \sin\theta\, \mathbf{e}_y\right]\ ,\end{aligned} \tag{1.186}$$

where $\Delta n = n_+ - n_-$, $< n >= (n_+ + n_-)/2$ and $\theta = -q\, \Delta n\, z/2 = -q\, \varkappa\, z$. *Refer to the calculation of the previous lecture for Faraday rotation.* Thus, for the linearly polarized wave which passed a distance z in the medium, the polarization plane is rotated by the angle θ proportional to the distance z.

1.9 Spatial dispersion. Link between local and nonlocal description

Useful reading: book by Agranovich and Ginzburg [5].

To describe the properties of linear media, we have previously introduced the permittivity $\hat{\varepsilon}$ and permeability $\hat{\mu}$ tensors. To describe specific phenomena like optical activity, we have also introduced the bianisotropy tensors $\hat{\alpha}$ and $\hat{\beta}$.

Now the natural question is whether this "bianisotropic" framework is complete for linear media, or it requires further advancement. It turns out that in order to describe such phenomena as anisotropy of cubic crystals, or trirefringence, one needs to extend this framework and introduce *spatial dispersion*.

The most general link between the polarization of a medium (this medium is assumed to be linear, stationary and uniform) and electric field reads:

$$P_i(\mathbf{r}) = \int\limits_{-\infty}^{t} \hat{\chi}_{ij}\left(t-t', \mathbf{r}-\mathbf{r}'\right)\, E_j(\mathbf{r}')\, d^3\,\mathbf{r}'\ . \tag{1.187}$$

This said, the polarization in a given point depends on the fields in the previous moments of time (time of frequency dispersion) and in some neighboring regions of space (spatial dispersion).

Importantly, in spatial dispersion framework we do not distinguish the polarization current and the magnetization current, and always assume that $\mathbf{B} = \mathbf{H}$. It is possible since the fields $\mathbf{H}$ and $\mathbf{D}$ are considered as auxiliary.

By Fourier transforming Eq. (1.187), we obtain that

$$\begin{aligned}P_i(\omega, \mathbf{k}) = \chi_{ij}(\omega, \mathbf{k})\, E_j(\omega, \mathbf{k})\ ,\\ D_i(\omega, \mathbf{k}) = \varepsilon_{ij}(\omega, \mathbf{k})\, E_j(\omega, \mathbf{k})\ ,\end{aligned} \tag{1.188}$$

where $\varepsilon_{ij}(\omega, \mathbf{k}) = \delta_{ij} + 4\pi\, \chi_{ij}(\omega, \mathbf{k})$. Thus, the properties of the medium in spatial dispersion framework are described by the tensor $\hat{\varepsilon}(\omega, \mathbf{k})$. Since this is the most general framework, there should be a link between this framework and the approach based on local material parameters $\hat{\varepsilon}(\omega)$, $\hat{\mu}(\omega)$, $\hat{\alpha}(\omega)$, $\hat{\beta}(\omega)$, which are included in the material equations (1.175), (1.176).

We consider the fields $\mathbf{D}$ and $\mathbf{H}$ included in the local material equations (1.175), (1.176) as *auxiliary* and therefore we can *redefine* them, keeping the redefined fields consistent with Maxwell's equations. In physical terms, this corresponds to the inclusion of magnetization currents into polarization currents. The redefined magnetic field reads

$$\mathbf{H}' = \mathbf{H} - \mathbf{a}\,, \tag{1.189}$$

where $\mathbf{a}$ is some vector field, which will be chosen later. Since in the plane wave case $\mathbf{k} \times \mathbf{H} = -q\,\mathbf{D}$ and also $\mathbf{k} \times \mathbf{H}' = -q\,\mathbf{D}'$, electric displacement should be redefined as follows:

$$\mathbf{D}' = \mathbf{D} + \mathbf{k} \times \mathbf{a}/q\,. \tag{1.190}$$

Now we choose the vector field $\mathbf{a}$ from the requirement that $\mathbf{H}' = \mathbf{B}$ or, in other words,

$$\mathbf{H}' = \mathbf{B} = \hat{\beta}\,\mathbf{E} + \hat{\mu}\,\mathbf{H} = \hat{\beta}\,\mathbf{E} + \hat{\mu}\,(\mathbf{H}' + \mathbf{a})\,, \tag{1.191}$$

which yields

$$\mathbf{a} = \left[\hat{\mu}^{-1} - \hat{I}\right]\,\mathbf{H}' - \hat{\mu}^{-1}\,\hat{\beta}\,\mathbf{E}\,. \tag{1.192}$$

This choice leads to

$$\mathbf{H}' = \mathbf{B} = \mathbf{k}^{\times}\,\mathbf{E}/q\,, \tag{1.193}$$

$$\mathbf{H} = \mathbf{H}' + \mathbf{a} = \hat{\mu}^{-1}\,\mathbf{k}^{\times}\,\mathbf{E}/q - \hat{\mu}^{-1}\,\hat{\beta}\,\mathbf{E}\,. \tag{1.194}$$

Now we can evaluate the redefined electric displacement

$$\mathbf{D}' = \mathbf{D} + \frac{\mathbf{k}^{\times}}{q}\,\mathbf{a} = \hat{\varepsilon}\,\mathbf{E} + \hat{\alpha}\,\mathbf{H} + \frac{\mathbf{k}^{\times}}{q}\,\mathbf{a}\,. \tag{1.195}$$

Finally, we get the following material equations:

$$\mathbf{D}' = \hat{\varepsilon}(\omega, \mathbf{k})\,\mathbf{E}\,, \tag{1.196}$$

$$\mathbf{B} = \mathbf{H}'\,, \tag{1.197}$$

where the spatially dispersive permittivity tensor is given by the expression:

$$\hat{\varepsilon}(\omega, \mathbf{k}) = \left[\hat{\varepsilon} - \hat{\alpha}\,\hat{\mu}^{-1}\,\hat{\beta}\right] + \frac{1}{q}\,\left[\hat{\alpha}\,\hat{\mu}^{-1}\mathbf{k}^{\times} - \mathbf{k}^{\times}\,\hat{\mu}^{-1}\,\hat{\beta}\right] + \frac{1}{q^2}\,\mathbf{k}^{\times}\,\left[\hat{\mu}^{-1} - \hat{I}\right]\,\mathbf{k}^{\times}\,. \tag{1.198}$$

Matrix $\mathbf{k}^{\times}$ is given by the formula

$$\vec{k}^{\times} = \begin{pmatrix} 0 & -k_z & k_y \\ k_z & 0 & -k_x \\ -k_y & k_x & 0 \end{pmatrix} \tag{1.199}$$

Equation (1.198) demonstrates that the corrections to the nonlocal permittivity tensor linear with respect to $\mathbf{k}$ are related to the bianisotropy of the structure, whereas some of the corrections proportional to k^2 can be related to the magnetic response. *In other words, bianisotropy is a first-order spatial dispersion effect, whereas magnetism can be viewed as a second-order spatial dispersion effect.* It is evident, however, that not every nonlocal permittivity tensor $\hat{\varepsilon}(\omega, \mathbf{k})$ can be presented in the form Eq. (1.198).

Note that the nonlocal permittivity tensor for bi-isotropic medium with $\mu = 1$ is given by

$$\hat{\varepsilon}(\omega, \mathbf{k}) = \varepsilon - \varkappa^2 + 2i\varkappa/q\,\mathbf{k}^{\times}\,. \tag{1.200}$$

There is a similarity of this expression with magneto-optical medium with the permittivity

$$\hat{\varepsilon}(\omega, \mathbf{H_0}) = \varepsilon - i\,f\,\mathbf{H}_0^{\times}\,. \tag{1.201}$$

1.10 Optical effects due to spatial dispersion: "additional" waves and additional boundary conditions

After the discussion of the link between local ($\hat{\varepsilon}$, $\hat{\mu}$, $\hat{\alpha}$, $\hat{\beta}$) and nonlocal $[\varepsilon(\hat{\omega}, \mathbf{k})]$ description, it is instructive to analyze the new optical effects stemming from spatial dispersion.

Longitudinal waves

As a simplest example, we consider some isotropic medium possessing inversion symmetry. The effective permittivity tensor of such a medium ε_{il} can only contain the Kronecker symbol δ_{il} and the tensor product $k_i\,k_l$. Generally, the permittivity tensor has the form

$$\varepsilon_{il}(\omega, \mathbf{k}) = \varepsilon_t\,\left[\delta_{il} - k_i\,k_l/k^2\right] + \varepsilon_l\,k_i\,k_l/k^2\,, \tag{1.202}$$

where ε_t and ε_l are some scalar functions of frequency and the absolute value of wave vector that are called the transverse and longitudinal permittivity, respectively. The dispersion equation reads

$$0 = \left|q^2\,\hat{\varepsilon} - k^2\,\hat{I} + \mathbf{k}\otimes\mathbf{k}\right| = \left|(q^2\,\varepsilon_t - k^2)\,\left[\hat{I} - \mathbf{k}\otimes\mathbf{k}/k^2\right] + q^2\,\varepsilon_l\,\mathbf{k}\otimes\mathbf{k}/k^2\right|\,. \tag{1.203}$$

This equation decouples into two independent dispersion equations:

(i)

$$k^2 = q^2\,\varepsilon_t(\omega,k)\;, \tag{1.204}$$

which describes the waves with electric field orthogonal to $\mathbf{k}$. These transverse waves are the direct analogues of those existing in local medium.

(ii)

$$\varepsilon_l(\omega,k) = 0\;, \tag{1.205}$$

which describes the waves with electric field aligned parallel to $\mathbf{k}$. Such waves are called *longitudinal*, and they are characteristic to media with spatial dispersion.

"Additional" waves

Useful reading: paper by Orlov et al. on multilayered structures [6], paper by Gorlach and Belov on uniaxial structures [7].

An interesting phenomenon possible in spatially dispersive medium is the so-called trirefringence, when the light beam incident at the boundary of the structure generates three transmitted beams (not two, as in the case of anisotropic dielectric). The phenomenon of trirefringence may happen in many cases, here we will focus on two special situations.

Discuss the first situation of $\varepsilon \approx 0$. Skip the second case $\varepsilon \to \infty$. Stress that we analyze TM waves. TE case is trivial. The first situation corresponds to the uniaxial medium with the anisotropy axis perpendicular to the boundary as shown in Fig. 1.4(a), when the only essential component of permittivity tensor is along anisotropy axis (z).

Permittivity is approximated as

$$\varepsilon_{zz}(\omega,\mathbf{k}) \approx \varepsilon_{\text{loc}} + \alpha\,k_z^2 + \tilde{\alpha}\,k_x^2\,. \tag{1.206}$$

To simplify the analysis even further, we assume that $\tilde{\alpha}$ is negligible in comparison

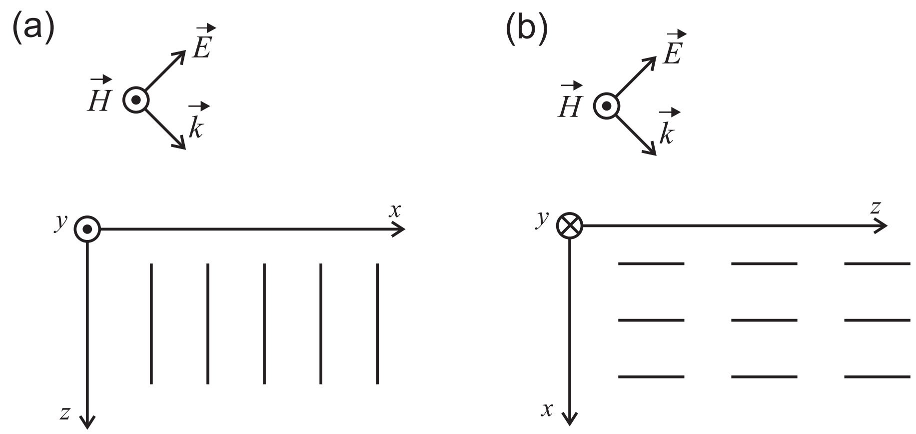

Figure 1.4: Geometry of the problem. (a) Trirefringence in ε near zero regime. (b) Trirefringence in $\varepsilon \to \infty$ regime.

with α. The dispersion equation for TM waves yields

$$\frac{k_x^2}{\varepsilon_{zz}} + k_z^2 = q^2 \Rightarrow (q^2 - k_z^2)\,\varepsilon_{zz}(\omega,\mathbf{k}) = k_x^2 \Rightarrow$$
$$\alpha\, k_z^4 - k_z^2\,\left(\alpha\, q^2 - \varepsilon_{\rm loc}\right) + \left(k_x^2 - q^2\,\varepsilon_{\rm loc}\right) = 0\,. \tag{1.207}$$

Thus, k_z (the component of wave vector normal to the boundary) satisfies the biquadratic equation, which generally has four solutions. Selecting the waves propagating *into* the structure, we get two solutions. Both solutions describe TM-polarized waves, whereas TE-polarized waves do not interact with the structure. **Thus, the incident beam generates one TE transmitted wave and two TM waves.** Depending on parameters, TM-waves can be both propagating, both evanescent or one of them is propagating and another one is evanescent. *Point out that evanescent waves have elliptic polarization, whereas propagating solutions are linearly polarized.*

To get further insights into the nature of trirefringence, we analyze the polarization state of TM solutions for the specific case of $k_x = 0$ (normal incidence). One of the solutions has $k_{z1}^2 = q^2$, which corresponds to the transverse wave polarized along x axis, which does not interact with the structure. The second solution has $k_{z2}^2 = -\varepsilon_{\rm loc}/\alpha$, i.e. $\varepsilon_{zz}(\omega,\mathbf{k}) = 0$. This describes the longitudinal wave with electric field parallel to the wave vector. Note that such modes can not be excited by the wave from vacuum at normal incidence. Quite importantly, this "additional" solution will be manifested if $\varepsilon_{\rm loc}$ is sufficiently small which would ensure that k_{z1} and k_{z2} have comparable magnitude.

In a similar way, Eq. (1.207) can be analyzed for oblique incidence. In this case, the transverse and longitudinal modes are hybridized, and the eigenmodes are neither purely transverse, nor purely longitudinal. Both of them can be excited by the incident wave.

The second scenario of trirefringence may take place when the anisotropy axis is parallel to the interface, but the effective permittivity is very large (i.e. the frequency of excitation is close to some resonance of the medium). In this case, we consider the expansion of *inverse permittivity* $\hat{\eta} = \hat{\varepsilon}^{-1}$:

$$\eta_{zz}(\omega,\mathbf{k}) = \eta_{\rm loc} + \beta\, k_x^2 + \tilde{\beta}\, k_z^2\,. \tag{1.208}$$

For simplicity we assume that $|\tilde{\beta}| \ll |\beta|$. The dispersion equation for TM waves then yields

$$k_x^2\,\eta_{zz} + k_z^2 = q^2 \Rightarrow \beta\, k_x^4 + \eta_{\rm loc}\, k_x^2 + \left(k_z^2 - q^2\right) = 0\,. \tag{1.209}$$

Thus, we again obtain two solutions propagating into the structure and having TM-like polarization. In this case, the spatial dispersion effects will be strongly manifested for sufficiently small $|\eta_{\rm loc}|$ which corresponds to very high permittivity.

To summarize, the phenomenon of trirefringence is expected either in the

vicinity of zeros or in the vicinity of poles of the effective permittivity. The specific range of parameters favouring the trirefringence is determined for the specific model of the structure.

Additional boundary conditions

Trying to calculate reflection or transmission coefficients from the boundary of spatially dispersive medium, we need to determine the amplitudes of the two transmitted waves and one reflected wave (overall, three parameters). However, for a fixed polarization (TM, in our case), we have only two boundary conditions which require the continuity of electric and magnetic field tangential components. Thus, it is evident that an additional boundary condition is required.

These additional boundary conditions can be derived from the microscopic theory (e.g., the *discrete dipole model* which we will discuss in the second part of the course) or, sometimes, from some macroscopic considerations.

For instance, for the wire medium with the wires perpendicular to the boundary, the additional boundary condition requires the continuity of $\varepsilon_h\, E_n$ at the interface [8]. Here, ε_h is the permittivity of the host medium, and E_n is the component of the average electric field normal to the boundary.

In another example of the 3D array of scatterers, an additional boundary conditions requires that

$$Q_{nn} = 0 \tag{1.210}$$

where tensor $\hat{Q}$ includes both quadrupole moment density and magnetic moment of the unit cell [9].

1.11 Spatial-dispersion-induced birefringence

Useful reading: Landau and Lifshitz [1], par. 105. Agranovich and Ginzburg [5], par. 8. Paper by Chebykin et al. [10].

Symmetry analysis

We consider a crystal possessing cubic symmetry (i.e. characterized by the symmetry groups T, T_h, T_d, O, O_h) and aim to find the restrictions on the structure of permittivity and permeability tensors $\hat{\varepsilon}(\omega)$ and $\hat{\mu}(\omega)$ dictated by symmetry.

First, we notice that the crystal has mirror symmetry with respect to Oxy, Oxz and Oyz planes. As a consequence, permittivity should be invariant under mirror reflections including, in particular, the transformation $T = \text{diag}\,(1, 1, -1)$. On the other hand, by doing this transformation, we see that $\varepsilon'_{xz} = -\varepsilon_{xz}$. This said, the off-diagonal components of the permittivity tensor vanish: $\varepsilon_{xz} = 0$.

Second, the crystal is invariant under rotation by 90° with respect to axes x, y and z. Consider, for instance, rotation with respect to z axis. Matrix of transformation is given by

$$T = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{1.211}$$

After this transformation, we find that $\varepsilon'_{xx} = \varepsilon_{yy}$, i.e. $\varepsilon_{xx} = \varepsilon_{yy}$.

The permeability tensor, obviously, shares the same properties. To conclude, if a crystal has cubic symmetry and is characterized by $\hat{\varepsilon}(\omega)$ and $\hat{\mu}(\omega)$ then these tensors are necessarily isotropic.

However, the experiment shows that some of natural cubic crystals do exhibit an anisotropy, which is the topic of this paragraph.

General treatment of the problem

To provide simple explanation of anisotropy emerging in cubic crystals, we consider the expansion of inverse permittivity tensor ($\hat{\eta} = \hat{\varepsilon}^{-1}$) of a cubic crystal with respect to wave vector:

$$\eta_{ik}(\omega, \mathbf{k}) = \eta_0(\omega)\,\delta_{ik} + \beta_{iklm}\,k_l\,k_m\,. \tag{1.212}$$

Terms of this expansion linear in k vanish due to the inversion symmetry of the crystal. Coefficients β_{iklm} are symmetric with respect to the indices i, k (due to symmetry of permittivity tensor) and also with respect to the indices l and m. Thus, without any crystal symmetries the 4^{th} rank tensor β_{iklm} has 36 independent components.

Highlight that generally second-order spatial dispersion effects scale as $(a/\lambda)^2$.

From Maxwell's equations we get the equation for the electric displacement vector

$$\left[\hat{I}/n^2 - \left(\hat{I} - \mathbf{n}\otimes\mathbf{n}\right)\,\hat{\eta}\right]\,\mathbf{D} = 0\,, \tag{1.213}$$

where n is the refraction index for the direction of wave vector given by the unit vector $\mathbf{n}$. The operator $\hat{I} - \mathbf{n}\otimes\mathbf{n} = -\left(\mathbf{n}^{\times}\right)^2$ simply substracts the part of the vector which is orthogonal to the direction of $\mathbf{n}$. Electric displacement vector $\mathbf{D}$ is always orthogonal to the direction of $\mathbf{n}$.

The origin of anisotropy

We align z axis parallel to wave vector (i.e. along $\mathbf{n}$). In this case, the dispersion equation reads:

$$0 = \det\,\left[\delta_{\mu\nu}/n^2 - \eta_{\mu\nu}\right] = \begin{pmatrix} \frac{1}{n^2} - \eta_{11} & \eta_{12} \\ \eta_{21} & \frac{1}{n^2} - \eta_{22} \end{pmatrix}\,. \tag{1.214}$$

where the Greek indices μ, ν are equal to 1 or 2. Quite obviously, this equation is quadratic with respect to $1/n^2$, and, therefore, it will have two solutions. In the general case this means birefringence.

Optical axes of cubic crystals

However, so far we have not used the symmetry of the crystal. By using the group theory, it can be shown that in the structures with cubic symmetry T or T_h, the β_{iklm} tensor has only 4 independent components. In the crystals with T_d, O and O_h symmetry group, the number of independent components is limited to 3.

Consider the crystal with O symmetry group. Calculate the number of independent components of β_{iklm} tensor.

Furthermore, with the help of group theory it can be shown that these independent components are

$$\beta_1 = \beta_{xxxx} = \beta_{yyyy} = \beta_{zzzz} \,, \tag{1.215}$$
$$\beta_2 = \beta_{yyxx} = \beta_{zzyy} = \beta_{xxzz} = \beta_{xxyy} = \beta_{yyzz} = \beta_{zzxx} \,, \tag{1.216}$$
$$\beta_3 = \beta_{xyxy} = \beta_{yzyz} = \beta_{zxzx} \,, \tag{1.217}$$

where the coordinate axes are aligned *parallel to the crystallographic axes*. The rest of the coefficients that cannot be obtained from Eqs. (1.215)-(1.217) by the permutation of the first or second pair of indices are zero.

We analyze now the dispersion equation (1.214) for some specific directions of propagation. Assume that $\mathbf{n}$ is aligned along the z axis. Then $\eta_{11} = \eta_{xx} = \eta_0 + \beta_2\, k^2$, $\eta_{22} = \eta_{yy} = \eta_0 + \beta_2\, k^2$, i.e. $\eta_{11} = \eta_{22}$. $\eta_{12} = \eta_{xy} = 0$. Thus, for this direction of propagation the dispersion equation yields doubly degenerate solution, i.e. the directions of propagation along the edges of cubic unit cell are the optical axes of the crystal.

Now assume that $\mathbf{n}$ is aligned along the crystallographic direction $[1, 1, 1]$. Two directions orthogonal to the wave vector are specified by the unit vectors $\mathbf{s_1} = [-1, -1, 2]/\sqrt{6}$ and $\mathbf{s_2} = [1, -1, 0]/\sqrt{2}$. $\eta_{\mu\nu} = \mathrm{s}_\mu \hat{\eta} \mathrm{s}_\nu$. It can be shown that this direction is also an optical axis.

Verify that the direction $[1, 1, 1]$ is an optical axis of the cubic crystal.

Answer.

$$\eta_{xx} = \eta_{yy} = \eta_{zz} = \eta_0 + k^2/3\,(\beta_1 + 2\,\beta_2)\,,$$
$$\eta_{xy} = \eta_{xz} = \text{off-diagonal components} = 2\,\beta_3\, k^2/3\,,$$
$$\eta_{11} = \eta_{22} = \eta_0 + (\beta_1 + 2\,\beta_2 - 2\,\beta_3)\ k^2/3\,,$$
$$\eta_{12} = 0\,.$$

Thus, the quadratic equation (1.214) yields a doubly degenerate solution.

Cubic crystal has seven optical axes: three of them correspond to the edges of the cubic unit cell, and four more axes correspond to the diagonals of the cube.

Quantifying spatial-dispersion-induced birefringence

Now consider the direction of wave vector given by $\mathbf{n} = [1, 1, 0]/\sqrt{2}$, which corresponds to the diagonal of the cube. Straightforward calculation yields

$$\eta_{xx} = \eta_{yy} = \eta_0 + (\beta_1 + \beta_2)\ k^2/2\,, \tag{1.218}$$
$$\eta_{zz} = \eta_0 + \beta_2\, k^2\,, \tag{1.219}$$
$$\eta_{xy} = \beta_3\, k^2\,, \tag{1.220}$$
$$\eta_{xz} = \eta_{yz} = 0\,. \tag{1.221}$$

Two directions orthogonal to $\mathbf{n}$ are chosen as $\mathbf{s_1} = [0,0,1]$ and $\mathbf{s_2} = [1,-1,0]/\sqrt{2}$. Then

$$\eta_{11} = \eta_{zz} = \eta_0 + \beta_2\, k^2\,, \tag{1.222}$$
$$\eta_{22} = \left(\eta_{xx} + \eta_{yy} - 2\,\eta_{xy}\right)/2 = \eta_0 + \left(\beta_1 + \beta_2 - 2\,\beta_3\right)\, k^2/2\,, \tag{1.223}$$
$$\eta_{12} = 0\,. \tag{1.224}$$

Thus, the difference of the refractive indices can be estimated as

$$\Delta\, n = n_{1\bar{1}0} - n_{001} \approx \frac{n_0^5\, q^2}{4}\, \left(\beta_1 - \beta_2 - 2\,\beta_3\right)\,. \tag{1.225}$$

It is this quantity that characterizes the magnitude of spatial-dispersion-induced birefringence.

1.12 Nonlinear susceptibilities

Additional reading: book on nonlinear optics by Boyd [11].

In the previous discussion we assumed that the medium polarization is linear with respect to the applied field. However, linear approximation of this kind breaks down once the fields in the medium become strong enough. Physical effects stemming from the medium nonlinear response are studied by *nonlinear optics*.

Some of the natural nonlinear media respond to electric field nonlinearly, and so

$$\begin{aligned} P_i(\omega) =& \chi^{(1)}_{ij}(\omega)\, E_j(\omega) + \sum_{\omega_1+\omega_2=\omega} \chi^{(2)}_{ijk}(\omega;\omega_1,\omega_2)\, E_j(\omega_1)\, E_k(\omega_2) + \\ &+ \sum_{\omega_1+\omega_2+\omega_3=\omega} \chi^{(3)}_{ijkl}(\omega;\omega_1,\omega_2,\omega_3)\, E_j(\omega_1)\, E_k(\omega_2)\, E_l(\omega_3) + \ldots\,. \end{aligned} \tag{1.226}$$

The coefficients $\chi^{(2)}$, $\chi^{(3)}$, etc. comprising this expansion are called *nonlinear susceptibilities*. Their values can be calculated analogously to the linear susceptibilities once the microstructure of the medium is specified. *Mention anharmonic oscillator model here.*

Symmetries of nonlinear susceptibilities

The effective susceptibilities $\chi^{(2)}_{ijk}(\omega;\omega_1,\omega_2)$ ($\chi^{(3)}_{ijkl}(\omega;\omega_1,\omega_2,\omega_3)$) are symmetric with respect to permutation of the indices j, k (j, k, l) once the frequencies ω_1, ω_2 (ω_1, ω_2, ω_3) are permuted accordingly:

$$\chi^{(2)}_{ijk}(\omega;\omega_1,\omega_2) = \chi^{(2)}_{ikj}(\omega;\omega_2,\omega_1)\,. \tag{1.227}$$

Furthermore, the nonlinear susceptibility $\chi^{(2)}$ vanishes in the media with inversion symmetry. Indeed, the tensor $E_j\, E_k$ is even under inversion, whereas P_i is odd. This implies that $\chi^{(2)}$ should be odd under inversion. On the other hand, the inversion symmetry of the system means that the inversion does not change $\chi^{(2)}$. Thus, $\chi^{(2)} = 0$ for inversion-symmetric media.

Additionally, it can be shown that in the absence of losses, the nonlinear susceptibilities defined by Eq. (1.226) are purely real (see the derivation of anharmonic oscillator nonlinear susceptibility). In this case, an additional symmetry called *full permutation symmetry* holds. For instance,

$$\chi^{(2)}_{ijk}(\omega;\omega_1,\omega_2) = \chi^{(2)}_{jki}(\omega_1;-\omega_2,\omega)\,. \tag{1.228}$$

$-$ sign in frequency arguments is included in order to ensure that the first argument is equal to the sum of the rest of frequencies.

If the frequencies of interest are much lower that the frequencies of the medium resonances ω_{0i}, the dependence of the nonlinear susceptibilities on frequency can be omitted. As a result, nonlinear susceptibility happens to be symmetric with respect to all its indices (Kleinman symmetry).

Crystalline symmetries further reduce the number of the independent components of nonlinear susceptibility. For instance, in the most simple isotropic case $\chi^{(2)} \equiv 0$, whereas $\chi^{(3)}$ has three independent components (see Table 1.5.4 of Boyd [11]):

$$\chi^{(3)}_{yyzz} = \chi^{(3)}_{zzyy} = \chi^{(3)}_{zzxx} = \chi^{(3)}_{xxzz} = \chi^{(3)}_{xxyy} = \chi^{(3)}_{yyxx}\,, \tag{1.229}$$
$$\chi^{(3)}_{yzyz} = \chi^{(3)}_{zyzy} = \chi^{(3)}_{zxzx} = \chi^{(3)}_{xzxz} = \chi^{(3)}_{xyxy} = \chi^{(3)}_{yxyx}\,, \tag{1.230}$$
$$\chi^{(3)}_{yzzy} = \chi^{(3)}_{zyyz} = \chi^{(3)}_{zxxz} = \chi^{(3)}_{xzzx} = \chi^{(3)}_{xyyx} = \chi^{(3)}_{yxxy}\,, \tag{1.231}$$
$$\chi^{(3)}_{xxxx} = \chi^{(3)}_{yyyy} = \chi^{(3)}_{zzzz} = \chi^{(3)}_{xxyy} + \chi^{(3)}_{xyxy} + \chi^{(3)}_{xyyx} \tag{1.232}$$

Omit this formulas until the topic of nonlinear self-action.

Wave equation for nolinear optical media

$$\mathrm{rot}\,\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{H}}{\partial t}\,, \tag{1.233}$$
$$\mathrm{rot}\,\mathbf{H} = \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t}\,. \tag{1.234}$$

These equations yield that

$$\mathrm{rot}\,\mathrm{rot}\,\mathbf{E} \equiv \nabla\left(\mathrm{div}\,\mathbf{E}\right) - \Delta\,\mathbf{E} = -\frac{1}{c^2}\frac{\partial^2 D}{\partial t^2}\,. \tag{1.235}$$

In many cases the term $\nabla\left(\mathrm{div}\,\mathbf{E}\right)$ is zero or negligibly small. After omitting this term and substituting

$$\mathbf{D} = \varepsilon^{(1)}\,\mathbf{E} + 4\pi\,\mathbf{P}^{\mathrm{NL}} \tag{1.236}$$

we get:

$$\Delta\,\mathbf{E} - \frac{\varepsilon^{(1)}}{c^2}\,\frac{\partial^2\mathbf{E}}{\partial t^2} = \frac{4\pi}{c^2}\,\frac{\partial^2\mathbf{P}^{\rm NL}}{\partial t^2}\,. \tag{1.237}$$

This said, the nonlinear polarization of the medium plays the role of the source term in the wave equation.

If the medium is dispersive, each frequency component of the field should be considered separately, and we get:

$$\Delta\,\mathbf{E}(\omega) + \frac{\varepsilon^{(1)}(\omega)\,\omega^2}{c^2}\,\mathbf{E}(\omega) = -\frac{4\pi\,\omega^2}{c^2}\,\mathbf{P}^{\rm NL}(\omega)\,. \tag{1.238}$$

1.13 Sum frequency generation

Equations for sum frequency generation

As a first example of nonlinear optical process we consider the medium characterized by the second-order nonlinearity. For the fixed geometry (i.e. fixed polarization and fixed propagation direction), it is possible to introduce some effective nonlinearity such that

$$P(\omega) = 4\,d_{\rm eff}\,E(\omega_1)\,E(\omega_2)\,, \tag{1.239}$$

where projections on suitable coordinate axes are considered. We assume that the medium is pumped by the plane waves with the frequencies ω_1, ω_2, amplitudes A_1, A_2 and with the wave vectors k_1, k_2 directed along z axis, such that $E(\omega) = A(z)\,e^{ikz}$. We also apply the slowly varying amplitude approximation, neglecting second-order derivatives d^2A_n/dz^2. With these assumptions we analyze sum harmonic generation and get the system of equations

$$\begin{aligned}\left[2i\,k_1\,\frac{dA_1}{dz} - k_1^2\,A_1 + \frac{\varepsilon^{(1)}(\omega_1)\,\omega_1^2}{c^2}\,A_1\right]\,e^{ik_1\,z} &= -\frac{4\pi\,\omega_1^2}{c^2}\,P^{\rm NL}(\omega_1) = \\ &= -\frac{16\pi\,\omega_1^2}{c^2}\,d_{\rm eff}\,A_3\,A_2^*\,e^{i(k_3-k_2)\,z}\,,\end{aligned} \tag{1.240}$$

$$\begin{aligned}\left[2i\,k_2\,\frac{dA_2}{dz} - k_2^2\,A_2 + \frac{\varepsilon^{(1)}(\omega_2)\,\omega_2^2}{c^2}\,A_2\right]\,e^{ik_2\,z} &= -\frac{4\pi\,\omega_2^2}{c^2}\,P^{\rm NL}(\omega_2) = \\ &= -\frac{16\pi\,\omega_2^2}{c^2}\,d_{\rm eff}\,A_3\,A_1^*\,e^{i(k_3-k_1)\,z}\,,\end{aligned} \tag{1.241}$$

$$\left[2i\,k_3\,\frac{dA_3}{dz} - k_3^2\,A_3 + \frac{\varepsilon^{(1)}(\omega_3)\,\omega_3^2}{c^2}\,A_3\right]\,e^{ik_3\,z} = -\frac{4\pi\,\omega_3^2}{c^2}\,P^{\mathrm{NL}}(\omega_3) = \\ = -\frac{16\pi\,\omega_3^2}{c^2}\,d_{\mathrm{eff}}\,A_1\,A_2\,e^{i(k_1+k_2)\,z}\,. \tag{1.242}$$

Note that in all three equations the second and the third terms from the left-hand side mutually cancel. Thus, we get the system of differential equations for the amplitudes of interacting waves:

$$\frac{dA_1}{dz} = \frac{8\pi\,i\,\omega_1^2}{k_1\,c^2}\,d_{\mathrm{eff}}\,A_3\,A_2^*\,e^{-i\Delta k\,z}\,, \tag{1.243}$$

$$\frac{dA_2}{dz} = \frac{8\pi\,i\,\omega_2^2}{k_2\,c^2}\,d_{\mathrm{eff}}\,A_3\,A_1^*\,e^{-i\Delta k\,z}\,, \tag{1.244}$$

$$\frac{dA_3}{dz} = \frac{8\pi\,i\,\omega_3^2}{k_3\,c^2}\,d_{\mathrm{eff}}\,A_1\,A_2\,e^{i\Delta k\,z}\,, \tag{1.245}$$

where $\Delta k = k_1 + k_2 - k_3$. *Same coupling coefficient due to full permutation symmetry. Neglect other nonlinear processes.*

Phase-matching conditions

Now we analyze the efficiency of sum frequency generation for the fixed nonlinearity strength d_{eff}. For simplicity we employ so-called *undepleted pump approximation* assuming that $A_1 = A_2 = \mathrm{const}$.

$$A_3(L) = \frac{8\pi\,i\,\omega_3^2}{k_3\,c^2}\,d_{\mathrm{eff}}\,A_1\,A_2\int_0^L e^{i\Delta k\,z}\,dz = \frac{8\pi\,\omega_3^2}{k_3\,c^2}\,d_{\mathrm{eff}}\,A_1\,A_2\,\frac{e^{i\Delta k\,L}-1}{\Delta k} = \\ = \frac{8\pi\,\omega_3^2\,d_{\mathrm{eff}}}{c^2\,k_3}\,A_1\,A_2\,L\,e^{i\Delta k L/2}\,\mathrm{sinc}\,(\Delta k\,L/2)\;, \tag{1.246}$$

where $\mathrm{sinc}\,x \equiv \sin x/x$. Thus, the intensity of the sum harmonic signal will be proportional to $\mathrm{sinc}^2\,(\Delta k\,L/2)$. The plot of this function is presented in Fig. 1.5.

Thus, in order to achieve the maximum harmonic generation efficiency, one needs to ensure that $k_3 = k_1 + k_2$ which is known as *phase-matching condition*. We explore the possibility to realize phase matching on the example of second harmonic generation. In this case, $2k_1 = k_3$ or $2n(\omega)\,\omega/c = n(2\omega)\,2\omega/c$, i.e. $n(2\omega) = n(\omega)$.

In the transparency windows of the medium, the normal dispersion takes place: $n(2\omega) > n(\omega)$. The way to circumvent this difficulty is based on on birefringent crystals for which it is possible to ensure that $n_o(2\omega) = n_e(\omega)$ or $n_e(2\omega) = n_o(\omega)$. Normally, this happens only for some specific propagation directions in the crystal.

The Manley-Rowe relations

For further understanding of the three-wave mixing process, we consider energy relations for the three propagating waves (ω_1, ω_2, ω_3). The time-averaged energy

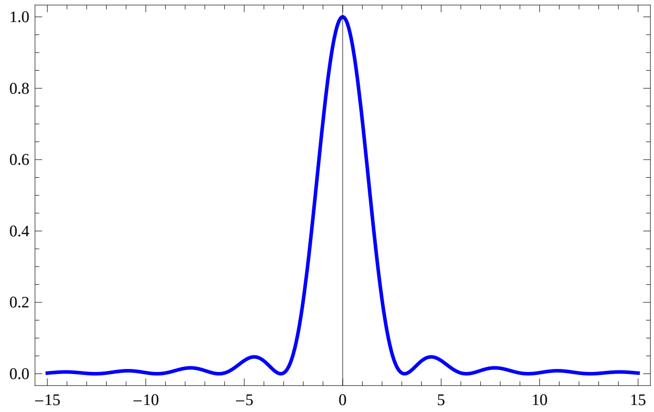

Figure 1.5: Plot of $\mathrm{sinc}^2 x$ function.

flow is given by

$$I = \frac{c}{4\pi}\,\langle E\,H\rangle = \frac{c}{8\pi}\,\mathrm{Re}\,[E_0^*\,H_0] = \frac{c\,n}{8\pi}|E_0|^2 = \frac{c\,n}{2\pi}|A|^2 = \frac{c^2\,k}{2\pi\,\omega}\,|A|^2\,, \tag{1.247}$$

where we take into account that the amplitude of the wave is given by $E_0 = 2|A|$. Therefore,

$$\frac{dI}{dz} = \frac{c^2\,k}{2\pi\,\omega}\left[\frac{dA}{dz}\,A^* + A\,\frac{dA^*}{dz}\right]\,. \tag{1.248}$$

Making use of Eqs. (1.243)-(1.245), we calculate the z derivatives of intensities:

$$\frac{dI_1}{dz} = 4d_{\mathrm{eff}}\,\omega_1\,\left[iA_3A_2^*A_1^*\,e^{-i\Delta k\,z} - iA_3^*A_2A_1\,e^{i\Delta k\,z}\right]\,, \tag{1.249}$$

$$\frac{dI_2}{dz} = 4d_{\mathrm{eff}}\,\omega_2\,\left[iA_3A_1^*A_2^*\,e^{-i\Delta k\,z} - iA_3^*A_1A_2\,e^{i\Delta k\,z}\right]\,, \tag{1.250}$$

$$\frac{dI_3}{dz} = 4d_{\mathrm{eff}}\,\omega_3\,\left[iA_1A_2A_3^*\,e^{i\Delta k\,z} - iA_1^*A_2^*A_3\,e^{-i\Delta k\,z}\right]\,. \tag{1.251}$$

First, we notice that since $\omega_3 = \omega_1 + \omega_2$

$$\frac{d}{dz}\,[I_1 + I_2 + I_3] = 0\,, \tag{1.252}$$

which simply means the energy conservation in the system (note that we have assumed zero dissipation above).

Second,

$$\frac{d}{dz}\left(\frac{I_1}{\omega_1}\right) = \frac{d}{dz}\left(\frac{I_2}{\omega_2}\right) = -\frac{d}{dz}\left(\frac{I_3}{\omega_3}\right)\,. \tag{1.253}$$

Eqs. (1.253) are known as Manley-Rowe relations. Since the energy of a photon with frequency ω is equal to $\hbar\,\omega$, Manley-Rowe relations simply indicate that the emission of each photon with frequency ω_3 is accompanied by the absorption of ω_1

and ω_2 photons, as illustrated in Fig. 1.6.

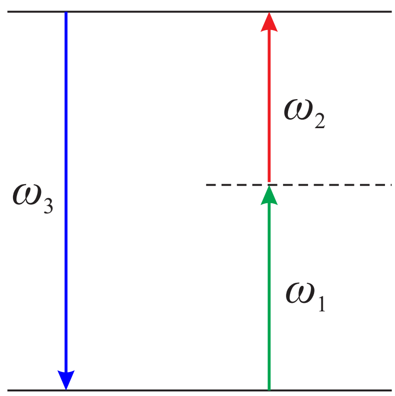

Figure 1.6: Illustration of the three-wave mixing process and the Manley-Rowe relations.

1.14 Nonlinear self-action effects

In this paragraph, we examine the nonlinear optical effects which arise at the frequency of impinging wave. To analyze such effects one has to consider cubic nonlinearity ($\omega = \omega + \omega - \omega$).

Expression for nonlinear polarization of isotropic medium

Can skip the details and just provide the final expression for the nonlinear polarization of isotropic medium with $\chi^{(3)}$.

We consider an *isotropic* nonlinear medium. In this case, according to Eq. (1.229)-(1.232), the only nonzero components of nonlinear susceptibility tensor read (no summation over the repeated indices here):

$$\chi^{(3)}_{iikk}(\omega;\omega,\omega,-\omega) = \chi^{(3)}_{ikik}(\omega;\omega,\omega,-\omega) \equiv \alpha(\omega)/(8\pi)\,, \quad (i \neq k) \tag{1.254}$$

$$\chi^{(3)}_{ikki}(\omega;\omega,\omega,-\omega) \equiv \beta(\omega)/(4\pi)\,, \quad (i \neq k) \tag{1.255}$$

$$\begin{aligned}\chi^{(3)}_{iiii}(\omega;\omega,\omega,-\omega) &= \chi^{(3)}_{iikk}(\omega;\omega,\omega,-\omega) + \chi^{(3)}_{ikik}(\omega;\omega,\omega,-\omega)\\ &+\chi^{(3)}_{ikki}(\omega;\omega,\omega,-\omega) = (\alpha+\beta)/(4\pi)\,,\end{aligned} \tag{1.256}$$

and additionally at low frequencies $\alpha(0) = 2\beta(0)$ due to Kleimann symmetry. The nonlinear polarization reads

$$\begin{aligned}&P^{(3)}_i(\omega) = \sum_{j,k,l} \chi^{(3)}_{ijkl}\, E_j\, E_k\, E^*_l = \\ &\chi^{(3)}_{iiii}\, E_i^2\, E_i^* + \sum_{k\neq i} \chi^{(3)}_{iikk}\, E_i\, E_k\, E^*_k + \sum_{k\neq i} \chi^{(3)}_{ikik}\, E_k\, E_i\, E^*_k + \sum_{k\neq i} \chi^{(3)}_{ikki}\, E_k\, E_k\, E^*_i\end{aligned} \tag{1.257}$$

where all field components are taken at frequency ω and frequency arguments of nonlinear susceptibilities are given in the order $(\omega;\omega,\omega,-\omega)$. Therefore, the nonlinear contribution to the displacement

$$D_i^{(3)}(\omega) = 4\pi\, P_i^{(3)}(\omega) = (\alpha+\beta)\; E_i^2\, E_i^* + \alpha\, E_i\, \left(|\mathbf{E}|^2 - |E_i|^2\right) + \beta\, E_i^*\, \left(\mathbf{E}^2 - E_i^2\right)\,. \tag{1.258}$$

Finally in vector form

$$\mathbf{D}^{(3)}(\omega) = \alpha(\omega)\, |\mathbf{E}|^2\, \mathbf{E} + \beta(\omega)\, \mathbf{E}^2\, \mathbf{E}^*\,. \tag{1.259}$$

Plane-wave solution and self-action

We seek the solution of wave equation in the form of plane wave: $\mathbf{E} = \mathbf{E}_0\, e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t}$ with $\mathbf{E}_0$ orthogonal to the direction of wave vector. In the case of linearly and circularly polarized waves, the electric displacement will be parallel to $\mathbf{E}$:

$$\mathbf{D} = \left(\varepsilon + \frac{2\,c^2}{\omega^2}\,\eta\,|\mathbf{E}_0|^2\right)\,\mathbf{E}\,, \tag{1.260}$$

where $\eta = \omega^2\,(\alpha+\beta)/(2\,c^2)$ for the linearly polarized wave and $\eta = \omega^2\,\alpha/(2\,c^2)$ for the circularly polarized wave. Note that such solution satisfies the condition $\operatorname{div}\mathbf{E} = 0$ due to $\operatorname{div}\mathbf{D} = 0$. The wave equation yields:

$$0 = \Delta\,\mathbf{E} + \frac{\omega^2}{c^2}\,\mathbf{D} = \left[-\mathbf{k}^2 + q^2\,\varepsilon + 2\eta\,|\mathbf{E}_0|^2\right]\,\mathbf{E} \tag{1.261}$$

and, thus, the dispersion equation reads

$$\mathbf{k}^2 = q^2\,\varepsilon + 2\eta\,|\mathbf{E}_0|^2\,. \tag{1.262}$$

In other words, the wave experiences the intensity-dependent refractive index

$$n \approx \sqrt{\varepsilon} + \frac{\eta\,|\mathbf{E}_0|^2}{q^2\,\sqrt{\varepsilon}}\,, \tag{1.263}$$

the effect known as the *optical Kerr effect*.

However, if the wave has finite extent (i.e. differs from the plane wave), an instability occurs. Here we discuss the origin of this instability only qualitatively. The wave propagating in the medium modifies the refractive index according to Eq. (1.263). This self-induced lens causes the wave to deflect from the lower-index region towards the higher-index region. Therefore, in the case of $\eta > 0$ the finite beam tends to focus; the nonlinearity is called *focusing*. On the contrary, if $\eta < 0$, the finite-size beam tends to defocus and the nonlinearity is called *defocusing*. This reasoning is illustrated in Fig. 1.7. On the other hand, any beam with a finite radius tends to broaden due to the diffraction (see theory of this effect in the textbook [12]).

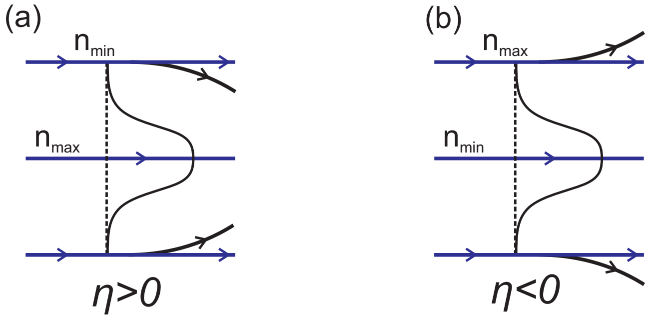

Figure 1.7: Illustration of (a) self-focusing; (b) self-defocusing processes happening for $\eta > 0$ and $\eta < 0$, respectively.

Solitons in the nonlinear medium

Thus, the propagation of the beams in the nonlinear medium is determined by the combination of the two factors: (i) self-focusing or self-defocusing due to nonlinearity; (ii) broadening of the beam due to diffraction. It occurs that the effects of self-focusing and diffraction can be exactly balanced leading to the emergence of optical soliton.

We seek the solution of the wave equation in the form

$$\mathbf{E} = F(y)\, e^{i\,(k_0+\varkappa)\,x - i\omega\, t}\,\mathbf{e}_z\,, \tag{1.264}$$

where $k_0 = q\sqrt{\varepsilon}$, $\varkappa$ is the parameter of the soliton providing the intensity-dependent correction to the propagation constant, and $F(y)$ is an unknown real function. For this ansatz $\operatorname{div}\mathbf{E} = 0$, and the wave equation yields

$$\Delta\, E_z + \left[q^2\,\varepsilon + 2\,\eta\,|E_z|^2\right]\, E_z = 0\,. \tag{1.265}$$

This gives the differential equation with respect to the unknown function $F(y)$:

$$-\frac{1}{2}\,\frac{d^2\,F}{dy^2} + k_0\,\varkappa\,F - \eta\,F^3 = 0\,. \tag{1.266}$$

Note that this equation is known as the *nonlinear Schrödinger equation* (also known as the Gross-Pitaevskii equation and the Ginzburg-Landau equation), and it appears in the variety of contexts including nonlinear optics, and interacting many-body quantum systems. In the latter case the canonical form reads:

$$-\frac{\hbar^2}{2m}\,\frac{d^2\psi}{dy^2} + \left[V(y) - \epsilon\right]\,\psi + g|\psi|^2\,\psi = 0\,. \tag{1.267}$$

Integration with respect to F gives:

$$-\frac{1}{4}\,\left(F'\right)^2 + k_0\,\varkappa\,\frac{F^2}{2} - \frac{\eta\,F^4}{4} = C_1\,. \tag{1.268}$$

Since we look for the solution with $F \to 0$ and $F' \to 0$ for $y \to \infty$, we set $C_1 = 0$. Then

$$\frac{dF}{dy} = -\sqrt{2k_0\, \varkappa\, F^2 - \eta\, F^4}\,, \tag{1.269}$$

($-$ sign choice to ensure the decrease of F). Next we do the substitution $F = 1/\psi$ and get

$$\frac{d\psi}{dy} = \sqrt{2k_0\, \varkappa\, \psi^2 - \eta} \tag{1.270}$$

which yields

$$y = \frac{1}{\sqrt{2k_0\, \varkappa}}\, \mathrm{arch}\left(\sqrt{\frac{2k_0\, \varkappa}{\eta}}\, \psi\right) + C_2\,. \tag{1.271}$$

By omitting the inessential constant (related to the shift of axis origin) we finally get the expression for the field profile:

$$F(y) = \sqrt{\frac{2k_0\, \varkappa}{\eta}}\, \frac{1}{\mathrm{ch}\left(\sqrt{2k_0\, \varkappa}\, y\right)}\,. \tag{1.272}$$

Equation (1.272) describes the soliton which is the solution of nonlinear Schrödinger equation and which appears due to the balance of diffraction mechanism and focusing nonlinearity. The soliton profile is depicted in Fig. 1.8.

1.15 Stimulated Raman scattering

Nonlinear processes described in the previous paragraphs are called *parametric* since they are energy-conserving (for instance, two pump photons are transformed into a single second-harmonic photon). We consider now the *non-parametric* processes accompanied by the change of the nonlinear medium state.

One of important processes of this kind is the *Raman scattering* in which the

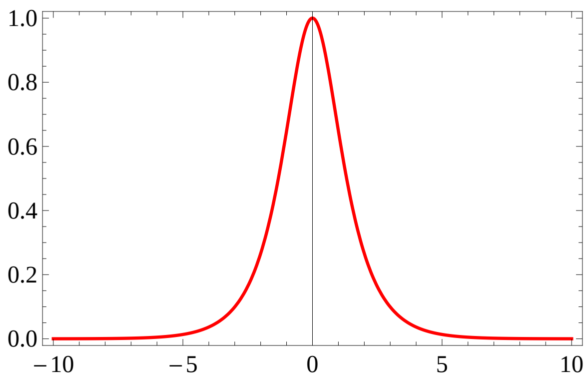

Figure 1.8: Field profile of the soliton in the nonlinear medium with $\chi^{(3)}$ nonlinearity.

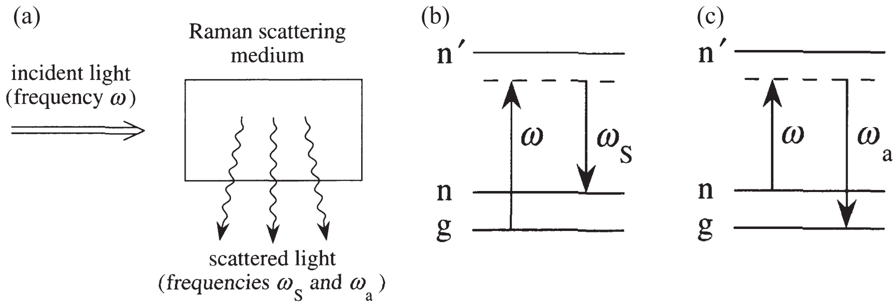

Figure 1.9: (a) A scheme of the Raman scattering process. (b,c) Raman Stokes and anti-Stokes scattering.

incident light at frequency ω is scattered either into the mode with frequency $\omega_s = \omega - \omega_v$ (the Stokes component) or to the component with the frequency $\omega_a = \omega + \omega_v$ (the anti-Stokes component) as illustrated in Fig. 1.9. Typically, $\omega_v \ll \omega$.

Microscopically, the Raman scattering originates from the coupling of the molecule vibrational mode (with frequency ω_v) to the light mode. In quantum-mechanical picture, the origin of the Stokes and anti-Stokes components in Raman signal is illustrated by Fig. 1.9. From these pictures it is clear that the intensity of the anti-Stokes component is usually much smaller than that of Stokes component.

Raman effect was discovered independently by the Soviet scientists Mandelstam and Landsberg in Moscow State University and by the Indian scientist Raman in Kolkata, both groups made their discoveries in February 1928. However, the Nobel Prize in Physics for the newly discovered type of scattering was awarded in 1930 to Raman only. Since then, the process has been called "Raman scattering", while in Russian literature the term "combination scattering" is used instead.

Two types of the Raman scattering are distinguished: spontaneous and stimulated. The latter occurs when the medium is pumped by intense laser light which causes highly efficient Raman scattering. On the contrary, the spontaneous process has extremely low efficiency.

The importance of the Raman spectroscopy for applications comes from the fact that the transitions between $|\, n \,\rangle$ and $|\, g \,\rangle$ are forbidden in dipole approximation. However, the Raman spectroscopy provides a tool to probe them. Raman signal provides the information about the molecule vibrational modes, which are considered as fingerprints of a molecule in spectroscopy. The so-called surface-enhanced Raman scattering (SERS) is one of important experimental techniques.

Classical analysis of the Raman scattering

The key assumption of this approach is the dependence of the molecule polarizability on the vibrational coordinate q:

$$\alpha(q) \approx \alpha_0 + \frac{\partial \alpha}{\partial q} q(t) \,. \tag{1.273}$$

Hence, the polarization of the medium induced by the incident wave is given by

$$\mathbf{P} = n\,\alpha[q(t)]\,\mathbf{E}\,e^{-i\omega\,t} = n\left(\alpha_0 + \frac{\partial\alpha}{\partial q}\,q(t)\right)\,\left[A\,e^{-i\omega\,t} + A^*\,e^{i\omega\,t}\right]\,, \tag{1.274}$$

where n is a number of molecules per unit volume. The molecule vibration occurs with the vibrational frequency ω_v, i.e. $q(t) = q_0\,e^{-i\omega_v\,t} + q_0^*\,e^{i\omega_v\,t}$. This gives for the polarization

$$P(t) = n\,\alpha_0\,A\,e^{-i\omega\,t} + n\,\alpha_0\,A^*\,e^{i\omega\,t} + n\,\frac{\partial\alpha}{\partial q}\,\Big[A\,q_0\,e^{-i\,(\omega+\omega_v)\,t} + A\,q_0^*\,e^{-i\,(\omega-\omega_v)\,t}$$
$$+A^*\,q_0^*\,e^{i\,(\omega+\omega_v)\,t} + A^*\,q_0\,e^{i(\omega-\omega_v)\,t}\Big]\,, \tag{1.275}$$

which, indeed, explains the origin of Stokes $\omega_s = \omega - \omega_v$ and anti-Stokes $\omega_a = \omega + \omega_v$ components of Raman signal.

Relation to nonlinear susceptibilities

On the other hand, a similar form of nonlinear polarization can be written in terms of nonlinear susceptibilities:

$$P(\omega_1) = 6\,\chi^{(3)}(\omega_1;\omega_1,\omega,-\omega)\,A_1\,|A|^2 \equiv 6\,\chi_R(\omega_1)\,A_1\,|A|^2\,, \tag{1.276}$$

where A and A_1 are the amplitudes of the incident wave and scattered light with shifted frequency, respectively. To make a comparison of Eqs. (1.275) and (1.276) and find the Raman susceptibility, we need to calculate the amplitude of molecule vibrations q_0.

The energy of a molecule in the external field is given by

$$W = -\frac{1}{2}\,\alpha\,\left\langle E^2\right\rangle \tag{1.277}$$

so that the derivative $-\partial\,W/\partial\,E$ yields the molecule dipole moment. The force acting on the molecule reads:

$$F = -\frac{\partial W}{\partial q} = \frac{1}{2}\frac{\partial\alpha}{\partial q}\,\left\langle E^2\right\rangle\,. \tag{1.278}$$

The field in the medium is presented as

$$E = A\,e^{-i\omega\,t} + A^*\,e^{i\omega\,t} + A_1\,e^{-i\omega_1\,t} + A_1^*\,e^{i\omega_1\,t} \tag{1.279}$$

and thus the amplitude of the force at frequency $\omega - \omega_1$ is given by $F(\omega-\omega_1) = \frac{\partial\alpha}{\partial q}\,A\,A_1^*$. Further, we consider the molecule as a classical oscillator and get the equation

$$\ddot{q} + 2\gamma\,\dot{q} + \omega_v^2\,q = F(\omega-\omega_s)\,e^{-i(\omega-\omega_1)\,t}/m + \text{c.c.}\,, \tag{1.280}$$

which has a steady state solution $q(t) = q_0 \, e^{-i(\omega-\omega_1)\,t} + \text{c.c.}$ with the amplitude q_0 given by

$$q_0 = \frac{1}{m}\frac{\partial\alpha}{\partial q}\,\frac{A\,A_1^*}{-(\omega-\omega_1)^2 - 2i\gamma\,(\omega-\omega_1) + \omega_v^2}\;. \tag{1.281}$$

The polarization at frequency ω_1 thus reads

$$P(\omega_1) = n\,\frac{\partial\alpha}{\partial q}\,q_0^*\,A = \frac{n}{m}\left|\frac{\partial\alpha}{\partial q}\right|^2 A_1\,|A|^2\,\left[-(\omega-\omega_1)^2 + 2i\gamma\,(\omega-\omega_1) + \omega_v^2\right]^{-1}\;, \tag{1.282}$$

and the Raman susceptibility is given by

$$\chi_R(\omega_1) = \frac{n}{6m}\left|\frac{\partial\alpha}{\partial q}\right|^2\,\left[-(\omega-\omega_1)^2 + 2i\gamma\,(\omega-\omega_1) + \omega_v^2\right]^{-1}\;. \tag{1.283}$$

Quite naturally, the Raman susceptibility reaches its maximum at resonance when $\omega - \omega_1 = \omega_v$. The width of the Raman peak is determined by the magnitude of loss γ.

1.16 Electromagnetic field of a particle moving in the continuous medium

Useful reading: book by Landau and Lifshits [1], paragraph 114

In this paragraph, we aim to calculate the electromagnetic fields created by a charged particle moving through the medium. First, we discuss the applicability range of the macroscopic treatment of the medium. If v is a particle velocity, a is the typical distance from the charged particle to the atom, then the spectrum of radiation has a maximum at frequencies around v/a. In order to cause ionization of the atoms, the frequency of radiation should be larger than the frequency of atomic transitions ω_0. The classical treatment will be adequate, provided the discrete energy spectrum of the atoms can be ignored, i.e. the frequency $v/a \gg \omega_0$. Otherwise (i.e. in the case of slow particles), one has to treat excitation of the medium quantum-mechanically.

We consider Maxwell's equations in non-magnetic medium:

$$\operatorname{rot}\mathbf{H} = \frac{1}{c}\frac{\partial\mathbf{D}}{\partial t} + \frac{4\pi}{c}\mathbf{j}_{\text{ext}}\;, \tag{1.284}$$

$$\operatorname{div}\mathbf{D} = 4\pi\,\rho_{\text{ext}}\;, \tag{1.285}$$

$$\operatorname{rot}\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{H}}{\partial t}\;, \tag{1.286}$$

$$\operatorname{div}\mathbf{H} = 0 \tag{1.287}$$

We assume that the particle moves through this medium with a constant speed $\mathbf{v}$ so the external charge and current densities are defined as

$$\mathbf{j}_{\rm ext} = Q\,\mathbf{v}\,\delta\,(\mathbf{r}-\mathbf{v}t)\ , \tag{1.288}$$
$$\rho_{\rm ext} = Q\,\delta\,(\mathbf{r}-\mathbf{v}t)\ , \tag{1.289}$$

where Q is the particle charge. We introduce the vector and scalar potentials $\mathbf{A}$ and ϕ as

$$\mathbf{H} = \mathrm{rot}\,\mathbf{A}\ , \tag{1.290}$$
$$\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi \tag{1.291}$$

with an additional gauge condition

$$\mathrm{div}\,\mathbf{A} + \frac{1}{c}\frac{\partial\,(\hat{\varepsilon}\,\phi)}{\partial t} = 0\ . \tag{1.292}$$

Note that we use a special type of gauge here: it is neither the Lorenz gauge nor the Coulomb one. The nonlocal operator $\hat{\varepsilon}$ used here incorporates the effect of frequency dispersion as follows:

$$\hat{\varepsilon}\,\phi = \iint \varepsilon(\omega)\,\phi_{\mathbf{k}}(\omega)\,e^{i\mathbf{k}\cdot\mathbf{r}-i\omega\,t}\,\frac{d\mathbf{k}\,d\omega}{(2\pi)^4} \tag{1.293}$$

and commutes with the derivatives with respect to time or coordinates. With the definitions Eqs. (1.290)-(1.291) the Eqs. (1.286)-(1.287) are satisfied identically. The remaining two equations yield:

$$\Delta\mathbf{A} - \frac{\hat{\varepsilon}}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} = -\frac{4\pi}{c}\,Q\,\mathbf{v}\,\delta\,(\mathbf{r}-\mathbf{v}t)\ . \tag{1.294}$$
$$\hat{\varepsilon}\,\Delta\phi - \frac{\hat{\varepsilon}^2}{c^2}\frac{\partial^2\phi}{\partial t^2} = -4\pi\,Q\,\delta\,(\mathbf{r}-\mathbf{v}t)\ . \tag{1.295}$$

Next, we decompose the potentials into Fourier integrals in space (i.e. perform the plane wave expansion):

$$\begin{aligned} \mathbf{A} &= \int \mathbf{A}_k\,e^{i\mathbf{k}\cdot\mathbf{r}}\,\frac{d\mathbf{k}}{(2\pi)^3}\ , \\ \phi &= \int \phi_k\,e^{i\mathbf{k}\cdot\mathbf{r}}\,\frac{d\mathbf{k}}{(2\pi)^3}\ . \end{aligned} \tag{1.296}$$

The Fourier transform of the δ-functon reads:

$$\int \delta(\mathbf{r}-\mathbf{v}t)\,e^{-i\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{r} = e^{-i\mathbf{v}\cdot\mathbf{k}\,t}\ . \tag{1.297}$$

Thus, we get ordinary differential equations for the Fourier transformed fields:

$$k^2\,\mathbf{A}_k + \frac{\hat{\varepsilon}}{c^2}\,\ddot{\mathbf{A}}_k = \frac{4\pi}{c}\,Q\,\mathbf{v}\,e^{-i\mathbf{v}\cdot\mathbf{k}\,t}\,, \tag{1.298}$$

$$k^2\,\hat{\varepsilon}\,\phi_k + \frac{\hat{\varepsilon}}{c^2}\,\ddot{\phi}_k = 4\pi\,Q\,e^{-i\mathbf{v}\cdot\mathbf{k}\,t} \tag{1.299}$$

Equations (1.298)-(1.299) suggest that the Fourier components of potentials oscillate with the frequency $\omega = \mathbf{v}\cdot\mathbf{k}$. *Stress here that the Fourier components of the fields are monochromatic.* Therefore, the action of the operator $\hat{\varepsilon}$ is equivalent to the multiplication by $\varepsilon(\omega)$, and the solutions of Eqs. (1.298)-(1.299) read:

$$\mathbf{A}_k = \frac{4\pi\,e^{-i\omega\,t}}{c}\,\frac{Q\,\mathbf{v}}{k^2 - \varepsilon(\omega)\,\omega^2/c^2}\,, \tag{1.300}$$

$$\phi_k = \frac{4\pi\,e^{-i\omega\,t}}{\varepsilon(\omega)}\,\frac{Q}{k^2 - \varepsilon(\omega)\,\omega^2/c^2}\,, \tag{1.301}$$

where the frequency $\omega = \mathbf{v}\cdot\mathbf{k}$. Furthermore, the Fourier components of the electric and magnetic fields created by the particle read

$$\mathbf{E}_k = i\omega/c\,\mathbf{A}_k - i\mathbf{k}\,\phi_k\,, \mathbf{H}_k = i\,[\mathbf{k}\times\mathbf{A}_k]\ . \tag{1.302}$$

Thus, magnetic field created by the moving particle is perpendicular to the plane determined by the vectors $\mathbf{k}$ *and* $\mathbf{v}$*, while electric field lies in this plane.*

The force acting on the particle is calculated as

$$\begin{aligned}\mathbf{F} &= \int \left(\rho_{\text{ext}}\,\mathbf{E} + \frac{1}{c}\,[\mathbf{j}_{\text{ext}}\times\mathbf{H}]\right)\,dV = Q\,\left(\mathbf{E}(\mathbf{v}t) + \frac{1}{c}\,[\mathbf{v}\times\mathbf{H}(\mathbf{v}t)]\right)\\ &= Q\int\left(\mathbf{E}_k + \frac{1}{c}\,[\mathbf{v}\times\mathbf{H}_\mathbf{k}]\right)\,e^{i\mathbf{k}\cdot\mathbf{v}t}\,\frac{d\mathbf{k}}{(2\pi)^3}\,.\end{aligned} \tag{1.303}$$

Here, the expression

$$f_k = \mathbf{E}_k + \frac{1}{c}\,[\mathbf{k}\times\mathbf{H}_k] = -\frac{4\pi\,i\,Q\,\mathbf{k}\,e^{-i\omega\,t}}{k^2 - \varepsilon(\omega)\,\omega^2/c^2}\,\left[\frac{1}{\varepsilon(\omega)} - \frac{v^2}{c^2}\right]\,. \tag{1.304}$$

Eventually, this yields the expression for the force acting on the particle:

$$\mathbf{F} = -4\pi\,iQ^2\int\frac{\varepsilon^{-1}(\omega) - v^2/c^2}{k^2 - \omega^2\,\varepsilon(\omega)/c^2}\,\mathbf{k}\,\frac{d\mathbf{k}}{(2\pi)^3}\,, \tag{1.305}$$

where $\omega = \mathbf{v}\cdot\mathbf{k}$. To simplify the calculations further, we align z axis along the velocity $\mathbf{v}$ and so $k_z = \omega/v$. We denote $p^2 = k_x^2 + k_y^2$, and $dk_x\,dk_y \to 2\pi\,p\,dp$. The length of wave vector thus reads $k^2 = p^2 + \omega^2/v^2$. The force acting on the particle is rewritten in a scalar form

$$F = -\frac{iQ^2}{\pi} \int_{-\infty}^{\infty} \int_{0}^{q_{max}} \frac{\left[\frac{1}{v^2} - \frac{\varepsilon(\omega)}{c^2}\right] \omega\, p\, dp\, d\omega}{\varepsilon(\omega) \left(p^2 + \omega^2 \left[\frac{1}{v^2} - \frac{\varepsilon(\omega)}{c^2}\right]\right)} \tag{1.306}$$

Generally, there are two physical reasons why the particle slows down. First, the charged particle excites the atoms of the medium, which transit from the ground state to the excited state and possibly become ionized. Therefore, such mechanism of loss is called *ionization losses*. Macroscopically, this mechanism is associated with the imaginary part of the medium permittivity. Quite importantly, this mechanism is active for arbitrary slow particles. Here we skip the detailed discussion of ionization losses and move to the discussion of the second source of losses which is *Cherenkov radiation*.

Note that an alternative way to calculate the radiation from the moving particle is the evaluation of the Poynting vector in the far-field zone, followed by the integration over the surface with infinite radius.

1.17 Cherenkov radiation

The Cherenkov radiation (also known as the Vavilov-Cherenkov radiation) is a type of electromagnetic radiation emitted by the charged particle passing through the medium, provided that the speed of the particle is larger than the phase velocity of light in this medium. There are two important features associated with Cherenkov radiation: (a) it occurs even in the transparent dielectric medium; (b) the intensity of radiation does not depend on the particle mass, which is in contrast with the phenomenon of bremsstrahlung (emission of radiation by the decelerating particle).

Historically, the Cherenkov radiation was discovered in 1934 by the Soviet physicist Pavel Cherenkov supervised by Sergey Vavilov (for that reason, in Russian literature the effect is called the Vavilov-Cherenkov radiation). *Give a remark about S. Vavilov room at Birzhevaya and mention Nikolay Vavilov.* Cherenkov observed weak radiation emitted by the liquids irradiated by gamma-rays. Based on the experimental data, Vavilov made a conclusion that the radiation appears due to the fast electrons released by gamma-rays. In 1937, the Soviet physicists Igor Tamm and Ilya Frank proposed the theoretical interpretation of the effect. Later, in 1958, Cherenkov, Tamm and Frank were awarded a Nobel Prize in Physics for this discovery. *Discuss why this effect is so important in high energy physics.*

Importantly, the Cherenkov radiation is highly directional. For the particle moving with the velocity v, radiation is emitted in the direction that forms the angle θ with the direction of the particle velocity:

$$\cos\theta = \frac{c}{n\,v}\,. \tag{1.307}$$

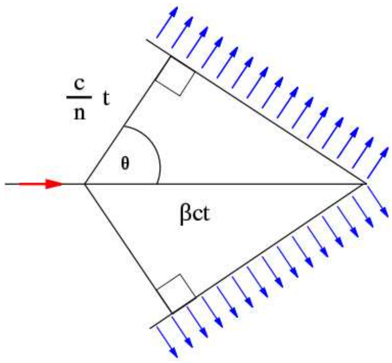

Figure 1.10: Illustration of the emergence of the Cherenkov radiation for the particle moving with the speed v larger than the phase velocity of light c/n in the medium.

Discuss simple explanation of that based on Hyugens-Fresnel principle.

From the solution of the previous paragraph, we find that electromagnetic fields of the particle oscillate with the frequency $\omega = v\,k_x$. On the other hand, any wave propagating in the medium obeys the dispersion equation $\omega\,n/c = k$. Combining these two equations, we immediately obtain the same result as given by Eq. (1.307).

However, by using electrodynamic treatment, we can actually go beyond Eq. (1.307) and calculate the *intensity* of the Cherenkov radiation. Note that the poles of expression Eq. (1.306) correspond to the condition

$$k^2 - \varepsilon(\omega)\,\omega^2/c^2 = 0$$

which describes the dispersion of the modes propagating in the medium. Thus, the contribution from these singularities gives the intensity of Cherenkov radiation.

To evaluate the contribution from the poles, we can use either contour integration technique or the Sokhotski formula which states:

$$\frac{1}{x \pm i\varepsilon} = \mathfrak{P}\,\frac{1}{x} \mp i\pi\delta(x)\,. \tag{1.308}$$

The proof of this identity is based on the fact that

$$\begin{aligned}\int\limits_a^b \frac{f(x)\,dx}{x \pm i\varepsilon} = \int\limits_a^b \frac{x \mp i\varepsilon}{x^2+\varepsilon^2}\,f(x)\,dx = \int\limits_a^b \frac{x^2}{x^2+\varepsilon^2}\,\frac{f(x)}{x}\,dx \mp \\ \mp i\pi \int\limits_a^b \frac{\varepsilon}{\pi\,(x^2+\varepsilon^2)}\,f(x)\,dx\end{aligned} \tag{1.309}$$

The first term here corresponds to the principal value of the integral since the factor $x^2/(x^2+\varepsilon^2)$ excludes the vicinity of $x=0$ and turns to 1 for $x \gg \varepsilon$. The second term yields $\mp i\pi\,f(0)$ because the function $\varepsilon/(\pi\,(x^2+\varepsilon^2))$ acts as a δ-function for sufficiently small ε.

We introduce an auxiliary variable $\xi = p^2 + \omega^2/v^2 - \varepsilon(\omega)\,\omega^2/v^2$. Since at the frequencies $\omega > 0$ ($\omega < 0$) permittivity of the medium has some small but nonzero imaginary part $\varepsilon''(\omega) > 0$ ($\varepsilon(\omega)'' < 0$), this auxiliary variable is written as $\xi - i0$ ($\omega > 0$) and $\xi + i0$ ($\omega < 0$).

$$\begin{aligned} \frac{dF}{d\omega} &= -\frac{iQ^2}{2\pi}\left(\frac{1}{v^2\,\varepsilon(\omega)} - \frac{1}{c^2}\right)\left[\omega \int\limits_{\xi_{min}}^{\xi_{max}} \frac{d\xi}{\xi - i0} + (-\omega)\int\limits_{\xi_{min}}^{\xi_{max}} \frac{d\xi}{\xi + i0}\right] \\ &= Q^2\,\omega\left(\frac{1}{v^2\,\varepsilon(\omega)} - \frac{1}{c^2}\right) = -\frac{Q^2\,\omega}{c^2}\left(1 - \frac{c^2}{n^2\,v^2}\right)\,. \end{aligned} \tag{1.310}$$

So, the closer the velocity of the particle is to the threshold velocity c/n, the smaller is the intensity of Cherenkov radiation. Combining Eqs. (1.307) and (1.310), we can also determine the angular distribution of the radiation.

Ideas for practice: Cherenkov radiation from the moving dipole.

The mechanism of Landau damping is somewhat inverse of the Cherenkov effect. In plasma, the charged particles are affected by the medium collective modes and can not only decelerate, but also accelerate.

Quite interestingly, the radiation from the particle moving with superluminal velocity in vacuum has been calculated by Sommerfeld. However, after the emergence of special relativity, Sommerfeld solution was considered unphysical, and only later a similar solution was found for the case of particles moving in the continuous medium with velocity $v > c/n$.

Semiclassical interpretation of the Cherenkov radiation

We consider the emission of a single photon of the Cherenkov radiation, using the conservation laws:

$$E(\mathbf{p}) = E(\mathbf{p}') + \hbar\,\omega\,, \tag{1.311}$$

$$\mathbf{p} = \mathbf{p}' + \hbar\,\mathbf{k}\,. \tag{1.312}$$

Then

$$\hbar\,\omega = E(\mathbf{p}) - E(\mathbf{p}') = E(\mathbf{p}) - E\left(\mathbf{p} - \hbar\,\mathbf{k}\right) \approx \frac{\partial E}{\partial \mathbf{p}} \cdot \hbar\,\mathbf{k} = \mathbf{v}\cdot\mathbf{k}\,\hbar\,. \tag{1.313}$$

As a consequence, we get the result $\omega = \mathbf{v}\cdot\mathbf{k}$, which we obtained previously from the classical treatment.

1.18 Transition radiation

A related phenomenon of radiation from the charged particle in rectilinear motion is the *transition radiation* which occurs when the particle passes from one medium to another. The theory of the transition radiation was developed by the Soviet physicists Ginzburg and Frank in 1945. Here we discuss the calculation of the transition radiation within the frame of classical electrodynamics, specifically, we aim to calculate spectral and angular distribution of the transition radiation.

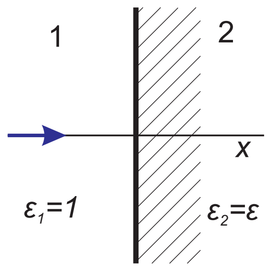

Figure 1.11: Transition radiation from the particle moving from vacuum to the continuous medium with permittivity ε. Geometry of the problem.

Electromagnetic field from the particle

Since the medium is non-homogeneous, we have to calculate the fields produced by the particle once again. We start from the equations

$$\Delta\tilde{\mathbf{A}} - \frac{\hat{\varepsilon}}{c^2}\frac{\partial^2\tilde{\mathbf{A}}}{\partial t^2} = -\frac{4\pi}{c}\,Q\,\mathbf{v}\,\delta(\mathbf{r}-\mathbf{v}t)\,, \tag{1.314}$$

$$\hat{\varepsilon}\left[\Delta\tilde{\phi} - \frac{\hat{\varepsilon}}{c^2}\frac{\partial^2\tilde{\phi}}{\partial t^2}\right] = -4\pi\,Q\,\delta(\mathbf{r}-\mathbf{v}t)\,. \tag{1.315}$$

The solution of these equations is presented by the sum of particular solution of inhomogeneous equations ($\phi^{(e)}$, $\mathbf{A}^{(e)}$) and general solution of homogeneous equations ($\phi^{(r)}$, $\mathbf{A}^{(r)}$). We perform the Fourier transform of the fields as follows:

$$\tilde{\phi} = \int \phi_{\omega\mathbf{k}}(x)\,e^{i\mathbf{p}\cdot\mathbf{r}_\perp - i\omega t}\,\frac{d\omega\,d^2\mathbf{p}}{(2\pi)^3}\,. \tag{1.316}$$

1. Note that we do Fourier transform differently from the analysis in the previous paragraphs. 2. Provide direct and inverse transformation. The Fourier transform of the δ-function reads:

$$\iint \delta(\mathbf{r}-\mathbf{v}t)\,e^{-i\mathbf{p}\cdot\mathbf{r}_\perp + i\omega t}\,d^2\mathbf{r}_\perp\,dt = \iint \delta(x-vt)\,\delta(\mathbf{r}_\perp)\,e^{-i\mathbf{p}\cdot\mathbf{r}_\perp}\,e^{i\omega t}d^2\mathbf{r}_\perp\,dt$$
$$= \frac{1}{v}\int \delta(x-\xi)\,e^{i\omega\,\xi/v}\,d\xi = \frac{1}{v}\,e^{i\omega\,x/v}\,. \tag{1.317}$$

Therefore, the equations for the Fourier-transformed fields read:

$$\frac{d^2 A}{dx^2} - p^2 A + \frac{\varepsilon(\omega)\,\omega^2}{c^2} A = -\frac{4\pi\,\mathbf{v}}{c\,v} Q\, e^{i\omega\, x/v} , \tag{1.318}$$

$$\frac{d^2 \phi}{dx^2} - p^2 \phi + \frac{\varepsilon(\omega)\,\omega^2}{c^2} \phi = -\frac{4\pi\, Q}{\varepsilon(\omega)\, v} e^{i\omega\, x/v} . \tag{1.319}$$

The particular solutions of the inhomogeneous equations read:

$$\phi^{(e)} = \frac{4\pi\, Q}{\varepsilon(\omega)\, v} e^{i\omega\, x/v} \left[p^2 + \frac{\omega^2}{v^2} - \frac{\omega^2}{c^2}\varepsilon(\omega)\right]^{-1} , \tag{1.320}$$

$$\mathbf{A} = \frac{\varepsilon(\omega)\,\mathbf{v}}{c}\phi . \tag{1.321}$$

The electric field is defined as

$$\tilde{\mathbf{E}} = -\frac{1}{c}\frac{\partial \tilde{\mathbf{A}}}{\partial t} - \nabla\tilde{\phi} , \tag{1.322}$$

i.e. the electric field corresponding to the inhomogeneous solution is

$$\mathbf{E}^{(e)} = i\frac{\omega}{c}\mathbf{A}^{(e)} - i\mathbf{p}\,\phi^{(e)} - \frac{\partial\phi^{(e)}}{\partial x}\mathbf{e}_x = i\left[\omega\,\mathbf{v}\left(\frac{\varepsilon(\omega)}{c^2} - \frac{1}{v^2}\right) - \mathbf{p}\right]\phi^{(e)} . \tag{1.323}$$

The solutions of the homogeneous for potentials are simply the plane waves. Accordingly, we assume that $E_x^{(r)} = i\,a\,e^{\pm ik_x\,x}$, where a is some constant, $k_x = \sqrt{\varepsilon(\omega)\,\omega^2/c^2 - p^2}$ is the wave vector along x and $+$ or $-$ sign are chosen for the domains with $x > 0$ and $x < 0$, respectively. This solution of homogeneous equations describes simply the waves reflected from the boundary between the media.

The transverse component of $\mathbf{E}^{(r)}$ is determined from the condition $\operatorname{div}\mathbf{D} = 0$ ($\mathbf{E}^{(e)}$ already satisfies this), i.e. $\varepsilon(\omega)\ (\mathbf{p} \pm k_x\,\mathbf{e}_x)\cdot\mathbf{E} = 0$. This yields the transverse component of the field (parallel to $\mathbf{p}$):

$$E_\perp^{(r)} = \mp\frac{ia}{p} k_x , \tag{1.324}$$

and thus

$$\mathbf{E}^{(r)} = ia\left[\mathbf{e}_x \mp \frac{\mathbf{p}}{p^2} k_x\right] \mathrm{e}^{\pm ik_x\,x} . \tag{1.325}$$

Finally, we get the following expression for the electric field $\mathbf{E} = \mathbf{E}^{(e)} + \mathbf{E}^{(r)}$ in media 1 and 2:

$$\mathbf{E}_{1,2} = i\left[\omega\,\mathbf{v}\left(\frac{\varepsilon_{1,2}}{c^2} - \frac{1}{v^2}\right) - \mathbf{p}\right]\phi_{1,2} + ia_{1,2}\left[\mathbf{e}_x \mp \frac{\mathbf{p}}{p^2} k_x^{(1,2)}\right] e^{\pm ik_x^{(1,2)}\,x} . \tag{1.326}$$

Specifically, if the medium 1 is vacuum, the electric field reads:

$$\mathbf{E}_1 = i\left[\omega\,\mathbf{v}\left(\frac{1}{c^2}-\frac{1}{v^2}\right)-\mathbf{p}\right]\phi_1 + i a_1\left[\mathbf{e}_x + \frac{\mathbf{p}}{p^2}\,k_x\right]e^{-ik_x x}\,. \tag{1.327}$$

Spectral and angular distribution of the transition radiation

The energy emitted by the particle when crossing the boundary of the two media can be evaluated as

$$U = \frac{1}{4\pi}\int dy\,dz\int_{-\infty}^{\infty} dx\,\left(\tilde{E}_1^{(r)}(r,t)\right)^2\,, \tag{1.328}$$

when the charged particle has already penetrated sufficiently far into the medium 2. We also take into account that in the far zone the electric and magnetic fields are equal. Now we substitute the expression for the electric field in terms of its Fourier components

$$U = \frac{1}{4\pi}\int dx\,dy\,dz\,\frac{d\omega\,d\omega'\,d\mathbf{p}\,d\mathbf{p}'}{(2\pi)^6}\,\mathbf{E}_{\omega\mathbf{p}}(x)\cdot\mathbf{E}^*_{\omega'\mathbf{p}'}(x)\,e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}_\perp - i(\omega-\omega')t} = \tag{1.329}$$

$$= \frac{1}{4\pi}\int dx\,\frac{d\omega\,d\omega'\,d\mathbf{p}\,d\mathbf{p}'}{(2\pi)^4}\,\mathbf{E}_{\omega\mathbf{p}}(x)\cdot\mathbf{E}^*_{\omega'\mathbf{p}'}(x)\delta(\mathbf{p}-\mathbf{p}')\,e^{-i\,(\omega-\omega')t} = \tag{1.330}$$

$$= \frac{1}{4\pi}\int dx\,\frac{d\omega\,d\omega'\,d\mathbf{p}}{(2\pi)^4}\,\mathbf{E}_{\omega\mathbf{p}}(x)\cdot\mathbf{E}^*_{\omega'\mathbf{p}}(x)\,e^{-i\,(\omega-\omega')t} = \tag{1.331}$$

$$= \frac{1}{4\pi}\int dx\,\frac{d\omega\,d\omega'\,d\mathbf{p}}{(2\pi)^4}\,|a_1|^2\left[1+\frac{k_x\,k'_x}{p^2}\right]e^{i(k'_x-k_x)x}\,e^{-i\,(\omega-\omega')t} = \tag{1.332}$$

$$= \frac{1}{2}\int\frac{d\omega\,d\omega'\,d\mathbf{p}}{(2\pi)^4}\,|a_1|^2\left[1+\frac{k_x\,k'_x}{p^2}\right]\delta(k'_x-k_x)\,e^{-i\,(\omega-\omega')t}\,. \tag{1.333}$$

Here, $k_x^2 = \omega^2/c^2 - p^2$. Therefore, if $k_x = k'_x$, $1 + k_x^2/p^2 = \omega^2/(c^2\,p^2)$. To evaluate the δ-function, we use the property

$$\delta(f(x)) = \sum_s \frac{\delta(x-x_s)}{|f'(x_s)|} \tag{1.334}$$

which guarantees that

$$\delta(k'_x-k_x) = \delta(\omega'-\omega)\,\frac{c^2\sqrt{\omega^2/c^2-p^2}}{\omega} = c\sqrt{1-\frac{p^2\,c^2}{\omega^2}}\,\delta(\omega'-\omega)\,. \tag{1.335}$$

Thus,

$$U = \frac{1}{2}\int\frac{d\omega\,d\mathbf{p}}{(2\pi)^4}\,|a_1|^2\,\frac{\omega^2}{c\,p^2}\sqrt{1-\frac{p^2\,c^2}{\omega^2}}\,. \tag{1.336}$$

Next, we introduce angle θ that characterizes the direction of emission: $p = \omega/c \sin\theta$ and

$$d^2\mathbf{p} = 2\pi p\, dp = 2\pi \frac{\omega^2}{c^2} \sin\theta \cos\theta\, d\theta = d\Omega \frac{\omega^2}{c^2} \cos\theta\,. \tag{1.337}$$

Then

$$U = \frac{1}{2} \int d\Omega \int_{-\infty}^{\infty} d\omega \frac{\omega^2/c^2 \cos\theta}{(2\pi)^4} |a_1|^2 \frac{c}{\sin^2\theta} \cos\theta = \tag{1.338}$$

$$= \frac{1}{c\,(2\pi)^4} \int d\Omega \int_0^{\infty} d\omega\, \omega^2 |a_1|^2 \,\mathrm{ctg}^2\theta\,. \tag{1.339}$$

Finally, we recast the expression for the radiated energy in the form

$$U = \int d\Omega \int_0^{\infty} d\omega\, \mathfrak{U}(\omega,\theta)\,, \tag{1.340}$$

$$\mathfrak{U}(\omega,\theta) = \frac{\omega^2}{c\,(2\pi)^4} |a_1|^2 \,\mathrm{ctg}^2\theta\,. \tag{1.341}$$

The function $\mathfrak{U}(\omega,\theta)$ characterizes the energy emitted into unit solid angle in the direction specified by θ and in the unit interval of frequencies around the frequency ω, i.e. it gives the spectral and angular distribution of the transition radiation. Here we consider the angles θ from 0 to $\pi/2$ (radiation emitted into the vacuum). Proceeding in a similar way, one can also calculate the radiation emitted into the medium 2, but then one has to evaluate the fields in the medium 2.

Boundary conditions and calculation of the coefficient a_1

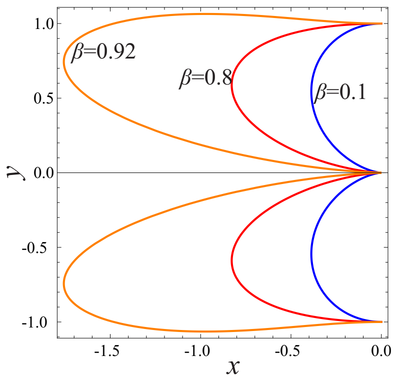

Figure 1.12: Angular dependence of the transition radiation for the particle entering into perfect electric conductor from vacuum.

To obtain the final closed-form solution for the transition radiation, we need to determine the coefficients a_1 and a_2. This can be done by applying the standard boundary conditions: continuity of the tangential components of electric field and continuity of the normal components of the electric displacement. The derivation in the general case appears very cumbersome, and here we do the calculation for the specific case when the medium 1 is vacuum and medium 2 is a perfect electric conductor. The perfect electric conductor is characterized by the vanishing tangential component of electric field. Using Eq. (1.327), we get

$$0 = E_\tau^{\rm tot} = -ip\,\phi_1 + ia_1\,k_x/p\,. \tag{1.342}$$

Thus,

$$a_1 = \frac{p^2\,\phi_1}{k_x} = \frac{4\pi\,Q\,p^2}{v}\left[p^2 + \frac{\omega^2}{v^2} - \frac{\omega^2}{c^2}\right]^{-1}\left[\frac{\omega^2}{c^2} - p^2\right]^{-1/2} = \tag{1.343}$$

$$= \frac{4\pi\,Q\,\beta\,\sin^2\theta}{\omega\,\cos\theta\,\left[1-\beta^2\,\cos^2\theta\right]}\,. \tag{1.344}$$

With this expression for a_1 coefficient, we obtain the spectral and angular distribution of the transition radiation:

$$\boxed{\mathfrak{U}(\omega,\theta) = \frac{Q^2\,\beta^2}{\pi^2\,c}\,\frac{\sin^2\theta}{(1-\beta^2\,\cos^2\,\theta)^2}\,.} \tag{1.345}$$

In the case of the perfect electric conductor, the spectral distribution of the transition radiation is uniform, whereas the angular distribution is illustrated in Fig. 1.12.

CHAPTER 2

Nanophotonics and metamaterials

2.1 Light propagation in planar stratified media: transfer matrix method

In this section, we consider the problem of light propagation in a stratified medium with permittivity which depends on a single Cartesian coordinate, $\varepsilon(x)$. While general treatment of this problem can be found in Ref. [13], we analyze here the most practical case when $\varepsilon(x)$ is a piecewise-constant function, i.e. the medium consists of layers with constant permittivities ε_n. For clarity, we consider the case of isotropic permittivity tensor.

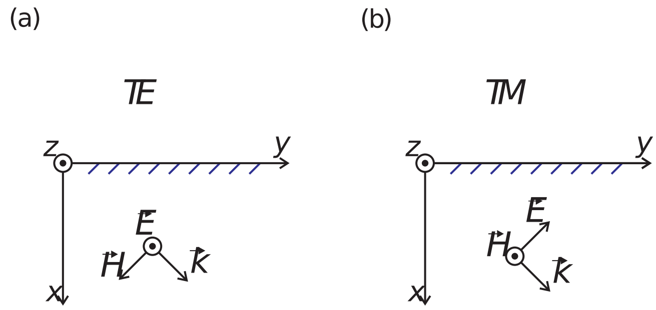

Figure 2.1: Two possible polarizations of the wave propagating in a stratified medium.

Without loss of generality, we assume that the wave vector of the incident wave lies in Oxy plane. Within a single layer, the solutions of Maxwell's equations can be presented as a superposition of plane waves. Boundary conditions fix the values of k_y and $k_z = 0$, and only k_x component of the wave vector varies from one layer to the other. Our goal here is to derive the link between the tangential components of the fields at two interfaces of a given layer with the thickness d. The matrix which relates these two sets of fields is called the *transfer matrix*.

TE-polarized waves

We consider first TE-polarized waves defining the transfer matrix as

$$\begin{pmatrix} E_z(d) \\ H_y(d) \end{pmatrix} = M_{\mathrm{TE}}(d) \begin{pmatrix} E_z(0) \\ H_y(0) \end{pmatrix} \tag{2.1}$$

For TE-polarized plane wave, the link between the tangential components of electric and magnetic fields is given by

$$H_y = -k_x/q\, E_z\ . \tag{2.2}$$

Hence,

$$E_z(0) = E_+ + E_- \,, \tag{2.3}$$

$$H_y(0) = -\frac{k_x}{q}\, E_+ + \frac{k_x}{q}\, E_- \,, \tag{2.4}$$

$$E_z(d) = E_+\, e^{ik_x\, d} + E_-\, e^{-ik_x\, d} \,, \tag{2.5}$$

$$H_y(d) = -\frac{k_x}{q}\, e^{ik_x\, d}\, E_+ + \frac{k_x}{q}\, e^{-ik_x\, d}\, E_- \,. \tag{2.6}$$

Here, $k_x = \sqrt{q^2\,\varepsilon - k_y^2}$ due to the dispersion law of plane waves in a homogeneous medium. Excluding the unknown amplitudes E_+ and E_-, we arrive to the equation Eq. (2.1) with transfer matrix

$$M_{\text{TE}}(d) = \begin{pmatrix} \cos k_x\, d & -\frac{iq}{k_x}\, \sin k_x\, d \\ -\frac{ik_x}{q}\, \sin k_x\, d & \cos k_x\, d \end{pmatrix} \,. \tag{2.7}$$

Note that the determinant of this matrix is equal to 1, while its inverse is obtained by replacing x by $-x$.

The rest of this topic is intended for self-study.

2.2 Image method in electrodynamics

In this section, we analyze the fields produced by the point dipole placed over perfectly conducting plane. The solution of the respective *electrostatic* problem is well-known, however, it is not immediately obvious that the similar approach is applicable for the time-varying fields.

Below, we show that replacing the field produced by the polarized plane by the mirror image of the dipole (Fig. 2.2) we can fulfill the standard PEC boundary conditions which require that $[\mathbf{n} \times \mathbf{E}] = 0$.

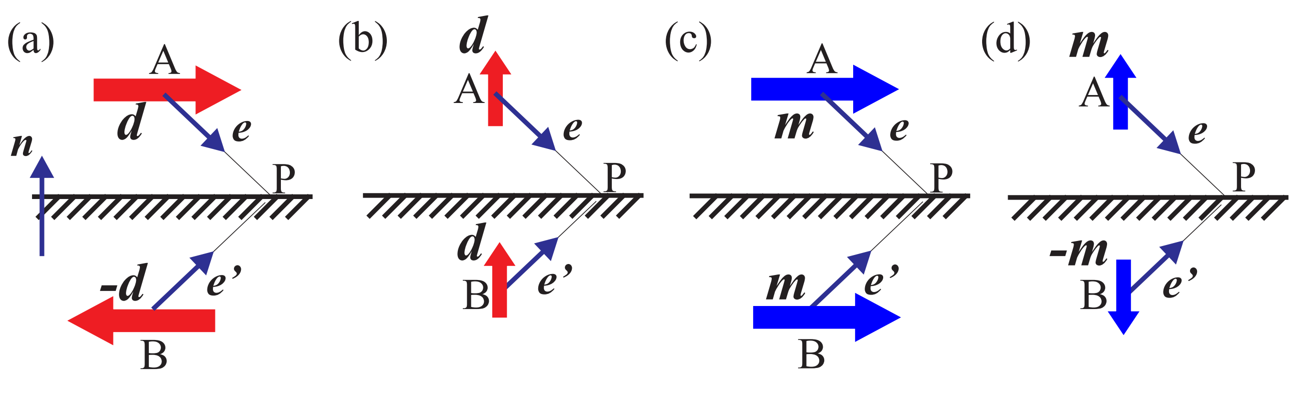

Figure 2.2: Illustration of image method in electrodynamics.

For the derivation below it is important that the dyadic Green's functions can be presented in the following form: $\hat{G}^{ee} = A(r)\,\hat{I} + B(r)\,\mathbf{n}\otimes\mathbf{n}$ and $\hat{G}^{em} = C(r)\,\mathbf{n}^{\times}$, where unit vector $\mathbf{n}$ points towards the observation point.

In geometry Fig. 2.2(a) the electric field at some point P at the surface of conducting plane

$$\begin{aligned}\mathbf{E}(P) &= \hat{G}^{ee}(AP)\,\mathbf{d}_{||} - \hat{G}^{ee}(BP)\,\mathbf{d}_{||} = B(r)\,\left[\mathbf{e}\,(\mathbf{e}\cdot\mathbf{d}_{||}) - \mathbf{e}'\,(\mathbf{e}'\cdot\mathbf{d}_{||})\right]\\ &= B(r)\,(\mathbf{e}\cdot\mathbf{d}_{||})\,(\mathbf{e}-\mathbf{e}')\;.\end{aligned} \tag{2.8}$$

Since $\mathbf{e}-\mathbf{e}'$ is normal to the plane, the field $\mathbf{E}(P)$ is also orthogonal to the plane.

In geometry Fig. 2.2(b) similar calculation yields:

$$\begin{aligned}\mathbf{E}(P) &= \hat{G}^{ee}(AP)\,\mathbf{d}_{\perp} + \hat{G}^{ee}(BP)\,\mathbf{d}_{\perp} = 2A(r)\,\mathbf{d}_{\perp} + B(r)\,[(\mathbf{e}\cdot\mathbf{d}_{\perp})\,\mathbf{e} + (\mathbf{e}'\cdot\mathbf{d}_{\perp})\,\mathbf{e}']\\ &= 2A(r)\,\mathbf{d}_{\perp} + B(r)\,(\mathbf{e}\cdot\mathbf{d}_{\perp})\,(\mathbf{e}-\mathbf{e}')\;.\end{aligned} \tag{2.9}$$

Both of these terms are orthogonal to the plane, which means that the standard boundary conditions are again fulfilled.

Note that the mirror image of magnetic dipole is constructed in a different way as shown in Figs. 2.2(c,d). *Provide a simple explanation for that.* Specifically, for the case shown in Fig. 2.2(c)

$$\mathbf{E}(P) = \hat{G}^{em}(AP)\,\mathbf{m}_{||} + \hat{G}^{em}(BP)\,\mathbf{m}_{||} = C(r)\,(\mathbf{e}+\mathbf{e}')\times\mathbf{m}_{||}\;. \tag{2.10}$$

The latter vector product is parallel to $\mathbf{n}$ and hence the field is normal to the surface.

In turn, in geometry of Fig. 2.2(d) the electric field

$$\mathbf{E}(P) = \hat{G}^{em}(AP)\,\mathbf{m}_{\perp} - \hat{G}^{em}(BP)\,\mathbf{m}_{\perp} = C(r)\,(\mathbf{e}-\mathbf{e}')\times\mathbf{m}_{\perp}\;. \tag{2.11}$$

The latter vector product vanishes since both vectors are normal to the plane.

Thus, the method of images summarized in Fig. 2.2 captures the fields of electric and magnetic dipoles in the general electrodynamic case. *As a follow-up, this approach can be generalized for higher-order multipoles as well.*

2.3 Substrate-induced bianisotropy (practice material)

Useful reading: Ref. [14].

In this paragraph we investigate effective bianisotropic response of particles induced by the presence of substrate. Using Green's functions method, we derive the effective polarizabilities of the particle renormalized due to substrate and analyze in detail the origin of the effective magneto-electric coupling. *Provide an intuitive picture of substrate-induced bianisotropy.*

We consider the particle illuminated by the incident wave with electric and magnetic fields $\mathbf{E}_0$ and $\mathbf{H}_0$. The incident field induces electric $\mathbf{d}$ and magnetic $\mathbf{m}$ dipole moments of the particle. The field radiated by the dipole moments is in turn reflected from the substrate. Hence, the total field acting on the particle

$$\mathbf{E} = \mathbf{E}_0 + \mathbf{E}_{\mathrm{ref}}^{(d)} + \mathbf{E}_{\mathrm{ref}}^{(m)} , \tag{2.12}$$

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_{\mathrm{ref}}^{(d)} + \mathbf{H}_{\mathrm{ref}}^{(m)} , \tag{2.13}$$

where the reflected fields are defined in terms of the dyadic Green's function for the reflected field as follows:

$$\mathbf{E}_{\mathrm{ref}}^{(d)} = \hat{G}_{\mathrm{ref}}^{ee} \, \mathbf{d} \, , \;\; \mathbf{E}_{\mathrm{ref}}^{(m)} = \hat{G}_{\mathrm{ref}}^{em} \, \mathbf{m} \, , \tag{2.14}$$

$$\mathbf{H}_{\mathrm{ref}}^{(d)} = \hat{G}_{\mathrm{ref}}^{me} \, \mathbf{d} \, , \;\; \mathbf{H}_{\mathrm{ref}}^{(m)} = \hat{G}_{\mathrm{ref}}^{mm} \, \mathbf{m} \, . \tag{2.15}$$

The particle responds to the total field as

$$\mathbf{d} = \alpha_0^e \, \mathbf{E} \, , \tag{2.16}$$

$$\mathbf{m} = \alpha_0^m \, \mathbf{H} \, . \tag{2.17}$$

We would like to rearrange Eqs. (2.16)-(2.17) excluding the reflected fields as follows:

$$\mathbf{d} = \hat{\alpha}^{ee} \, \mathbf{E}_0 + \hat{\alpha}^{em} \, \mathbf{H}_0 \, , \tag{2.18}$$

$$\mathbf{m} = \hat{\alpha}^{me} \, \mathbf{E}_0 + \hat{\alpha}^{mm} \, \mathbf{H}_0 \, , \tag{2.19}$$

where $\hat{\alpha}^{ee}$, $\hat{\alpha}^{em}$, $\hat{\alpha}^{me}$ and $\hat{\alpha}^{mm}$ are the *effective* polarizabilities which determine the response of the particle to the incident field and which incorporate the effect of substrate.

To evaluate the effective polarizabilities, we use Eqs. (2.16), (2.17) combining them with Eqs. (2.14), (2.15), which yield the system of equations

$$\left[\hat{I} - \alpha_0^e \, \hat{G}_{\mathrm{ref}}^{ee}\right] \, \mathbf{d} - \alpha_0^e \, \hat{G}_{\mathrm{ref}}^{em} \, \mathbf{m} = \alpha_0^e \, \mathbf{E}_0 \, , \tag{2.20}$$

$$-\alpha_0^m \, \hat{G}_{\mathrm{ref}}^{me} \, \mathbf{d} + \left[\hat{I} - \alpha_0^m \, \hat{G}_{\mathrm{ref}}^{mm}\right] \, \mathbf{m} = \alpha_0^m \, \mathbf{H}_0 \, . \tag{2.21}$$

Solving the system of equations Eqs. (2.20), (2.21) with respect to the unknown $\mathbf{d}$ and $\mathbf{m}$, we extract the effective polarizabilities Eqs. (2.18), (2.19).

Note that the effective polarizabilities can be presented in the form [14]:

$$\hat{\alpha}^{ee} = \hat{N}_e^{-1} \, \alpha_0^e \, , \;\; \hat{\alpha}^{mm} = \hat{N}_m^{-1} \, \alpha_0^m \, , \tag{2.22}$$

$$\hat{\alpha}^{em} = \hat{N}_e^{-1} \, \alpha_0^e \, \hat{G}_{\mathrm{ref}}^{em} \, \left[\hat{I} - \alpha_0^m \, \hat{G}_{\mathrm{ref}}^{mm}\right]^{-1} \, \alpha_0^m \, , \tag{2.23}$$

$$\hat{\alpha}^{me} = \hat{N}_m^{-1} \, \alpha_0^m \, \hat{G}_{\mathrm{ref}}^{me} \, \left[\hat{I} - \alpha_0^e \, \hat{G}_{\mathrm{ref}}^{ee}\right]^{-1} \, \alpha_0^e \, , \tag{2.24}$$

where

$$\hat{N}_e = \hat{I} - \alpha_0^e\,\hat{G}^{ee}_{\text{ref}} - \alpha_0^e\,\hat{G}^{em}_{\text{ref}}\left[\hat{I} - \alpha_0^m\,\hat{G}^{mm}_{\text{ref}}\right]^{-1}\alpha_0^m\,\hat{G}^{me}_{\text{ref}}\,,$$

$$\hat{N}_m = \hat{I} - \alpha_0^m\,\hat{G}^{mm}_{\text{ref}} - \alpha_0^m\,\hat{G}^{me}_{\text{ref}}\left[\hat{I} - \alpha_0^e\,\hat{G}^{ee}_{\text{ref}}\right]^{-1}\alpha_0^e\,\hat{G}^{em}_{\text{ref}}\,.$$

Still, Eqs. (2.20), (2.21) are better suited for calculations than the cumbersome expressions Eqs. (2.22)-(2.24).

As a specific example, we consider a spherical particle placed at distance z_0 over perfectly conducting plane. In such case, effective bianisotropic response can be evaluated analytically, since the dyadic Green's function of the reflected light corresponds just to the image dipole:

$$\hat{G}^{ee}_{\text{ref}} = \begin{pmatrix} -A & 0 & 0 \\ 0 & -A & 0 \\ 0 & 0 & A+B \end{pmatrix}\,,\quad \hat{G}^{mm}_{\text{ref}} = \begin{pmatrix} A & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & -A-B \end{pmatrix}\,, \tag{2.25}$$

$$\hat{G}^{em}_{\text{ref}} = \hat{G}^{me}_{\text{ref}} = \begin{pmatrix} 0 & -C & 0 \\ C & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\,, \tag{2.26}$$

where the scalar coefficients A, B and C are defined as

$$A(r) = \frac{e^{iqr}}{r^3}\left[-1 + iqr + q^2\,r^2\right]\,, \tag{2.27}$$

$$B(r) = \frac{e^{iqr}}{r^3}\left[3 - 3\,iqr - q^2\,r^2\right]\,, \tag{2.28}$$

$$C(r) = \frac{e^{iqr}}{r^3}\left[-iqr - q^2\,r^2\right]\,, \tag{2.29}$$

and the argument of these functions is $r = 2\,z_0$, i.e. the distance between the dipole and its image.

With these expressions for the Green's function of the reflected field, we return to the system Eqs. (2.20), (2.21) and extract the associated effective polarizabilities:

$$\hat{\alpha}^{ee} = \begin{pmatrix} \alpha^{ee}_{||} & 0 & 0 \\ 0 & \alpha^{ee}_{||} & 0 \\ 0 & 0 & \alpha^{ee}_{\perp} \end{pmatrix}\,,\quad \hat{\alpha}^{mm} = \begin{pmatrix} \alpha^{mm}_{||} & 0 & 0 \\ 0 & \alpha^{mm}_{||} & 0 \\ 0 & 0 & \alpha^{mm}_{\perp} \end{pmatrix}\,, \tag{2.30}$$

$$\hat{\alpha}^{em} = \hat{\alpha}^{me} = \begin{pmatrix} 0 & -\alpha^{em}_{yx} & 0 \\ \alpha^{em}_{yx} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\,, \tag{2.31}$$

where

$$\alpha_\perp^{ee} = \frac{\alpha_0^e}{1-\alpha_0^e\,(A+B)}\,,\quad \alpha_\perp^{mm} = \frac{\alpha_0^m}{1+\alpha_0^m\,(A+B)}\,, \tag{2.32}$$

$$\alpha_{||}^{ee} = \alpha_0^e\,\frac{1-\alpha_0^m\,A}{1+(\alpha_0^e-\alpha_0^m)\,A+(C^2-A^2)\,\alpha_0^e\,\alpha_0^m}\,,$$

$$\alpha_{||}^{mm} = \alpha_0^m\,\frac{1+\alpha_0^e\,A}{1+(\alpha_0^e-\alpha_0^m)\,A+(C^2-A^2)\,\alpha_0^e\,\alpha_0^m}\,, \tag{2.33}$$

$$\alpha_{yx}^{em} = \frac{C\,\alpha_0^e\,\alpha_0^m}{1+(\alpha_0^e-\alpha_0^m)\,A+(C^2-A^2)\,\alpha_0^e\,\alpha_0^m}\,. \tag{2.34}$$

Importantly, for the emergence of the nonzero effective bianisotropy the particle should possess overlapping electric and magnetic dipole resonances which ensure sizeable magnitudes of α_0^e and α_0^m. Equation (2.34) shows also that magneto-electric coupling is proportional to the factor $C(2z_0)$, which describes the magnetic field produced by the electric dipole and electric field produced by the magnetic dipole. *In fact, effective bianisotropy arises due to electric field produced by magnetic image-dipole and due to magnetic field produced by electric image-dipole.*

2.4 General expression for the Purcell factor

Useful reading: chap. 10 of the book by Novotny and Hecht [12].

We consider an electric dipole radiating in some arbitrary linear environment. Our goal here is to express the power radiated by the dipole in terms of its dyadic Green's function.

To this end, we make use of the energy conservation law:

$$\begin{aligned} P &= -\int \langle \mathbf{j}\cdot\mathbf{E}\rangle = -\left\langle \dot{\mathbf{d}}\cdot\mathbf{E}\right\rangle = P_0 - \left\langle \dot{\mathbf{d}}\cdot\mathbf{E}_s\right\rangle \\ &= P_0 + \frac{\omega}{2}\,\mathrm{Im}\,(\mathbf{d}^*\cdot\mathbf{E}_s) = P_0 + \frac{\omega}{2}\,\mathrm{Im}\left(d_i^*\,G_{ik}^{(\mathrm{ref})}(0)\,d_k\right)\,, \end{aligned} \tag{2.35}$$

where the full field $\mathbf{E}$ is represented as a sum of vacuum dipole field $\mathbf{E}_0$ and the field scattered by the structure $\mathbf{E}_s$. P_0 is power radiated by the dipole in vacuum. Note that we use the following averaging formula:

$$\langle \dot{a}'(t)\,b'(t)\rangle = -\frac{\omega}{2}\,\mathrm{Im}\,(a^*\,b)\,, \tag{2.36}$$

where a and b are the complex amplitudes of $a'(t)$ and $b'(t)$. Further we note that power radiated by the dipole oscillating with the frequency ω in vacuum is given by

$$P_0 = \frac{\omega^4}{3\,c^3}\,|\mathbf{d}|^2\,. \tag{2.37}$$

Prove Eq. (2.37) by calculating the quantity $P_0 = \omega/2\,(\mathbf{d}^* \cdot \mathbf{E}_0)$. Use the representation of the Green's function

$$\hat{G}_0(r) = A(r,q)\,\hat{I} + B(r,q)\mathbf{n}\otimes\mathbf{n}\,,$$
$$A(r,q) = e^{iqr}/r^3\,\left[-1 + iqr + q^2\,r^2\right]\,,$$
$$B(r,q) = e^{iqr}/r^3\,\left[3 - 3iqr - q^2\,r^2\right]\,.$$

Finally, we obtain the expression for the Purcell factor:

$$\boxed{F = \frac{P}{P_0} = 1 + \frac{3}{2\,q^3}\,\mathrm{Im}\,\left[n_i^*\,G_{ik}^{(\mathrm{ref})}\,n_k\right]\,,} \tag{2.38}$$

where $n_k = d_k/|\mathbf{d}|$. Thus, in order to evaluate the Purcell factor, one only needs the reflected field in the point of dipole location.

2.5 Purcell factor for the dipole above the layered structure

Useful reading: chap. 10 of the textbook by Novotny and Hecht [12].

The idea of this calculation is as follows: we expand the field of the dipole into an infinite series of plane waves. Further we separate the s- and p-polarized plane waves. For each of the polarizations, we calculate the reflection coefficients using Fresnel's formulas. Sum of the reflected plane waves yields the reflected field. Finally, we calculate the Purcell factor using Eq. (2.38).

Expanding dipole field into plane waves

To decompose the field of the dipole into plane waves, we use the so-called Weyl identity:

$$\frac{e^{iqr}}{r} = \frac{i}{2\pi}\iint \frac{\exp\left(ik_x\,x + ik_y\,y + ik_z\,|z|\right)}{k_z}\,dk_x\,dk_y\,, \tag{2.39}$$

where $k_z = \sqrt{q^2 - k_x^2 - k_y^2}$. The sign of the square root is chosen such that $\mathrm{Im}\,k_z > 0$ for $k_{||} > q$ ($k_{||}^2 = k_x^2 + k_y^2$) and $\mathrm{Re}\,k_z > 0$ for $k_{||} < q$.

Next, we use the definition of the dyadic Green's function in vacuum:

$$\begin{aligned}\hat{G}_0(\mathbf{r}) &= \left(\nabla\otimes\nabla + q^2\,\hat{I}\right)\left[\frac{e^{iqr}}{r}\right] = \\ &= \left(\nabla\otimes\nabla + q^2\,\hat{I}\right)\frac{i}{2\pi}\iint\frac{\exp\left(ik_x\,x + ik_y\,y + ik_z|z|\right)}{k_z}\,dk_x\,dk_y \\ &= \frac{i}{2\pi}\iint\frac{q^2\,\hat{I} - \mathbf{k}\otimes\mathbf{k}}{k_z}\,\exp\left(ik_x\,x + ik_y\,y + ik_z\,|z|\right)\,dk_x\,dk_y\,,\end{aligned} \tag{2.40}$$

where $\mathbf{k} = (k_x, k_y, \pm k_z)$ ($\pm$ corresponds to the sign of z). Assuming that the dipole is placed in the point $\mathbf{r}_0 = (0, 0, z_0)$, we obtain the field of the dipole in the form:

$$\mathbf{E}_0(\mathbf{r}-\mathbf{r}_0) = \hat{G}_0(\mathbf{r}-\mathbf{r}_0)\,\mathbf{d} = \frac{i}{2\pi}\iint \hat{M}\,\mathbf{d}\,\exp\left(ik_x\,x + ik_y\,y + ik_z\,|z-z_0|\right)\,, \tag{2.41}$$

where matrix $\hat{M}$ is defined by

$$\hat{M} = \frac{1}{k_z}\left(q^2\,\hat{I} - \mathbf{k}\otimes\mathbf{k}\right) = \frac{1}{k_z}\begin{pmatrix} q^2 - k_x^2 & -k_x\,k_y & \mp k_x\,k_z \\ -k_x\,k_y & q^2 - k_y^2 & \mp k_y\,k_z \\ \mp k_x\,k_z & \mp k_y\,k_z & q^2 - k_z^2 \end{pmatrix}\,. \tag{2.42}$$

The upper (lower) sign is chosen if $z > z_0$ ($z < z_0$). Note that the matrix $\hat{M}$ projects the dipole moment onto the plane orthogonal to $\mathbf{k}$. This means that all the plane waves in expansion Eq. (2.41) are transverse.

Substracting the s- and p-polarized contributions

In our geometry, the plane of incidence is determined by the vectors $\mathbf{k}$ and $\mathbf{e}_z$. The unit vector

$$\tau = [\mathbf{e}_z \times \mathbf{k}]/k_{||} = (-k_y/k_{||}, k_x/k_{||}, 0) \tag{2.43}$$

is orthogonal to the plane of incidence. Thus, in the case of s-polarized wave, the electric field should be directed along τ. Matrix $\hat{M}$ is decomposed as $\hat{M} = \hat{M}^{(s)} + \hat{M}^{(p)}$ with:

$$\hat{M}^{(s)} = \tau\otimes\tau\hat{M} = \frac{q^2}{k_z\,k_{||}^2}\begin{pmatrix} k_y^2 & -k_x\,k_y & 0 \\ -k_x\,k_y & k_x^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}\,, \tag{2.44}$$

$$\hat{M}^{(p)} = \hat{M} - \hat{M}^{(s)} = \frac{1}{k_{||}^2}\begin{pmatrix} k_x^2\,k_z & k_x\,k_y\,k_z & \mp k_x\,k_{||}^2 \\ k_x\,k_y\,k_z & k_y^2\,k_z & \mp k_y\,k_{||}^2 \\ \mp k_x\,k_{||}^2 & \mp k_y\,k_{||}^2 & k_{||}^4/k_z \end{pmatrix}\,. \tag{2.45}$$

Reflection of the s- and p-polarized waves is described by the formulas

$$\tilde{E}_r^{(s)}(\mathbf{k}) = r^{(s)}(k_x, k_y)\,\tilde{E}_{in}^{(s)}(\mathbf{k})\,, \tag{2.46}$$

$$\tilde{E}_r^{(p)}(\mathbf{k}) = r^{(p)}(k_x, k_y)\,\mathrm{diag}\,(-1, -1, 1)\,\tilde{E}_{in}^{(p)}(\mathbf{k})\,, \tag{2.47}$$

where the Fresnel reflection coefficients read:

$$r^{(s)}(k_x, k_y) = \frac{\mu_2\,k_{z1} - \mu_1\,k_{z2}}{\mu_2\,k_{z1} + \mu_1\,k_{z2}}\,, \tag{2.48}$$

$$r^{(p)}(k_x, k_y) = \frac{\varepsilon_2\,k_{z1} - \varepsilon_1\,k_{z2}}{\varepsilon_2\,k_{z1} + \varepsilon_1\,k_{z2}}\,, \tag{2.49}$$

With these expressions, we deduce that

$$\hat{M}^{(s)}_{ref} = \frac{r^{(s)}(\mathbf{k})\, q^2}{k_z\, k_{||}^2} \begin{pmatrix} k_y^2 & -k_x\, k_y & 0 \\ -k_x\, k_y & k_x^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} , \tag{2.50}$$

$$\hat{M}^{(p)} = -\frac{r^{(p)}(\mathbf{k})}{k_{||}^2} \begin{pmatrix} k_x^2\, k_z & k_x\, k_y\, k_z & k_x\, k_{||}^2 \\ k_x\, k_y\, k_z & k_y^2\, k_z & k_y\, k_{||}^2 \\ -k_x\, k_{||}^2 & -k_y\, k_{||}^2 & -k_{||}^4/k_z \end{pmatrix} , \tag{2.51}$$

Here we used the fact that in the point of reflection $0 = z < z_0$. The total reflected field

$$\mathbf{E}_{ref}(\mathbf{r}) = \frac{i}{2\pi} \iint \left[\hat{M}^{(s)}_{ref} + \hat{M}^{(p)}_{ref}\right] \mathbf{d} \exp\left(ik_x\, x + ik_y\, y + ik_z\,(z+z_0)\right)\, dk_x\, dk_y\, . \tag{2.52}$$

Purcell factor calculation

The reflected field acting on the scatterer reads

$$\mathbf{E}_{ref}(\mathbf{r}_0) = \frac{i}{2\pi} \iint \left[\hat{M}^{(s)}_{ref} + \hat{M}^{(p)}_{ref}\right] \mathbf{d}\, e^{2ik_z\, z_0}\, dk_x\, dk_y \tag{2.53}$$

$$= \frac{i}{2\pi} \int_0^\infty \int_0^{2\pi} \left[\hat{M}^{(s)}_{ref} + \hat{M}^{(p)}_{ref}\right] \mathbf{d}\, e^{2ik_z\, z_0}\, k_{||}\, dk_{||}\, d\varphi \tag{2.54}$$

$$= i \int_0^\infty \left[\left\langle \hat{M}^{(s)}_{ref} \right\rangle + \left\langle \hat{M}^{(p)}_{ref} \right\rangle\right] \mathbf{d}\, e^{2ik_z\, z_0}\, k_{||}\, dk_{||}\, . \tag{2.55}$$

Here, φ is the angle between the wave vector and x axis, and $< .. >$ means averaging over the angle. Specifically,

$$\left\langle \hat{M}^{(s)}_{ref} \right\rangle = \frac{r^{(s)}(k_{||})\, q^2}{k_z} \begin{pmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 0 \end{pmatrix} ,$$

$$\left\langle \hat{M}^{(p)}_{ref} \right\rangle = -\frac{r^{(p)}}{k_z} \begin{pmatrix} k_z^2/2 & 0 & 0 \\ 0 & k_z^2/2 & 0 \\ 0 & 0 & -k_{||}^2 \end{pmatrix} \tag{2.56}$$

Thus, the expression for the Purcell factor reads:

$$F = 1 + \frac{3}{2\,q^3\,|\mathbf{d}|^2}\ \mathrm{Im}\ [\mathbf{d}^* \cdot \mathbf{E}_{ref}(\mathbf{r}_0)] =$$
$$= 1 + \frac{3}{2\,q^3\,|\mathbf{d}|^2}\ \mathrm{Im}\left[\int_0^\infty \mathbf{d}^* \left(\left\langle M_{ref}^{(s)}\right\rangle + \left\langle M_{ref}^{(s)}\right\rangle\right)\mathbf{d}\, e^{2ik_z\,z_0}\, k_{||}\, dk_{||}\right]\ . \quad (2.57)$$

Finally, using expressions for $\left\langle M_{ref}^{(s,p)}\right\rangle$ and making the substitutions $s = k_{||}/q$ and $s_z = k_z/q = \sqrt{1-s^2}$, we get:

$$\boxed{\begin{aligned} F = 1 + \frac{3}{4}\frac{|d_x|^2+|d_y|^2}{|\mathbf{d}|^2}\ \mathrm{Re}\int_0^\infty \frac{\left(r^{(s)} - r^{(p)}\,s_z^2\right)\ s}{s_z}\, e^{2iq\,z_0\,s_z}\, ds+ \\ +\frac{3}{2}\frac{|d_z|^2}{|\mathbf{d}|^2}\ \mathrm{Re}\int_0^\infty \frac{r^{(p)}\,s^3}{s_z}\, e^{2iq\,z_0\,s_z}\, ds\ . \end{aligned}} \quad (2.58)$$

2.6 Discrete dipole model and lattice summation techniques

Poisson summation formula

One of the powerful tools in lattice sums evaluation is provided by the Poisson summation formula. It allows one to replace the summation in the real space by the summation in reciprocal space, which in many cases greatly improves the convergence of the series.

We consider a function $\phi(x) = \sum\limits_{n=-\infty}^{\infty} \delta(x - na)$. Since this function is periodic with the period a, it can be expanded in the Fourier series:

$$\phi(x) = \sum_{n=-\infty}^{\infty} \phi_n\, e^{inbx}\ , \quad (2.59)$$

where $b = 2\pi/a$ and the coefficients of the Fourier expansion read

$$\phi_n = \frac{1}{a}\int_{-a/2}^{a/2} \phi(x)\, e^{-inbx}\, dx = \frac{1}{a}\sum_{m=-\infty}^{\infty}\ \int_{-a/2}^{a/2} \delta(x - ma)\, e^{-inbx}\, dx = \frac{1}{a} \quad (2.60)$$

since only one of the δ-functions is nonzero in the interval of integration $[-a/2, a/2]$.

Thus, we obtain an important identity:

$$\phi(x) = \sum_{n=-\infty}^{\infty} \delta(x - na) = \frac{1}{a} \sum_{n=-\infty}^{\infty} e^{inbx} \equiv \frac{1}{a} \sum_{n=-\infty}^{\infty} e^{-inbx}\,, \tag{2.61}$$

where $b = 2\pi/a$.

Next, we consider the sum

$$\sum_{n=-\infty}^{\infty} f(n\,a) = \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \delta(x - na)\, f(x)\, dx = \int_{-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \delta(x - na)\, f(x)\, dx \tag{2.62}$$

$$= \frac{1}{a} \int_{-\infty}^{\infty} \sum_{n=-\infty}^{\infty} e^{-inbx}\, f(x)\, dx = \frac{1}{a} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-inbx}\, f(x)\, dx = \frac{1}{a} \sum_{n=-\infty}^{\infty} \tilde{f}(nb) \tag{2.63}$$

where $b = 2\pi/a$, and the Fourier transform of the function is defined as

$$\tilde{f}(p) \equiv \int_{-\infty}^{\infty} f(x)\, e^{-ipx}\, dx\,. \tag{2.64}$$

Thus, we finally get the *Poisson summation formula*:

$$\sum_{n=-\infty}^{\infty} f(na) = \frac{1}{a} \sum_{n=-\infty}^{\infty} \tilde{f}(nb)\,, \tag{2.65}$$

which converts the sum in the real space into the sum in reciprocal space, provided that the Fourier transform of $f(x)$ is well defined for all $x_n = n\,a$. *Note that the Poisson summation formula can be applied also to the double and triple sums.*

Properties of the Fourier transform

$$\mathfrak{F}_{x\to p}\,[f(x)] \equiv \int_{-\infty}^{\infty} f(x)\, e^{-ipx}\, dx\,, \tag{2.66}$$

$$\mathfrak{F}_{x\to p}\,[f(x+a)] = e^{ipa}\,\mathfrak{F}_{x\to p}\,[f(x)]\;, \tag{2.67}$$

$$\mathfrak{F}_{x\to p}\left[f(x)\, e^{-ikx}\right] = \mathfrak{F}_{x\to (p+k)}\,[f(x)]\;, \tag{2.68}$$

$$\mathfrak{F}_{x\to p}\,[f'(x)] = ip\,\mathfrak{F}_{x\to p}\,[f(x)]\;, \tag{2.69}$$

$$(2.70)$$

$$\mathfrak{F}_{x\to p, y\to s}\left[\frac{e^{iq\sqrt{x^2+y^2+z^2}}}{\sqrt{x^2+y^2+z^2}}\right] = 2\pi\, i\,\frac{e^{i|z|t}}{t}, \quad t=\sqrt{q^2-p^2-s^2},\ \mathrm{Im}\, t>0\,. \tag{2.71}$$

$$\mathfrak{F}_{y\to p}\left[H_0^{(1)}(\varkappa\sqrt{x^2+y^2})\right] = 2\,\frac{e^{itx}}{t}, \quad t=\sqrt{\kappa^2-p^2},\ \mathrm{Im}\, t>0\,. \tag{2.72}$$

Exercise Using the Poisson summation formula, evaluate the sum

$$S=\sum_{n=1}^{\infty}\frac{1}{n^2+a^2}\,,$$

where a is some positive parameter. How many terms are needed in order to evaluate the sum with the precision 10^{-4} with (a) direct summation; (b) summation in reciprocal space?

Answer. The Fourier transform of the function $f(x)=1/(x^2+a^2)$ is equal to $\tilde{f}(p) = \pi\, e^{-|p|a}/a$. Now the series has exponential convergence. $S=\pi\coth(\pi\, a)/(2\, a) - 1/(2\, a^2)$. In the limiting cases, we can derive the sums $\sum\limits_{n=1}^{\infty} 1/n^2=\pi^2/6$ and $\sum\limits_{n=1}^{\infty} 1/n^4=\pi^4/90$.

Dyadic Green's function.

Next, we apply the Poisson summation formula to investigate the fields created by the periodic arrays of scatterers. To write down the field of a single scatterer, we use the *dyadic Green's functions*, which are defined as

$$\mathbf{E}(\mathbf{r}) = \hat{G}^{\mathrm{ee}}(\mathbf{r})\,\mathbf{d} + \hat{G}^{\mathrm{em}}(\mathbf{r})\,\mathbf{m}\,, \tag{2.73}$$

$$\mathbf{H}(\mathbf{r}) = -\hat{G}^{\mathrm{em}}(\mathbf{r})\,\mathbf{d} + \hat{G}^{\mathrm{ee}}(\mathbf{r})\,\mathbf{m}\,, \tag{2.74}$$

where $\mathbf{d}$ and $\mathbf{m}$ are the electric and magnetic dipole moments of the particle located in the coordinate origin, and $\hat{G}^{ee}$ and $\hat{G}^{\mathrm{em}}$ are the tensors defined as follows:

$$\hat{G}^{\mathrm{ee}}(\mathbf{r}) = \left[\nabla\otimes\nabla + q^2\,\hat{I}\right]\left(\frac{e^{iqr}}{r}\right)\,, \tag{2.75}$$

$$\hat{G}^{\mathrm{em}}(\mathbf{r}) = iq\,\nabla^X\left(\frac{e^{iqr}}{r}\right)\,. \tag{2.76}$$

In the framework of Green's functions, in the following we examine the response of two-dimensional periodic array.

Floquet expansion. Grid of electric dipoles.

As an illustration of Poisson summation formula, we consider now the field from the discrete array of scatterers and expand it into the so-called Floquet harmonics. The terms of this Floquet expansion include a propagating wave, possible diffracted waves and a whole set of evanescent waves.

We analyze first the contribution from electric dipole moments of the particles. The particles are located at the sites of rectangular lattice in Oxy plane. We assume the following distribution of the dipole moments:

$$\mathbf{d}_{mn} = \mathbf{d}\, e^{i\mathbf{k}\cdot\mathbf{r}_{mn}}\,, \tag{2.77}$$

where $\mathbf{k}$ is the Bloch wave vector with x and y components. The field from the grid reads:

$$\begin{aligned}
\mathbf{E} &= \sum_{l,n} \hat{G}(\mathbf{r}-\mathbf{r}_{ln})\,\mathbf{d}\, e^{i\mathbf{k}\cdot\mathbf{r}_{ln}} = \sum_{l,n} \hat{G}(\mathbf{r}+\mathbf{r}_{ln})\, e^{-i\mathbf{k}\cdot r_{ln}}\,\mathbf{d}\\
&= \sum_{l,n} \left[\nabla\otimes\nabla + q^2\,\hat{I}\right] \left(\frac{e^{iq|\mathbf{r}+\mathbf{r}_{ln}|}}{|\mathbf{r}+\mathbf{r}_{ln}|}\right) e^{-i\mathbf{k}\cdot\mathbf{r}_{ln}}\,\mathbf{d}\\
&= \frac{1}{a\,b}\sum_{l,n} \mathfrak{F}_{\tilde{x}\to 2\pi\, l/a,\tilde{y}\to 2\pi\, n/b} \left[\left(\nabla\otimes\nabla + q^2\,\hat{I}\right) \left(\frac{e^{iq|\mathbf{r}+\tilde{\mathbf{r}}|}}{|\mathbf{r}+\tilde{\mathbf{r}}|}\right) e^{-i\mathbf{k}\cdot\tilde{\mathbf{r}}}\right]\mathbf{d}\\
&= \frac{1}{a\,b}\sum_{l,n} \mathfrak{F}_{\tilde{x}\to(2\pi\, l/a+k^x),\tilde{y}\to(2\pi\, n/b+k^y)} \left[\left(\nabla\otimes\nabla + q^2\,\hat{I}\right) \left(\frac{e^{iq|\mathbf{r}+\tilde{\mathbf{r}}|}}{|\mathbf{r}+\tilde{\mathbf{r}}|}\right)\right]\mathbf{d}\\
&= \frac{1}{a\,b}\left[\nabla\otimes\nabla + q^2\,\hat{I}\right] \sum_{l,n} \mathfrak{F}_{\tilde{x}\to k_l^x,\tilde{y}\to k_n^y} \left[\frac{e^{iq|\tilde{\mathbf{r}}+z\,\mathbf{e}_z|}}{|\tilde{\mathbf{r}}+z\,\mathbf{e}_z|}\right] e^{ik_l^x\,x+ik_n^y\,y}\,\mathbf{d}
\end{aligned}$$

$$\begin{aligned}
&= \frac{2\pi\, i}{a\,b}\left(\nabla\otimes\nabla + q^2\,\hat{I}\right)\sum_{l,n}\frac{e^{\pm ik_{ln}^z\,z}}{k_{ln}^z}\, e^{ik_l^x\,x+ik_n^y\,y}\,\mathbf{d}\\
&= \frac{2\pi\, i}{a\,b}\sum_{l,n}\left[-\mathbf{k}_{ln}^{(\pm)}\otimes\mathbf{k}_{ln}^{(\pm)} + q^2\right]\frac{e^{i\mathbf{k}_{ln}^{(\pm)}\cdot\mathbf{r}}}{k_{ln}^z}\,\mathbf{d}
\end{aligned} \tag{2.78}$$

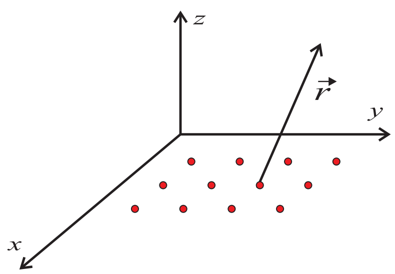

Figure 2.3: Calculation of the fields from the two-dimensional discrete array.

Thus, the electric field from the grid of electric dipoles reads:

$$\mathbf{E} = \frac{2\pi\, i}{a\, b} \sum_{l,n} \left[-\mathbf{k}_{ln}^{(\pm)} \otimes \mathbf{k}_{ln}^{(\pm)} + q^2 \right] \frac{e^{i\mathbf{k}_{ln}^{(\pm)}\cdot\mathbf{r}}}{k_{ln}^z}\, \mathbf{d}\,, \tag{2.79}$$

where $\mathbf{d}$ is the amplitude of the dipole moment of the particles in the grid, a and b are the periods of the grid, $q = \omega/c$, $\mathbf{k}_{ln}^{(\pm)} = (k_l^x, k_n^y, \pm k_{ln}^z)^T$, $k_l^x = k^x + 2\pi\, l/a$, $k_n^y = k^y + 2\pi\, n/b$, $k_{ln}^z = \sqrt{q^2 - (k_l^x)^2 - (k_n^y)^2}$ with the sign of the square root chosen such that $\mathrm{Im}\, k_{ln}^z \geq 0$. In case if k_{ln}^z is purely real, we choose the branch with the positive real part. $\pm$ sign choice in the expression for $k_{ln}^{(\pm)}$ is determined by the choice of the observation point ($z > 0$ or $z < 0$). The summation includes all integer values of indices l and n.

To get some insight on the Floquet expansion, we inspect the Floquet harmonic $l = n = 0$ more closely. We denote $\mathbf{k}_{00}^{(\pm)} = \mathbf{p}^{(\pm)}$:

$$\mathbf{E}_{00} = \frac{2\pi\, i\, q^2}{p_z} \left[1 - \mathbf{p}^{(\pm)} \otimes \mathbf{p}^{(\pm)}/q^2 \right] \mathfrak{P}\, e^{i\mathbf{p}^{(\pm)}\cdot\mathbf{r}}\,, \tag{2.80}$$

where $\mathfrak{P}$ is the average polarization of the metasurface. But this expression actually represents the electric field of the sheet with the continuous polarization distribution. Such an expression can be derived, for example, by matching the plane wave solutions at the boundary of the metasurface or by using the solution of Maxwell's equations via retarded potentials. Operator in the square brackets in Eq. (2.80) simply projects the polarization on the plane orthogonal to the wave vector.

Field from the grid of magnetic dipoles

Quite analogously, we can also compute the electric field radiated by the grid of magnetic dipoles oscillating with the frequency ω, located in Oxy plane, with the amplitude $\mathbf{m}$.

$$\mathbf{E} = \sum_{l,n} \hat{G}^{\mathrm{em}}(\mathbf{r} - \mathbf{r}_{ln})\, \mathbf{m}\, e^{i\mathbf{k}\cdot\mathbf{r}_{ln}} = \sum_{l,n} \hat{G}^{\mathrm{em}}(\mathbf{r} + \mathbf{r}_{ln})\, e^{-i\mathbf{k}\cdot r_{ln}}\, \mathbf{m} \tag{2.81}$$

$$= \sum_{l,n} iq\, \nabla^X \left(\frac{e^{iq|\mathbf{r}+\mathbf{r}_{ln}|}}{|\mathbf{r} + \mathbf{r}_{ln}|} \right) e^{-i\mathbf{k}\cdot\mathbf{r}_{ln}}\, \mathbf{m} \tag{2.82}$$

$$= \frac{iq}{a\, b} \sum_{l,n} \mathfrak{F}_{\tilde{x}\to 2\pi\, l/a, \tilde{y}\to 2\pi\, n/b} \left[\nabla^X \left(\frac{e^{iq|\mathbf{r}+\tilde{\mathbf{r}}|}}{|\mathbf{r} + \tilde{\mathbf{r}}|} \right) e^{-i\mathbf{k}\cdot\tilde{\mathbf{r}}} \right] \mathbf{m} \tag{2.83}$$

$$= \frac{iq}{a\,b}\,\nabla^X \sum_{l,n} \mathfrak{F}_{\tilde{x}\to k_l^x,\tilde{y}\to k_n^y} \left[\frac{e^{iq|\mathbf{r}+\tilde{\mathbf{r}}|}}{|\mathbf{r}+\tilde{\mathbf{r}}|}\right] \mathbf{m} \tag{2.84}$$

$$= \frac{iq}{a\,b}\,\nabla^X \sum_{l,n} e^{i\,k_l^x\,x+i\,k_n^y\,y}\,\mathfrak{F}_{\tilde{x}\to k_l^x,\tilde{y}\to k_n^y} \left[\frac{e^{iq\,|\tilde{\mathbf{r}}+z\,\mathbf{e}_z|}}{|\tilde{\mathbf{r}}+z\,\mathbf{e}_z|}\right] \mathbf{m} \tag{2.85}$$

$$= -\frac{2\pi\,q}{a\,b}\,\nabla^X \sum_{l,n} e^{i\,k_l^x+i\,k_n^y\,y}\,\frac{e^{\pm ik_{ln}^z\,z}}{k_{ln}^z}\,\mathbf{m} \tag{2.86}$$

$$= -\frac{2\pi\,i\,q}{a\,b} \sum_{l,n} \frac{e^{i\mathbf{k}_{ln}^{(\pm)}\cdot\mathbf{r}}}{k_{ln}^z} \left[\mathbf{k}_{ln}^{(\pm)}\times\mathbf{m}\right] . \tag{2.87}$$

Finally, we get the following result for the field from the grid of magnetic dipoles:

$$\mathbf{E} = -\frac{2\pi\,i\,q}{a\,b} \sum_{l,n} \frac{e^{i\mathbf{k}_{ln}^{(\pm)}\cdot\mathbf{r}}}{k_{ln}^z} \left[\mathbf{k}_{ln}^{(\pm)}\times\mathbf{m}\right] . \tag{2.88}$$

If the particles of the array simultaneously have nonzero electric and magnetic moments, the full electric field from the grid reads:

$$\boxed{\mathbf{E}_{\text{tot}} = -\frac{2\pi\,i}{a\,b} \sum_{l,n} \left\{\mathbf{k}_{ln}^{(\pm)}\,\left(\mathbf{k}_{ln}^{(\pm)}\cdot\mathbf{d}\right) - q^2\,\mathbf{d} + q\,\left[\mathbf{k}_{ln}^{(\pm)}\times\mathbf{m}\right]\right\} \frac{e^{i\mathbf{k}_{ln}^{(\pm)}\cdot\mathbf{r}}}{k_{ln}^z}} \tag{2.89}$$

Again, we inspect the Floquet harmonic with the indices $(0,0)$ more closely:

$$\mathbf{E}_{00} = -\frac{2\pi\,i}{p_z\,a\,b} \left\{\mathbf{p}^{(\pm)}\,\left(\mathbf{p}^{(\pm)}\cdot\mathbf{d}\right) - q^2\,\mathbf{d} + q\,\left[\mathbf{p}^{(\pm)}\times\mathbf{m}\right]\right\} e^{i\mathbf{p}^{(\pm)}\cdot\mathbf{r}} . \tag{2.90}$$

From Maxwell's equations (namely, using that $\operatorname{rot}\mathbf{E} = iq\,\mathbf{B}$) we can immediately calculate also the magnetic field of the mode:

$$\mathbf{H}_{00} = -\frac{2\pi\,i}{p_z\,a\,b} \left\{\mathbf{p}^{(\pm)}\,\left(\mathbf{p}^{(\pm)}\cdot\mathbf{m}\right) - q^2\,\mathbf{m} - q\,\left[\mathbf{p}^{(\pm)}\times\mathbf{d}\right]\right\} e^{i\mathbf{p}\cdot\mathbf{r}} . \tag{2.91}$$

Note the dual symmetry of the Eqs. (2.90) and (2.91).

Huygens' metasurface

It turns out that by combining the electric and magnetic responses, one can fully suppress the reflection from the metasurface or, alternatively, suppress the transmission. *Note that the full suppression of transmission is prohibited by the optical theorem, which relates forward scattering with the total scattering cross-section.* The underlying mechanism is the so-called Kerker effect (unidirectional scattering by the single particle with mutually orthogonal electric and magnetic dipole moments).

For simplicity, we assume normal incidence of light at the metasurface. Analyzing Eq. (2.90), we deduce that: (i) if $m_y = -d_x$, the transmitted field is suppressed. *Note that since electric and magnetic polarizability of passive structure both have positive imaginary part, it is impossible to fulfill this condition exactly.* (ii) if $m_y = d_x$, the reflected field is suppressed.

Floquet expansion: grid of wires

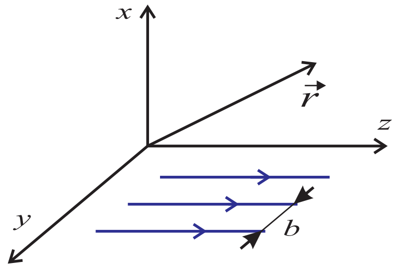

Figure 2.4: To the calculation of the fields from the grid of parallel wires.

Now we consider a somewhat different problem of the field calculation for the grid of parallel wires of negligibly small cross-section. The field of the individual wire with a negligibly small cross-section reads:

$$E_z = -\frac{\pi\,\varkappa^2}{q\,c}\,I_0\,H_0^{(1)}(\varkappa\,\sqrt{x^2+y^2})\,e^{ik^z\,z}\,, \tag{2.92}$$

where $q = \omega/c$, $\varkappa = \sqrt{q^2-(k^z)^2}$ and $H_0^{(1)}(\varkappa\rho)$ is the Hankel function of the first kind. Therefore, the field from the entire grid is represented as

$$E_z = -\frac{\pi\,\varkappa^2}{q\,c}\,I_0\,\sum_{n=-\infty}^{\infty}\,H_0^{(1)}(\varkappa\,\sqrt{x^2+(y-nb)^2})\,e^{ik^z\,z+ik^y\,n\,b}\,, \tag{2.93}$$

where we assume that the amplitudes of the current in the wires of the grid are modulated as $I_n = I_0\,e^{ik^y\,n\,b}$. To evaluate the sum Eq. (2.93), we change the summation index $n \to -n$ and apply again the same procedure based on the Poisson summation formula.

$$E_z = -\frac{\pi\,\varkappa^2}{q\,c}\,I_0\,e^{ik^z\,z}\,\sum_{n=-\infty}^{\infty}\,H_0^{(1)}(\varkappa\,\sqrt{x^2+(y+nb)^2})\,e^{-ik^y\,n\,b} \tag{2.94}$$

$$= -\frac{\pi\,\varkappa^2}{q\,c\,b}\,I_0\,e^{ik^z\,z}\,\sum_{n=-\infty}^{\infty}\,\mathfrak{F}_{y\to 2\pi\,n/b}\left[H_0^{(1)}(\varkappa\sqrt{x^2+(y+nb)^2})\,e^{-ik^y\,n\,b}\right] \tag{2.95}$$

$$= -\frac{\pi\,\varkappa^2}{q\,c\,b}\,I_0\,e^{ik^y y+ik^z z}\sum_{n=-\infty}^{\infty}\mathfrak{F}_{y\to(2\pi\,n/b+k^y)}\left[H_0^{(1)}(\varkappa\sqrt{x^2+n^2\,b^2})\right] \tag{2.96}$$

$$= -\frac{2\pi\,\varkappa^2}{q\,c\,b}\,I_0\,e^{ik^y y+ik^z z}\sum_{n=-\infty}^{\infty}\frac{e^{\pm ik_n^x x}}{k_n^x}\,, \tag{2.97}$$

where the sign choice corresponds to the sign of x coordinate. Thus, we get the result

$$\boxed{E_z = -\frac{2\pi\,\varkappa^2}{q\,c\,b}\,I_0\sum_{n=-\infty}^{\infty}\frac{e^{i\mathbf{k}_n^{(\pm)}\cdot\mathbf{r}}}{k_n^x}\,,} \tag{2.98}$$

where $\mathbf{k}_n^{(\pm)} = (\pm k_n^x, k_n^y, k^z)^T$, $k_n^x = \sqrt{\varkappa^2-(k_n^y)^2} = \sqrt{q^2-(k_n^y)^2-k_z^2}$, $k_n^y = 2\pi\,n/b + k^y$ and the sign of the square root is chosen such that $\mathrm{Im}\,k_n^x > 0$.

Based on Eq. (2.98), we again inspect the zeroth order Floquet harmonics, taking into account that the current amplitude is related to the average polarization of the grid as $I_0 = -i\omega\,\mathfrak{P}\,b$. We also denote $\mathbf{p}^{(\pm)} \equiv k_0^{(\pm)}$. Then

$$E_0^z = \frac{2\pi\,i\,q^2}{p_x}\left(1-\frac{p_z^2}{q^2}\right)e^{i\mathbf{p}^{\pm}\cdot\mathbf{r}}\,. \tag{2.99}$$

Comparing this result with Eq. (2.80), we conclude that the expression for the zeroth Floquet harmonic stays essentially the same, being determined only by the average polarization of the metasurface. The details about the structure of the metasurface are only manifested in higher-order Floquet harmonics, which (in metasurface regime) exponentially decay with the distance.

2.7 Dielectric slab waveguide

Equations for TE and TM modes

In this section, we consider wave propagation in dielectric waveguides characterized by the refractive index exceeding that of the surrounding medium. We analyze the geometry depicted in Fig. 2.5 assuming that $\varepsilon_2 > \varepsilon_3 > \varepsilon_1$.

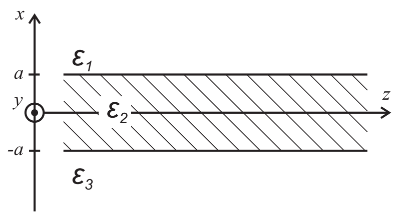

Figure 2.5: A scheme of a planar waveguide. a is half-thickness of the waveguide.

We seek the solution of Maxwell's equations in the form

$\mathbf{E},\mathbf{H}(\mathbf{r},t) \propto \mathbf{E},\mathbf{H}(x)\, e^{ikz-i\omega\, t}$, where k is the propagation constant and $q=\omega/c$ is the normalized frequency. In this geometry, Maxwell's equations

$$\mathrm{rot}\,\mathbf{E} = i\,q\,\mathbf{H}\,, \tag{2.100}$$

$$\mathrm{rot}\,\mathbf{H} = -iq\,\varepsilon(x)\,\mathbf{E}\,. \tag{2.101}$$

split into two sets of independent equations:

$$-ik\,E_y = iq\,H_x\,, \tag{2.102}$$

$$ik\,H_x - \frac{\partial H_z}{\partial x} = -iq\,\varepsilon(x)\,E_y\,, \tag{2.103}$$

$$\frac{\partial E_y}{\partial x} = iq\,H_z\,, \tag{2.104}$$

which correspond to TE waves ($H_y=0$) and

$$ik\,H_y = iq\,\varepsilon(x)\,E_x\,, \tag{2.105}$$

$$ik\,E_x - \frac{\partial E_z}{\partial x} = iq\,H_y\,, \tag{2.106}$$

$$\frac{\partial H_y}{\partial x} = -iq\,\varepsilon(x)\,E_z\,, \tag{2.107}$$

which correspond to TM waves ($E_y=0$).

To summarize, in the case of **TE waves** all fields are expressed through E_y: $H_x = -k\,E_y/q$ and $H_z = -i/q\,dE_y/dx$. In turn, E_y satisfies the equation

$$\frac{d^2\,E_y}{dx^2} + \left(q^2\,\varepsilon(x) - k^2\right)\,E_y = 0\,. \tag{2.108}$$

In the case of **TM waves**, all fields are expressed via H_y: $E_x = k/(q\,\varepsilon(x))\,H_y$ and $E_z = i/(q\,\varepsilon(x))\,dH_y/dx$, whereas H_y satisfies the equation:

$$\frac{d}{dx}\left[\frac{1}{\varepsilon(x)}\,\frac{dH_y}{dx}\right] + \left[q^2 - \frac{k^2}{\varepsilon(x)}\right]\,H_y = 0\,. \tag{2.109}$$

In Eqs. (2.108), (2.109) $\varepsilon(x)$ is a piecewise function: $\varepsilon(x)=\varepsilon_1$ for $x\geq a$, $\varepsilon(x)=\varepsilon_2$ for $-a\leq x\leq a$ and $\varepsilon(x)=\varepsilon_3$ for $x<-a$.

Solution for TE modes

The solution of Eq. (2.108) can be presented in the form

$$E_y = \begin{cases} A\,\cos(u-\varphi)\,e^{-w'(x-a)/a}\,, & x\geq a\,,\\ A\,\cos(u\,x/a-\varphi)\,, & -a\leq x\leq a\,,\\ A\,\cos(u+\varphi)\,e^{w(x+a)/a}\,, & x\geq -a\,,\end{cases} \tag{2.110}$$

with the continuity of E_y at $x = \pm a$ fulfilled automatically. Here,

$$w = a\sqrt{k^2 - q^2\,\varepsilon_3}\,, \;\; w' = a\sqrt{k^2 - q^2\,\varepsilon_1}\,, \;\; u = a\sqrt{q^2\,\varepsilon_2 - k^2}\,. \tag{2.111}$$

Additionally, the continuity of H_z should be ensured: $H_z = -i/q\,dE_y/dx$. This yields the set of two equations:

$$\tan(u + \varphi) = \frac{w}{u}\,, \tag{2.112}$$

$$\tan(u - \varphi) = \frac{w'}{u}\,. \tag{2.113}$$

Excluding φ from this system, we derive:

$$u = \frac{\pi\,m}{2} + \frac{1}{2}\arctan\left(\frac{w}{u}\right) + \frac{1}{2}\arctan\left(\frac{w'}{u}\right)\,, \tag{2.114}$$

where $m = 0, 1, 2, \ldots$ Besides that, Eq. (2.111) imposes a constraint on variables w and u:

$$u^2 + w^2 = v^2 \equiv q^2\,a^2\,(\varepsilon_2 - \varepsilon_3)\,. \tag{2.115}$$

We also introduce a variable γ that characterizes the asymmetry of the cladding:

$$\gamma = \frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_2 - \varepsilon_3} \tag{2.116}$$

and the dimensionless parameter characterizing the dispersion of the waveguide mode:

$$b = \frac{k^2/q^2 - \varepsilon_3}{\varepsilon_2 - \varepsilon_3}\,. \tag{2.117}$$

Note that the borderline between the waveguide modes and the leaky modes is defined by the condition $b = 0$. With these designations, $w = v\sqrt{b}$, $u = v\sqrt{1-b}$, $w' = v\sqrt{b+\gamma}$, while Eq. (2.114) takes the form:

$$v\sqrt{1-b} = \frac{\pi\,m}{2} + \frac{1}{2}\arctan\sqrt{\frac{b}{1-b}} + \frac{1}{2}\arctan\sqrt{\frac{b+\gamma}{1-b}}\,. \tag{2.118}$$

To determine the dispersion of the waveguide mode, one has to solve Eq. (2.118) numerically with respect to the unknown b for the given frequency and given mode order m. The cutoff frequency of the waveguide mode is determined by the condition

$$v_c = \frac{\pi\,m}{2} + \frac{1}{2}\arctan\sqrt{\gamma}\,. \tag{2.119}$$

Solution for TM modes

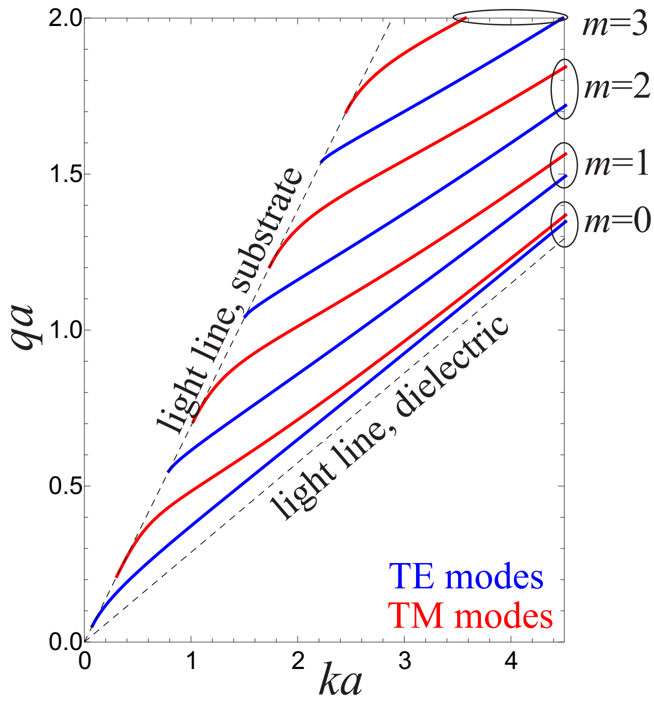

Figure 2.6: Modes in slab waveguide depicted in Fig. 2.5 calculated for $n_1 = 1$, $n_2 = 3.4799$ and $n_3 = 1.4446$, neglecting the frequency dispersion of permittivity.

In a similar manner we present the solutions of Eq. (2.109) in the form

$$H_y = \begin{cases} A\,\cos(u-\varphi)\,e^{-w'(x-a)/a}\,, & x \geq a\,, \\ A\,\cos(ux/a-\varphi)\,, & -a \leq x \leq a\,, \\ A\,\cos(u+\varphi)\,e^{w(x+a)/a}\,, & \end{cases} \tag{2.120}$$

with the same formulas Eq. (2.111) for u, w and w'. Solution (2.120) automatically fulfills the continuity of magnetic field H_y, whereas the continuity of $E_z = i/(q\,\varepsilon(x))\,dH_y/dx$ has to be checked. This yields the set of two equations:

$$\tan(u-\varphi) = \frac{w'\,\varepsilon_2}{u\,\varepsilon_1}\,, \tag{2.121}$$

$$\tan(u+\varphi) = \frac{w\,\varepsilon_2}{u\,\varepsilon_3}\,, \tag{2.122}$$

which can be combined into a single equation for u variable:

$$u = \frac{\pi m}{2} + \frac{1}{2}\,\arctan\left(\frac{\varepsilon_2\,w}{\varepsilon_3\,u}\right) + \frac{1}{2}\,\arctan\left(\frac{\varepsilon_2\,w'}{\varepsilon_1\,u}\right) \tag{2.123}$$

Converting Eq. (2.123) into the dimensionless units, we derive:

$$v\,\sqrt{1-b} = \frac{\pi\,m}{2} + \frac{1}{2}\,\arctan\left(\frac{\varepsilon_2}{\varepsilon_3}\sqrt{\frac{b}{1-b}}\right) + \frac{1}{2}\,\arctan\left(\frac{\varepsilon_2}{\varepsilon_1}\sqrt{\frac{b+\gamma}{1-b}}\right)\,. \tag{2.124}$$

In particular, it is seen that the cutoff frequency for TM modes is a bit different from TE case:

$$v_c = \frac{\pi\, m}{2} + \frac{1}{2}\arctan\left(\frac{\varepsilon_2}{\varepsilon_1}\sqrt{\gamma}\right)\,. \tag{2.125}$$

To illustrate the dispersion of the modes in a slab waveguide, we consider the case when $n_1 = 1$ (air), $n_2 = 3.4799$ (crystalline silicon at 1.5 um) and $n_3 = 1.4446$ (fused silica at 1.5 um). Calculated modes are presented in Fig. 2.6.

To conclude, Eqs. (2.118) and (2.124) are also valid for the case of dispersive media when ε_1, ε_2 and ε_3 depend on frequency. Still, the numerical solution for the mode dispersion can be readily obtained.

2.8 Elements of semiconductor physics. Excitons. Polaritons

Semiconductors. Energy bands. Excitons: Brief overview

The properties of solids are usually described within the so-called single-particle approximation: to calculate the energy bands of a solid, one considers the motion of a single electron in a field created by the lattice of ions and the rest of electrons. For a wide class of problems this description is sufficient.

Within this single-particle scheme, each solid is characterized by the set of energy bands parametrized by the electron wave vector. *Comment on the distinction between semiconductors and dielectrics, 3 eV bandgap.*

However, there is a number of physical phenomena which lies beyond such a simplified treatment of electronic states. An example of this kind is the correlated pair of electron and hole termed *exciton*. The limiting cases of strongly (weakly) bound electron-hole pair are called the Frenkel (the Wannier-Mott) excitons. In experiment, excitons were observed by examining the absorption spectra of Cu_2O and detecting the series of peaks described by the formula $\omega = \omega_0 - R/n^2$ [1952, Gross and Karriev].

The theoretical interpretation of those peaks is based on the assumption of bound electron-hole pairs emergence with the energies given by the formula similar to that of hydrogen atom.

Later, the microscopic theory of excitons was developed, and the impact of excitons on electromagnetic properties of solids was investigated. Specifically, it occurs that exciton resonances in solids give rise to spatial dispersion effects (which we discussed earlier in our course).

In this lecture we will mostly focus on another interesting phenomenon, namely, the hybridization of excitons with light and formation of polaritons.

Exciton-polaritons and their dispersion

We consider light absorption by excitons. In the two-particle scheme, absorption means photon conversion into the exciton. Therefore, momentum and energy conservation require that the absorption process can happen only for the particular energies and momenta when the photon and exciton dispersions cross. At this degeneracy point, even a small coupling between photons and excitons leads to their hybridization in the resulting stationary states. Such mixed states of exciton and photon are called *exciton-polaritons*.

Below, we deduce the dispersion of exciton-polaritons, adopting a simplified model for excitons and describing light-matter interaction semiclassically.

We describe the matter degrees of freedom with the Schrödinger equation

$$i\hbar \frac{\partial \mid \psi \rangle}{\partial t} = \hat{H} \mid \psi \rangle \ , \tag{2.126}$$

where system Hamiltonian is the sum of exciton Hamiltonian and the interaction term describing the coupling of light to excitons:

$$\hat{H} = \left(\varepsilon_{exc} + \frac{\hbar^2 k^2}{2\,M} \right) \hat{c}^\dagger \hat{c} - \left[\hat{\mathbf{d}} \cdot \mathbf{E}^{(+)} e^{-i\omega\, t} + \text{H.c.} \right] . \tag{2.127}$$

Electric field $\mathbf{E}$ introduced here is considered a *classical* one, which is the basis of *semiclassical* description of light-matter interaction. $\mid \psi \rangle$ is the wave function of the system:

$$\mid \psi \rangle = N \mid 0 \rangle + \sum_\alpha C_\alpha \mid exc, \alpha \rangle \ , \tag{2.128}$$

where $\mid 0 \rangle$ describes the ground state of the system (no excitons) and $\mid exc, \alpha \rangle$ is the exciton wave function with the dipole moment of the exciton aligned parallel to x_α axis. We assume that the exciton wave function oscillates with frequency ω so that $i\hbar\, \partial \mid \psi \rangle / \partial t = \hbar\omega \mid \psi \rangle$. With these assumptions, the Schrödinger equation yields:

$$\hbar\, \omega\, C_\alpha = \left(\varepsilon_{exc} + \frac{\hbar^2 k^2}{2M} \right) C_\alpha - d\, E_\alpha^{(+)} \, . \tag{2.129}$$

In the adopted semiclassical framework, we describe electromagnetic degrees of freedom with Maxwell's equations. This yields wave equation

$$\Delta\, \mathbf{E} - \frac{\varepsilon_b}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} = \frac{4\pi}{c^2} \frac{\partial^2 \mathbf{P}}{\partial t^2} \, , \tag{2.130}$$

where ε_b describes the response of the medium without the exciton contribution, whereas P term on the right-hand side describes the medium polarization due to excitons: $P_\alpha = C_\alpha\, d$. Therefore, we get

$$\left(-k^2 + \varepsilon_b\, \omega^2 / c^2 \right) \, E_\alpha^{(+)} = -4\pi\omega^2 / c^2 \, d\, C_\alpha \, . \tag{2.131}$$

Eventually, Eqs. (2.129), (2.131) yield the system of two equations with two unknowns, C_α and $E_\alpha^{(+)}$:

$$\left(\varepsilon_{exc} + \frac{\hbar^2\, k^2}{2\, M} - \hbar\, \omega\right)\, C_\alpha - d\, E_\alpha^{(+)} = 0\,, \tag{2.132}$$

$$4\pi\, \frac{\omega^2}{c^2}\, d\, C_\alpha + \left(\frac{\omega^2}{c^2}\, \varepsilon_b - k^2\right)\, E_\alpha^{(+)} = 0\,, \tag{2.133}$$

which yield the following dispersion law:

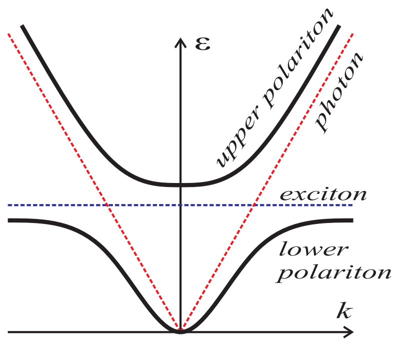

Figure 2.7: Schematic representation of the polariton dispersion.

$$\left(\varepsilon_{exc} + \frac{\hbar^2\, k^2}{2\, M} - \hbar\, \omega\right)\, \left(\frac{\omega^2}{c^2}\, \varepsilon_b - k^2\right) + 4\pi\, \frac{\omega^2}{c^2}\, d^2 = 0\,. \tag{2.134}$$

Note that $\hbar\omega = \varepsilon_{exc} + \hbar\, k^2/(2\, M)$ is the pure exciton dispersion, while $\omega^2/c^2\, \varepsilon_b = k^2$ is the pure photon dispersion. Light-matter coupling proportional to the square of exciton dipole moment gives rise to anticrossing behavior schematically illustrated in Fig. 2.7. Hybridization of the heavy exciton and light photon dispersions gives rise to two polariton states, namely, the lower and upper polariton branches. The states described by these dispersions are the superpositions of a photon and an exciton.

CHAPTER 3

Scattering on spherical and cylindrical particles

In the theory of scattering of electromagnetic waves, there are two important problems that can be solved analytically. They are related to the scattering of waves on a spherical particle and on the infinite cylinder. The solution of these problems provides valuable insights into the properties of Mie-resonant nanoparticles as well as metamaterials and metasurfaces composed of them.

3.1 Scalar spherical harmonics: brief summary

Useful reading: [3] on general derivation of multipole expansion, multipole coefficients and Mie theory. Definition of electric and magnetic dipole moments for current distribution which is not subwavelength can be found in [15] and in the further papers from the same group. Comprehensive textbook on scattering from small particles [16].

Separation of variables in a scalar wave equation

The Helmholtz equation (the wave equation for monochromatic waves):

$$\Delta\psi + k^2\,\psi = 0\,, \quad k = \omega/c\,, \tag{3.1}$$

separation of variables in spherical coordinates:

$$\psi(r,\theta,\varphi) = R(r)\,Y(\theta,\varphi)\,, \tag{3.2}$$

where the Laplacian

$$\Delta = \frac{1}{r}\,\frac{\partial^2}{\partial r^2}\,(r.) + \frac{1}{r^2}\,\Delta_{\theta,\varphi}\,, \tag{3.3}$$

$$\Delta_{\theta,\varphi} = \frac{1}{\sin\theta}\,\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial .}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\,\frac{\partial^2 .}{\partial\varphi^2}\,. \tag{3.4}$$

Hence, we get independent equations for angular and radial parts:

$$\Delta_{\theta,\varphi}\,Y(\theta,\varphi) + l(l+1)\,Y(\theta,\varphi) = 0\,, \quad l = 0,1,2,\ldots \tag{3.5}$$

$$\frac{1}{r}\,\frac{d^2}{dr^2}\,(rR) + \left[k^2 - \frac{l(l+1)}{r^2}\right]\,R = 0\,. \tag{3.6}$$

Radial functions

- Spherical Bessel function

$$j_l(x) = \sqrt{\frac{\pi}{2x}}\, J_{l+1/2}(x) = (-x)^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \left[\frac{\sin x}{x}\right]. \tag{3.7}$$

For $x \to 0$ $j_l(x) \approx x^l/(2l+1)!!$, i.e. it is regular at coordinate origin. For $x \to \infty$ $j_l(x) \approx \sin(x - l\pi/2)/x$, i.e. it shows a decaying and oscillatory behavior at large distances.

- Spherical Neumann function

$$n_l(x) = \sqrt{\frac{\pi}{2x}}\, N_{l+1/2}(x) = -(-x)^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \left[\frac{\cos x}{x}\right]. \tag{3.8}$$

For $x \to 0$ this function is singular $n_l(x) \approx -(2l-1)!!/x^{l+1}$. For $x \to \infty$ this function also has oscillatory decaying behavior $n_l(x) = -\cos(x - l\pi/2)/x$.

- Spherical Hankel functions

$$h_l^{(1,2)}(x) = j_l(x) \pm i n_l(x) = \mp i(-x)^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \left[\frac{e^{\pm ix}}{x}\right]. \tag{3.9}$$

If we use $e^{-i\omega t}$ time convention, $h_l^{(1)}(x)$ describes outgoing spherical waves, while $h_l^{(2)}(x)$ describes incoming waves. For $x \to \infty$ $h_l^{(1,2)}(x) \approx (\mp i)^{l+1}\, e^{\pm ix}/x$.

Recurrent formulas for radial functions:

$$j_l'(x) = j_{l-1}(x) - \frac{l+1}{x}\, j_l(x) = \frac{l j_l(x)}{x} - j_{l+1}(x)\,, \tag{3.10}$$

$$j_{l-1}(x) + j_{l+1}(x) = \frac{2l+1}{x}\, j_l(x)\,. \tag{3.11}$$

Integral representation of Bessel functions:

$$J_n(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ix\sin\varphi + in\varphi}\, d\varphi \tag{3.12}$$

$$e^{-ix\sin\varphi} = \sum_{-\infty}^{\infty} J_n(x)\, e^{-in\varphi}\,. \tag{3.13}$$

Angular part: spherical harmonics

Orthogonality property: $\int Y_{l,m}(\theta,\varphi)\, Y^*_{l',m'}(\theta,\varphi) d\Omega = \delta_{ll'}\, \delta_{mm'}$. Additionally, $Y_{l,-m}(\theta,\varphi) = (-1)^m\, Y^*_{lm}(\theta,\varphi)$.

"Addition theorem" for spherical harmonics:

$$P_l(\cos\gamma) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{lm}(\theta,\varphi)\, Y^*_{lm}(\theta',\varphi') \,, \tag{3.14}$$

where $\cos\gamma = \cos\theta\,\cos\theta' + \sin\theta\,\sin\theta'\,\cos(\varphi-\varphi')$.

Angular momentum operator

Quite a useful technique to deal with spherical harmonics is provided by the angular momentum operator defined as $\hat{L}_k = e_{klm}\hat{x}_l\,\hat{p}_m$, where $\hat{p}_m = -i\partial_m$. In these definitions, Cartesian components are considered.

It is straightforward to verify the following commutation relations:

$$[\hat{x}_j, \hat{p}_k] = i\delta_{jk} \,, \quad \left[\hat{L}_j, \hat{p}_k\right] = ie_{jkm}\,\hat{p}_m \,, \tag{3.15}$$

$$\left[\hat{L}_j, \hat{x}_k\right] = i\,e_{jkl}\,\hat{x}_l \,, \quad \left[\hat{L}_j, \hat{L}_k\right] = ie_{jkm}\,\hat{L}_m \,, \tag{3.16}$$

$$\left[L^2, L_k\right] = 0 \,. \tag{3.17}$$

Note that in spherical coordinates

$$\hat{L}_z = -i\frac{\partial}{\partial\varphi} \,, \tag{3.18}$$

$$\hat{L}_\pm = \hat{L}_x \pm i\,\hat{L}_y = e^{\pm i\varphi}\left(\pm\frac{\partial}{\partial\theta} + i\cot\theta\,\frac{\partial}{\partial\varphi}\right) \,, \tag{3.19}$$

$$\hat{L}^2 = -\Delta_{\theta,\varphi} \,. \tag{3.20}$$

Thus, spherical harmonics $Y_{lm}(\theta,\varphi)$ can be viewed as the system of eigenfunctions of two Hermitian operators $\hat{L}_z$ and $\hat{L}^2$, which is widely used in quantum mechanics:

$$\hat{L}^2\,Y_{lm} = l(l+1)\,Y_{lm} \,, \tag{3.21}$$

$$\hat{L}_z\,Y_{lm} = m\,Y_{lm} \,. \tag{3.22}$$

Additionally, it can be checked that $\left[\hat{L}_z, \hat{L}_\pm\right] = \pm\hat{L}_\pm$. Using this commutation relation in combination with Eqs. (3.21) and (3.22), we extract the following relations for scalar spherical harmonics:

$$\hat{L}_+\,Y_{lm} = \sqrt{(l-m)(l+m+1)}\,Y_{l,m+1} \,, \tag{3.23}$$

$$\hat{L}_-\,Y_{lm} = \sqrt{(l-m+1)(l+m)}\,Y_{l,m-1} \,. \tag{3.24}$$

Using Eqs. (3.23), (3.24) and definition of these operators in spherical coordinates, calculate all spherical harmonics with $l=1$. Use the fact that $Y_{lm}(\theta,\varphi) \propto e^{im\varphi}$.

3.2 Vector spherical harmonics. Multipole expansion

Our goal now is to construct the vector solutions of the Helmholtz equation, since electromagnetic field is a vector one. We assume that $\psi(\mathbf{r})$ is a solution of the scalar Helmholtz equation:

$$\Delta\psi + k^2\,\psi = 0\,, \tag{3.25}$$

where $k = \omega/c$. First, we show that $\mathbf{M} = \mathrm{rot}\,(\psi\,\mathbf{r})$ is a solution of the vector Helmholtz equation. We use two vector identities:

$$\mathrm{rot}(\mathbf{a}\cdot\mathbf{b}) = \mathbf{a}\;\mathrm{div}\,\mathbf{b} - \mathbf{b}\;\mathrm{div}\,\mathbf{a} + (\mathbf{b}\nabla)\mathbf{a} - (\mathbf{a}\nabla)\mathbf{b}\,, \tag{3.26}$$

$$\nabla(\mathbf{a}\cdot\mathbf{b}) = \mathbf{a}\times\mathrm{rot}\,\mathbf{b} + \mathbf{b}\times\mathrm{rot}\,\mathbf{a} + (\mathbf{a}\nabla)\mathbf{b} + (\mathbf{b}\nabla)\mathbf{a}\,. \tag{3.27}$$

$$\begin{aligned}\Delta\mathbf{M} + k^2\,\mathbf{M} &= \nabla(\mathrm{div}\,\mathbf{M}) - \mathrm{rot}\,\mathrm{rot}\,\mathbf{M} + k^2\,\mathbf{M} = \mathrm{rot}\,\big[-\mathrm{rot}\,\mathrm{rot}(\psi\mathbf{r}) + k^2\,\psi\,\mathbf{r}\big] = \\ &= \mathrm{rot}\,\big[-\nabla\psi + \mathbf{r}\Delta\psi - \nabla(\mathbf{r}\cdot\nabla\psi) + k^2\,\psi\,\mathbf{r}\big] = \mathrm{rot}\,\big[\mathbf{r}\,(\Delta\psi + k^2\,\psi)\big] = 0\,.\end{aligned} \tag{3.28}$$

Thus, $\mathbf{M}$ is a vector solution of the Helmholtz equation.

Similarly, we can construct two other vector solutions of Helmholtz equation: $\mathbf{N} = \mathrm{rot}\,\mathbf{M}$ and $\mathbf{P} = \nabla\psi$ with $\mathrm{rot}\,\mathbf{N} = \mathrm{rot}\,\mathrm{rot}\,\mathbf{M} = \nabla(\mathrm{div}\,\mathbf{M}) - \Delta\mathbf{M} = k^2\,\mathbf{M}$.

In turn, any solution of scalar Helmholtz equation can be represented as a series:

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_{lm}\,\psi_{lm}(\mathbf{r}) \tag{3.29}$$

with some constant coefficients f_{lm}. Analogously, vector solutions can be presented in the form

$$\mathbf{A} = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left[a_{lm}\,\mathbf{M}_{lm} + b_{lm}\,\mathbf{N}_{lm} + c_{lm}\,\mathbf{P}_{lm}\right]\,, \tag{3.30}$$

where we assume the Lorenz gauge $\mathrm{div}\,\mathbf{A} + \frac{1}{c}\frac{\partial\varphi}{\partial t} = 0$. Hence, the scalar potential can be written as

$$\varphi = -\frac{i}{k}\,\mathrm{div}\,\mathbf{A} = -\frac{i}{k}\sum_{l,m} c_{lm}\;\mathrm{div}\,\mathbf{P}_{lm} = -\frac{i}{k}\sum_{l,m} c_{lm}\,\Delta\psi_{lm} = ik\sum_{l,m} c_{lm}\,\psi_{lm}\,. \tag{3.31}$$

Therefore, the expressions for the electric and magnetic fields take the form:

$$\mathbf{B} = \mathrm{rot}\,\mathbf{A} = \sum_{l,m} \left[a_{lm}\ \mathrm{rot}\,\mathbf{M}_{lm} + b_{lm}\ \mathrm{rot}\,\mathbf{N}_{lm} + c_{lm}\ \mathrm{rot}\,\mathbf{P}_{lm}\right] =$$

$$= \sum_{l,m} \left[a_{lm}\,\mathbf{N}_{lm} + k^2\, b_{lm}\,\mathbf{M}_{lm}\right]\ , \tag{3.32}$$

$$\mathbf{E} = -\nabla\varphi - \frac{1}{c}\frac{\partial\mathbf{A}}{\partial t} = -ik\sum_{l,m} c_{lm}\,\mathbf{P}_{lm} + ik\sum_{l,m}\left[a_{lm}\,\mathbf{M}_{lm} + b_{lm}\,\mathbf{N}_{lm} + c_{lm}\,\mathbf{P}_{lm}\right] =$$

$$= ik\sum_{l,m}\left[a_{lm}\,\mathbf{M}_{lm} + b_{lm}\,\mathbf{N}_{lm}\right]\ . \tag{3.33}$$

Thus, only vector harmonics $\mathbf{M}_{lm}$ and $\mathbf{N}_{lm}$ are included in the expressions for the fields. The terms with $\mathbf{P}_{lm}$ are omitted out. Next, we examine the angular dependence of vector spherical harmonics:

$$\mathbf{M} = \mathrm{rot}\,(\psi\,\mathbf{r}) = -\mathbf{r}\times\nabla\psi = -i\hat{\mathbf{L}}\psi = -if(r)\,\hat{\mathbf{L}}\,Y(\theta,\varphi). \tag{3.34}$$

Hence, angular dependence of $\mathbf{M}$ harmonics is given by $\hat{\mathbf{L}}\,Y(\theta,\varphi)$, while $\mathbf{M}$ harmonics themselves do not contain the radial component of the field.

After making the normalization of $\hat{\mathbf{L}}\,Y$, using the Cartesian components of $\hat{\mathbf{L}}$ operator and Eqs. (3.23), (3.24), we get the following normalized vector spherical harmonics:

$$\mathbf{X}_{lm} = \frac{1}{\sqrt{l\,(l+1)}}\,\hat{\mathbf{L}}\,Y_{lm}(\theta,\varphi)\ , \tag{3.35}$$

where $\hat{\mathbf{L}} = (\frac{\hat{L}_+ + \hat{L}_-}{2}, \frac{\hat{L}_+ - \hat{L}_-}{2i}, \hat{L}_z)$, and which satisfy the condition

$$\int \mathbf{X}_{lm}(\theta,\varphi)\cdot\mathbf{X}^*_{l'm'}(\theta,\varphi)\,d\Omega = \delta_{ll'}\,\delta_{mm'}\ . \tag{3.36}$$

Note that the spherically symmetric solutions of Maxwell's equations described by $\mathbf{X}_{00}$ exist only in the static case. Thus, $\mathbf{M}_{lm} = f_l(kr)\,\mathbf{X}_{lm}$, $\mathbf{N}_{lm} = \mathrm{rot}\,[f_l(kr)\,\mathbf{X}_{lm}]$. Redefining the coefficients $a_{lm} = i\,a_M(l,m)/k$ and $b_{lm} = a_E(l,m)/k^2$, we arrive at the following multipole expansion:

$$\mathbf{E} = \sum_{l=1}^{\infty}\sum_{m=-l}^{l}\left[\frac{i}{k}\,a_E(l,m)\ \mathrm{rot}\,[f_l(kr)\,\mathbf{X}_{lm}] - a_M(l,m)\,g_l(kr)\,\mathbf{X}_{lm}\right]\ , \tag{3.37}$$

$$\mathbf{B} = \sum_{l=1}^{\infty}\sum_{m=-l}^{l}\left[a_E(l,m)\,f_l(kr)\,\mathbf{X}_{lm} + \frac{i}{k}\,a_M(l,m)\ \mathrm{rot}\,[g_l(kr)\,\mathbf{X}_{lm}]\right]\ . \tag{3.38}$$

Here, functions $f_l(kr)$ and $g_l(kr)$ are spherical Bessel/Neumann/Hankel functions and their combinations, which are the radial solutions of scalar Helmholtz equation.

$a_E(l,m)$ and $a_M(l,m)$ are known as multipole coefficients for electric and magnetic multipoles. "Electric" multipoles correspond to $B_r = 0$, "magnetic" multipoles – $E_r = 0$.

The form of the multipole expansion, Eqs. (3.37)-(3.38), reflects the dual symmetry of electrodynamics in vacuum.

$$\nabla = \mathbf{n}\,\frac{\partial}{\partial r} + \frac{1}{r}\,\nabla_{\theta,\varphi}\,, \tag{3.39}$$

$$\mathbf{X} = \frac{\hat{\mathbf{L}}Y}{\sqrt{l(l+1)}} = -i\,\frac{\mathbf{n}\times\nabla_{\theta,\varphi}Y}{\sqrt{l(l+1)}}\,, \tag{3.40}$$

$$\mathbf{Z} = \mathbf{n}\times\mathbf{X} = \frac{i\nabla_{\theta,\varphi}Y}{\sqrt{l(l+1)}}\,. \tag{3.41}$$

Clearly, $\mathbf{Z}_{lm}$ harmonics are also normalized to unity as $\int \mathbf{Z}_{lm}\cdot\mathbf{Z}^*_{l'm'}\,d\Omega = \delta_{ll'}\,\delta_{mm'}$. Finally, we note useful auxiliary expression:

$$i\,\mathrm{rot}\,\hat{\mathbf{L}} = \mathbf{r}\,\Delta - \nabla\left(1 + r\,\frac{\partial.}{\partial r}\right)\,. \tag{3.42}$$

With this, we can compute $\mathrm{rot}\,[f(kr)\,\mathbf{X}]$.

$$\begin{aligned}
\mathrm{rot}\,[f(kr)\,\mathbf{X}] &= \nabla(f(kr))\times\mathbf{X} + f(kr)\,\mathrm{rot}\,\mathbf{X} = \\
&= \frac{d}{dr}\,f(kr)\;[\mathbf{n}\times\mathbf{X}] + \frac{f(kr)}{\sqrt{l(l+1)}}\,\mathrm{rot}\,\hat{\mathbf{L}}Y = \\
&= \frac{df(kr)}{r}\,\mathbf{Z} + \frac{f(kr)}{\sqrt{l(l+1)}}\;(-i\mathbf{r}\Delta\,Y + i\nabla Y) = \\
&= \frac{df(kr)}{dr}\,\mathbf{Z} + \frac{f(kr)}{r\sqrt{l(l+1)}}\,(-i\mathbf{n}\Delta_{\theta,\varphi}Y + i\nabla_{\theta,\varphi}Y)\,.
\end{aligned}$$

Eventually,

$$\mathrm{rot}\,[f(kr)\,\mathbf{X}] = \frac{1}{r}\,\frac{d}{dr}\;[r\,f(kr)]\;\mathbf{Z} + i\sqrt{l(l+1)}\,\frac{f(kr)}{r}\,\mathbf{n}\,Y\,. \tag{3.43}$$

Example: finding the eigenmodes of a spherical cavity

To give a simple application of multipole expansion, we find the eigenmodes of a spherical cavity with perfectly conducting walls. In this case $f_l(kr)$ and $g_l(kr)$ correspond to the spherical Bessel function $j_l(kr)$, which is the only radial function regular in the coordinate origin. The boundary condition at the cavity wall reads: $\mathbf{n}\times\mathbf{E} = 0$.

Hence, for "electric" (or TM-like) modes we get:

$$\frac{d}{dr}\left[r j_l(kr)\right]\Bigg|_{r=a} = 0\,. \tag{3.44}$$

For "magnetic" (or TE-like) modes we get:

$$j_l(kr) = 0\,. \tag{3.45}$$

Hence, the eigenmodes are parametrized by the two indices: multipolar index l of the mode and number n of solution: $\omega_l^{(n)}$. Note that the modes are degenerate in m (since the sphere is rotationally-invariant) and the index l runs from 1 to infinity.

Below, we provide the values of dimensionless parameter $x = q\,a$ for the lowest eigenmodes. For TE-type modes: $x_1^{(1)} = 4.4934$, $x_2^{(1)} = 5.7635$, $x_3^{(1)} = 6.9879$, $x_1^{(2)} = 7.7253$,... For TM-type modes: $x_1^{(1)} = 2.7437$, $x_2^{(1)} = 3.8702$, $x_3^{(1)} = 4.9734$, $x_4^{(1)} = 6.0620$, $x_1^{(2)} = 6.1168$ ...

The lowest frequency TM eigenmode ($l = 1$, $n = 1$) has $\lambda_{11}^{\mathrm{TM}} = 2.29\,a$. The lowest frequency TE mode has $\lambda_{11}^{\mathrm{TE}} = 1.40\,a$.

Multipole expansion in a homogeneous medium

Let's assume now that we want to make a multipole expansion in some homogeneous medium with ε and μ. Our goal is to find out how Eqs. (3.37), (3.38) should be modified.

Maxwell's equations for monochromatic field in an isotropic homogeneous medium have the form:

$$\nabla \times \mathbf{E} = iq\,\mu\,\mathbf{H}\,, \tag{3.46}$$
$$\nabla \times \mathbf{H} = -iq\,\varepsilon\,\mathbf{E}\,, \tag{3.47}$$

where $q = \omega/c$. We do the transformation $\mathbf{E} = \mathbf{E}'/\sqrt{\varepsilon}$, $\mathbf{H} = \mathbf{H}'/\sqrt{\mu}$, $\mathbf{r} = \mathbf{r}'/\sqrt{\varepsilon\,\mu}$. Accordingly, nabla operator is transformed as $\nabla = \nabla'\sqrt{\varepsilon\,\mu}$. Note that this transformation changes the distances but does not change the angles between radius-vectors. Furthermore, the transformed fields satisfy Maxwell's equations in the vacuum:

$$\nabla' \times \mathbf{E}' = iq\,\mathbf{H}'\,, \tag{3.48}$$
$$\nabla' \times \mathbf{H}' = -iq\,\mathbf{E}'\,. \tag{3.49}$$

Hence, the transformed fields can be written as follows:

$$\mathbf{E}' = \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \left[\frac{i}{q}\, a_E(l,m)\, \nabla' \times [f_l(qr')\, \mathbf{X}_{lm}] - a_M(l,m)\, g_l(qr')\, \mathbf{X}_{lm} \right] , \tag{3.50}$$

$$\mathbf{H}' = \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \left[a_E(l,m)\, f_l(qr')\, \mathbf{X}_{lm} + \frac{i}{q}\, a_M(l,m)\, \nabla' \times [g_l(qr')\, \mathbf{X}_{lm}] \right] , \tag{3.51}$$

where the radial part is transformed, whereas the angular part stays the same. We denote $k = q\sqrt{\varepsilon\,\mu}$ and get

$$\mathbf{E} = \frac{1}{\sqrt{\varepsilon}} \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \left[\frac{i}{k}\, a_E(l,m)\, \nabla \times [f_l(kr)\, \mathbf{X}_{lm}] - a_M(l,m)\, g_l(kr)\, \mathbf{X}_{lm} \right] , \tag{3.52}$$

$$\mathbf{H} = \frac{1}{\sqrt{\mu}} \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \left[a_E(l,m)\, f_l(kr)\, \mathbf{X}_{lm} + \frac{i}{k}\, a_M(l,m)\, \nabla \times [g_l(kr)\, \mathbf{X}_{lm}] \right] , \tag{3.53}$$

3.3 Fields of multipoles. Link between multipole coefficients and multipole moments

Near fields of multipoles

Employing the general multipole expansion Eq. (3.37), we now evaluate the fields in the near zone of the source, i.e. for $qr \ll 1$. We choose $f_l(qr) = g_l(qr) = h_l^{(1)}(qr)$ for a finite distribution of charges, replacing the latter function by the leading term $-i\,(2l-1)!!/(qr)^{l+1}$. For simplicity, we consider only the electric multipoles.

$$\begin{aligned} \mathbf{E} &= \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \frac{i}{q}\, a_E(l,m)\ \mathrm{rot}\left[h_l^{(1)}(qr)\, \mathbf{X}_{lm} \right] \\ &= \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \frac{a_E(l,m)}{q^{l+2}}\, \frac{(2l-1)!!}{\sqrt{l(l+1)}}\ \mathrm{rot}\ \hat{\mathbf{L}} \frac{Y_{lm}}{r^{l+1}} \,. \end{aligned} \tag{3.54}$$

Next we use the identity $\mathrm{rot}\ \hat{\mathbf{L}} = -i\mathbf{r}\,\Delta + i\,\nabla\, \left(1 + r\,\frac{\partial.}{\partial r}\right)$. $\Delta(Y_{lm}/r^{l+1}) = 0$, since this function is one of the solutions of the scalar Laplace equation. Finally, we get:

$$\mathbf{E} = -\nabla \left\{ \sum_{l,m} i\, a_E(l,m) \sqrt{\frac{l}{l+1}}\, \frac{(2l-1)!!}{q^{l+2}}\, \frac{Y_{lm}(\theta,\varphi)}{r^{l+1}} \right\} , \tag{3.55}$$

so that the expression in the brackets yields the scalar potential of electrostatic field. On the other hand, the scalar potential of electrostatic field can be written in the form [see e.g. LL II]:

$$\varphi = \frac{\mathbf{d}\cdot\mathbf{n}}{r^2} + \frac{Q_{ij}\,n_i\,n_j}{2\,r^3} + \dots\,, \tag{3.56}$$

where $\mathbf{d}$ is the dipole moment, Q_{ij} is the tensor of quadrupole moment, etc.. Comparing Eqs. (3.55) and (3.56), we immediately find out that

$$\frac{i}{\sqrt{2}\,q^3}\sum_{m=-1}^{1} a_E(1,m)\,Y_{1m} = \mathbf{d}\cdot\mathbf{n}\,, \tag{3.57}$$

$$\frac{i\,\sqrt{6}}{q^4}\sum_{m=-2}^{2} a_E(2,m)\,Y_{2m} = \frac{1}{2}\,Q_{ij}\,n_i\,n_j\,. \tag{3.58}$$

A similar identification holds for the magnetic multipole moments:

$$\frac{i}{\sqrt{2}\,q^3}\sum_{m=-1}^{1} a_M(1,m)\,Y_{1m} = \mathbf{m}\cdot\mathbf{n}\,, \tag{3.59}$$

$$\frac{i\,\sqrt{6}}{q^4}\sum_{m=-2}^{2} a_M(2,m)\,Y_{2m} = \frac{1}{2}\,Q^{\mathrm{M}}_{ij}\,n_i\,n_j\,. \tag{3.60}$$

To establish Eqs. (3.57)-(3.60), we used the well-known definitions of multipole moments in the static case. Now, turning our attention to the dynamic case, we *define* multipole moments via multipole coefficients as specified by Eqs. (3.57) and (3.58).

Using an explicit expression for the first scalar spherical harmonics:

$$Y_{11} = -\sqrt{3/(8\pi)}\,\sin\theta\,e^{i\varphi}\,, \tag{3.61}$$

$$Y_{10} = \sqrt{3/(4\pi)}\,\cos\theta\,, \tag{3.62}$$

$$Y_{1,-1} = \sqrt{3/(8\pi)}\,\sin\theta\,e^{-i\varphi}\,, \tag{3.63}$$

and taking the expression for the unit vector $\mathbf{n} = (\sin\theta\,\cos\varphi, \sin\theta\,\sin\varphi, \cos\theta)$, we can now deduce the explicit expressions for the multipole coefficients $a_E(1,m)$ and $a_M(1,m)$ in terms of dipole moments:

$$\begin{aligned} a_E(1,1) = iq^3\,\sqrt{4\pi/3}\,(d_x - i\,d_y)\,,\ \ a_E(1,0) &= -iq^3\,\sqrt{8\pi/3}\,d_z\,,\\ a_E(1,-1) &= -iq^3\,\sqrt{4\pi/3}\,(d_x + i\,d_y)\,, \end{aligned} \tag{3.64}$$

and the similar relations hold for $a_M(1,m)$ and the components of magnetic dipole moment. This said, $a_E(1,0)$ is related to the radiation of z-oriented electric dipole, whereas $a_E(1,\pm 1)$ describe the radiation from the dipole rotating in the plane Oxy clockwise $[a_E(1,-1)]$ or counter-clockwise $[a_E(1,1)]$.

Expressions for the fields of oscillating electric and magnetic dipoles

Having the definitions of multipole moments, we are ready now to compute the fields produced by the oscillating electric and magnetic dipoles. Specifically, we focus on electric field from magnetic dipole.

$$
\begin{aligned}
\mathbf{E} &= -\sum_{m=-1}^{1} a_M(1,m)\, h_1^{(1)}(qr)\,\frac{1}{\sqrt{2}}\,\hat{\mathbf{L}}\,Y_{1m} = \\
&= -\sum_{m=-1}^{1} a_M(1,m)\,\frac{i}{q^2}\,\frac{d}{dr}\left(\frac{e^{iqr}}{r}\right)\frac{1}{\sqrt{2}}\,\hat{\mathbf{L}}\,Y_{1m} = \\
&= -q\,\frac{d}{dr}\left(\frac{e^{iqr}}{r}\right)\hat{\mathbf{L}}\sum_{m=-1}^{1}\frac{i}{\sqrt{2}\,q^3}\,a_M(1,m)\,Y_{1m} = \\
&= -q\,\frac{d}{dr}\left(\frac{e^{iqr}}{r}\right)\hat{\mathbf{L}}\,(\mathbf{m}\cdot\mathbf{n}) = \\
&= -\frac{q}{r}\,\frac{d}{dr}\left(\frac{e^{iqr}}{r}\right)\hat{\mathbf{L}}\,(\mathbf{m}\cdot\mathbf{r})\,.
\end{aligned}
\tag{3.65}
$$

Next, we analyze the expression $\hat{\mathbf{L}}(\mathbf{m}\cdot\mathbf{n})$ using the properties of angular momentum operator:

$$
\hat{L}_j\;(x_l\,m_l) = \left[\hat{L}_j, x_l\right]\,m_l + x_l\,\hat{L}_j\,m_l = ie_{jln}\,x_n\,m_l \tag{3.66}
$$

Therefore,

$$
E_j = q\,\frac{d}{dr}\left(\frac{e^{iqr}}{r}\right)\,i\,e_{jnl}\,\frac{x_n}{r}\,m_l = ik\,\frac{d}{dr}\left(\frac{e^{iqr}}{r}\right)\,[\mathbf{n}\times\mathbf{m}]_j\;. \tag{3.67}
$$

Finally, we find that

$$
\mathbf{E} = iq\,\nabla\left(\frac{e^{iqr}}{r}\right)\times\mathbf{m}\,. \tag{3.68}
$$

Magnetic field, in turn, reads:

$$
\begin{aligned}
\mathbf{H} &= -\frac{i}{q}\,\mathrm{rot}\,\mathbf{E} = \nabla\times(\nabla f\times\mathbf{m}) = -\mathbf{m}\,\Delta f + (\mathbf{m}\cdot\nabla)\nabla f = \\
&= q^2\,f\,\mathbf{m} + (\mathbf{m}\cdot\nabla)\,\nabla f = \left[\nabla\otimes\nabla + q^2\,\hat{I}\right]\left(\frac{e^{iqr}}{r}\right)\mathbf{m}\,,
\end{aligned}
\tag{3.69}
$$

where $f = e^{iqr}/r$. Field of the electric dipole can be calculated analogously, taking dual symmetry into account. Finally, we write the fields from the electric and magnetic dipoles in the following form:

$$\mathbf{E} = \hat{G}^{\rm ee}(\mathbf{r})\,\mathbf{d} + \hat{G}^{\rm em}(\mathbf{r})\,\mathbf{m}\,, \tag{3.70}$$

$$\mathbf{H} = -\hat{G}^{\rm em}(\mathbf{r})\,\mathbf{d} + \hat{G}^{\rm ee}(\mathbf{r})\,\mathbf{m}\,. \tag{3.71}$$

The matrices introduced here are known as *dyadic Green's functions*:

$$\hat{G}^{\rm ee} = \left[\nabla\otimes\nabla + q^2\,\hat{I}\right]\left(\frac{e^{iqr}}{r}\right) = \not\nabla\, f\,, \tag{3.72}$$

$$\hat{G}^{\rm em} = iq\,\nabla^{\times}\, f\,, \tag{3.73}$$

where we introduced $f = e^{iqr}/r$ which is the solution of scalar Helmgoltz equation, $\not\nabla_{ik} = \nabla_i\,\nabla_k + q^2\,\delta_{ik}$ and $\nabla^{\times}_{ik} = e_{ijk}\,\nabla_j$.

Fields of electric and magnetic quadrupoles

In a similar way we evaluate the fields produced by the oscillating electric or magnetic quadrupole. To this end we consider the magnetic field produced by the oscillating electric quadrupole:

$$\mathbf{H} = \sum_{m=-2}^{2} a_E(2,m)\,h_2^{(1)}(qr)\,\frac{1}{\sqrt{6}}\,\hat{\mathbf{L}}Y_{2m} = \frac{1}{\sqrt{6}}\,h_2^{(1)}(qr)\,\hat{\mathbf{L}}\sum_{m=-2}^{2} a_E(2,m)\,Y_{2m} \overset{Eq.\ (3.58)}{=}$$
$$= -\frac{ir^2}{\sqrt{6}\,q^3}\left(\frac{1}{r}\frac{d}{dr}\right)^2 f\,\hat{\mathbf{L}}\,\frac{q^4}{2\sqrt{6}\,i}\,Q_{jk}\,x_j\,x_k/r^2 = -\frac{q}{12}\left(\frac{1}{r}\frac{d}{dr}\right)^2 f\,Q_{jk}\,\hat{\mathbf{L}}\,x_j\,x_k \tag{3.74}$$

Using the properties of angular momentum operator, we calculate

$$\hat{L}_i\,\hat{x}_j\,\hat{x}_k = [\hat{L}_i,\hat{x}_j]\,\hat{x}_k + \hat{x}_j\,\hat{L}_i\,\hat{x}_k = ie_{ijl}\,\hat{x}_l\,\hat{x}_k + \hat{x}_j\,ie_{ikl}\,\hat{x}_l = -ix^{\times}_{ij}\,\hat{x}_k - ix^{\times}_{ik}\,\hat{x}_j\,. \tag{3.75}$$

Hence, the magnetic field of a quadrupole can be presented in the form

$$H_i = G^{meq}_{ijk}\,Q_{jk}\,,$$

where

$$G^{meq}_{ijk} = \frac{iq}{12}\,\left[x^{\times}_{ij}\,x_k + x^{\times}_{ik}\,x_j\right]\left(\frac{1}{r}\frac{d}{dr}\right)^2 f\,.$$

Taking into account that

$$\nabla_i\,f(r) = \frac{x_i}{r}\,\frac{df}{dr}\,, \tag{3.76}$$

we present the Green's function in the form

$$G^{meq}_{ijk} = \frac{iq}{12}\,\left(\nabla^{\times}_{ij}\,\nabla_k + \nabla^{\times}_{ik}\,\nabla_j\right)\,f\,. \tag{3.77}$$

Electric field from the quadrupole can be evaluated as

$$E_i = \frac{i}{q} \nabla^{\times}_{in} H_n = \frac{i}{q} \nabla^{\times}_{in} G^{meq}_{njk} Q_{jk} \,, \tag{3.78}$$

which means that the Green's function for electric field is equal to $G^{eeq}_{ijk} = i/q \, \nabla^{\times}_{in} G^{meq}_{njk}$. Next we take into account that

$$\nabla^{\times}_{in} \nabla^{\times}_{nj} = \nabla_i \nabla_j - \delta_{ij} \nabla^2 = \not\nabla_{ij} \,, \tag{3.79}$$

since $\nabla^2 f = -q^2 f$. Therefore,

$$G^{eeq}_{ijk} = -\frac{1}{12} \left(\not\nabla_{ij} \nabla_k + \not\nabla_{ik} \nabla_j \right) f \,. \tag{3.80}$$

Equations Eqs. (3.80) and (3.77) provide electric and magnetic fields produced by the arbitrary electric quadrupole moment Q_{ij}. The solution for magnetic quadrupole moment is immediately recovered from duality:

$$E_i = G^{eeq}_{ijk} Q_{jk} + G^{emq}_{ijk} Q^M_{jk} \,, \tag{3.81}$$

$$H_i = G^{meq}_{ijk} Q_{jk} + G^{mmq}_{ijk} Q^M_{jk} \,, \tag{3.82}$$

where $G^{emq}_{ijk} = -G^{meq}_{ijk}$ and $G^{mmq}_{ijk} = G^{eeq}_{ijk}$. Using expressions for the Green's functions Eqs. (3.80), (3.77), it is straightforward to obtain near and far fields produced by quadrupoles. For example, in the far-field zone ∇ operators should be replaced by

$$\nabla_k \to iq \, n_k \,, \tag{3.83}$$

$$\nabla^{\times}_{ik} \to iq \, n^{\times}_{ik} \,, \tag{3.84}$$

$$\not\nabla_{ik} \equiv \nabla^{\times}_{ij} \nabla^{\times}_{jk} = -q^2 \, n^{\times}_{ij} n^{\times}_{jk} \,. \tag{3.85}$$

3.4 Radiation of multipoles

In this paragraph, we consider the fields produced by some finite distribution of currents and charges at distances much larger than the wavelength ($kr \gg 1$). In this *far-field zone* the Hankel functions can be replaced by $h^{(1)}_l(kr) \approx (-i)^{l+1} e^{ikr}/(kr)$. In turn,

$$\begin{aligned} \mathrm{rot}\left[h^{(1)}_l(kr)\,\mathbf{X}_{lm}\right] &\overset{\text{Eq. (3.43)}}{=} \frac{1}{r}\frac{d}{dr}\left(r\,h^{(1)}_l(kr)\right)\mathbf{Z}_{lm} + i\sqrt{l(l+1)}\,\frac{h^{(1)}_l(kr)}{r}\,\mathbf{n}Y_{lm} \\ &\approx i\,(-i)^{l+1}\,\frac{e^{ikr}}{r}\,\mathbf{Z}_{lm} \,. \end{aligned} \tag{3.86}$$

Therefore, the far-field asymptotics of the multipole expansion reads:

$$\mathbf{E} = -\frac{e^{ikr}}{kr} \sum_{l=1}^{\infty} \sum_{m=-l}^{l} (-i)^{l+1} \left[a_E(l,m)\, \mathbf{Z}_{lm} + a_M(l,m)\, \mathbf{X}_{lm} \right] , \tag{3.87}$$

$$\mathbf{H} = \frac{e^{ikr}}{kr} \sum_{l=1}^{\infty} \sum_{m=-l}^{l} (-i)^{l+1} \left[a_E(l,m)\, \mathbf{X}_{lm} - a_M(l,m)\, \mathbf{Z}_{lm} \right] . \tag{3.88}$$

It is straightforward to verify that $\mathbf{H} = \mathbf{n} \times \mathbf{E}$, which means that the far-field has a local structure of a plane wave. Energy flux is then calculated as

$$\frac{dP}{d\Omega} = r^2\, S_r = r^2\, \frac{c}{8\pi}\, |\mathbf{E}|^2 . \tag{3.89}$$

Consider first the angular distribution of radiation for a single multipole:

$$\begin{aligned}\frac{dP_{lm}}{d\Omega} &= \frac{c}{8\pi\, k^2} |\mathbf{X}_{lm}|^2 \left[|a_E(l,m)|^2 + |a_M(l,m)|^2 \right] = \\ &= \frac{c}{16\pi\, k^2\, l(l+1)} \left[|a_E(l,m)|^2 + |a_M(l,m)|^2 \right] \times \left[(l-m)(l+m+1)\, |Y_{l,m+1}|^2 \right. \\ &\quad \left. + (l+m)(l-m+1)\, |Y_{l,m-1}|^2 + 2m^2\, |Y_{lm}|^2 \right] .\end{aligned} \tag{3.90}$$

This said, the radiation from the electric and magnetic multipoles simply adds up because of their mutually orthogonal polarization. Equation (3.90) determines the radiation pattern of a single multipole. Note that it depends on the angle θ being independent of φ. To calculate the full intensity of radiation, we take into account orthogonality of vector spherical harmonics and integrate Eq. (3.90) over 4π solid angle. As a result, we get:

$$P = \frac{c}{8\pi\, k^2} \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \left[|a_E(l,m)|^2 + |a_M(l,m)|^2 \right] \tag{3.91}$$

It is important to stress that after obtaining this general result, we can immediately calculate the power emitted by dipoles, quadrupoles, etc. To do this, we only need the identification of multipole moments previously made in Sec. 3.3. Additionally, we take into account two important identities:

$$\langle n_i\, n_k \rangle = \frac{1}{3}\, \delta_{ik} , \tag{3.92}$$

$$\langle n_i\, n_j\, n_k\, n_l \rangle = \frac{1}{15} \left[\delta_{ij}\, \delta_{kl} + \delta_{ik}\, \delta_{jl} + \delta_{il}\, \delta_{jk} \right] , \tag{3.93}$$

where < .. > operator means the integration over full 4π solid angle and division of the result by 4π.

We start from the definition of dipole moment

$$\frac{i}{\sqrt{2}\,q^3}\sum_{m=-1}^{1} a_E(1,m)\,Y_{1m} = d_j\,n_j$$

$$\frac{1}{2\,q^6}\sum_{m,m'}\int a_E(1,m)\,a_E^*(1,m')\,Y_{1m}\,Y_{1m'}^*\,d\Omega = \int d_j\,n_j\,d_k^*\,n_k\,d\Omega$$

$$\frac{1}{2\,q^6}\sum_{m=-1}^{1} |a_E(1,m)|^2 = \frac{4\pi}{3}\,d_j\,d_k^*\,\delta_{jk}$$

$$\sum_{m=-1}^{1} |a_E(1,m)|^2 = \frac{8\pi\,q^6}{3}\,|\mathbf{d}|^2\,. \tag{3.94}$$

In an analogous way, taking into account that $Q_{ij} = Q_{ji}$, $Q_{ii} = 0$ (the tensor of quadrupole moment is symmetric and traceless), we find that

$$\sum_{m=-2}^{2} |a_E(2,m)| = \frac{\pi\,q^8}{45}\,|Q_{ij}|^2\,, \tag{3.95}$$

where the summation is performed over all indices i and j (sum of squares of elements of quadrupole moment tensor). With Eqs. (3.94) and (3.95), we derive that

$$P = \frac{c\,q^4}{3}\left(|\mathbf{d}|^2 + |\mathbf{m}|^2\right) + \frac{c\,q^6}{360}\sum_{i,j}\left(|Q_{ij}^{\mathrm{E}}|^2 + |Q_{ij}^{\mathrm{M}}|^2\right)\,. \tag{3.96}$$

3.5 Eigenmodes of a spherical particle

As a next application of multipole expansion, we consider a particle made of dielectric material with permittivity $\varepsilon = n^2$ placed in vacuum and analyze the eigenmodes supported by such particle. The fields inside and outside of the particle read

$$\mathbf{E}^{\mathrm{in}} = \frac{1}{n}\sum_{l,m}\left\{\frac{i}{qn}\,a_E^{\mathrm{in}}(l,m)\ \mathrm{rot}\left[j_l(qnr)\,\mathbf{X}_{lm}\right] - a_M^{\mathrm{in}}(l,m)\,j_l(qnr)\,\mathbf{X}_{lm}\right\}\,, \tag{3.97}$$

$$\mathbf{H}^{\mathrm{in}} = \sum_{l,m}\left\{a_E^{\mathrm{in}}(l,m)\,j_l(qnr)\,\mathbf{X}_{lm} + \frac{i}{qn}\,a_M^{\mathrm{in}}\ \mathrm{rot}\left[j_l(qnr)\,\mathbf{X}_{lm}\right]\right\}\,, \tag{3.98}$$

$$\mathbf{E}^{\text{out}} = \sum_{l,m} \left\{ \frac{i}{q}\, a_E^{\text{out}}\, \text{rot}\,[h_l(qr)\,\mathbf{X}_{lm}] - a_M^{\text{out}}\, h_l(qr)\,\mathbf{X}_{lm} \right\} , \tag{3.99}$$

$$\mathbf{H}^{\text{out}} = \sum_{l,m} \left\{ a_E^{\text{out}}\, h_l(qr)\,\mathbf{X}_{lm} + \frac{i}{q}\, a_M^{\text{out}}\, \text{rot}\,[h_l(qr)\,\mathbf{X}_{lm}] \right\} . \tag{3.100}$$

Unknown multipole coefficients are found by matching the fields inside and outside of the particle. *In monochromatic case, it is sufficient to consider only the conditions for the tangential components of* $\mathbf{E}$ *and* $\mathbf{H}$*. The conditions for the normal components of* $\mathbf{B}$ *and* $\mathbf{D}$ *are then fulfilled automatically.* Boundary conditions yield:

$$\frac{i}{qn^2}\, a_E^{\text{in}}(l,m)\, \frac{1}{a}\, \frac{d}{dr}\,[r\, j_l(qnr)]\bigg|_{r=a} = \frac{i}{q}\, a_E^{\text{out}}(l,m)\, \frac{1}{a}\, \frac{d}{dr}\, [r\, h_l(qr)]|_{r=a} , \tag{3.101}$$

$$\frac{1}{n}\, a_M^{\text{in}}(l,m)\, j_l(qna) = a_M^{\text{out}}(l,m)\, h_l(qa) , \tag{3.102}$$

$$a_E^{\text{in}}(l,m)\, j_l(qna) = a_E^{\text{out}}(l,m)\, h_l(qa) , \tag{3.103}$$

$$\frac{i}{qn}\, a_M^{\text{in}}(l,m)\, \frac{1}{a}\, \frac{d}{dr}\, [r\, j_l(qnr)]|_{r=a} = \frac{i}{qn}\, a_M^{\text{out}}\, \frac{1}{a}\, \frac{d}{dr}\, [r\, h_l(qr)]|_{r=a} . \tag{3.104}$$

Here, $h_l(qr) \equiv h_l^{(1)}(qr)$. Quite importantly, the equations for the electric and magnetic multipoles of different order appear to be independent. Therefore, each of multipoles has its own set of eigenmodes:

$$\frac{\frac{d}{dr}\, [r\, h_l(qr)]|_{r=a}}{h_l(qa)} = \frac{1}{n^2}\, \frac{\frac{d}{dr}\, [r\, j_l(qnr)]|_{r=a}}{j_l(qna)} , \quad \text{electric multipole of the order } l \tag{3.105}$$

$$\frac{\frac{d}{dr}\, [r\, h_l(qr)]|_{r=a}}{h_l(qa)} = \frac{\frac{d}{dr}\, [r\, j_l(qnr)]|_{r=a}}{j_l(qna)} , \quad \text{magnetic multipole of the order } l\, . \tag{3.106}$$

The degeneracy of the modes with respect to m is due to the spherical symmetry of the particle. Taking the limit $n \to \infty$ (or just imposing boundary conditions corresponding to the perfect conductor), we derive the boundary conditions for the ideally conducting sphere:

$$\frac{d}{dr}\, [r\, h_l(qr)]|_{r=a} = 0\, , \quad \text{electric multipole of the order } l \tag{3.107}$$

$$h_l(qa) = 0\, , \quad \text{magnetic multipole of the order } l \tag{3.108}$$

Note that since the Hankel function is complex, the modes of a spherical particle are also complex. The imaginary part of the mode frequency is associated with losses ($\omega_{ln} = \omega'_{ln} - i\omega''_{ln}$ with $\omega''_{ln} > 0$). Therefore, solving the equations with respect to the mode frequency, we consider only the solutions with negative imaginary part of frequency.

It can be shown that the solutions for magnetic modes of PEC sphere are purely imaginary, whereas the solutions for electric modes have some nonzero real part.

3.6 Mie theory: scattering of a plane wave on a spherical particle

Decomposition of a plane wave into the spherical ones

A scalar plane wave can be decomposed in terms of scalar spherical harmonics in the following way:

$$e^{ikr\,\cos\theta} = \sum_{l=0}^{\infty} i^l\,(2l+1)\,j_l(kr)\,P_l(\cos\theta) = \sum_{l=0}^{\infty} i^l\,\sqrt{4\pi\,(2l+1)}\,j_l(kr)\,Y_{l0}(\theta,\varphi)\,. \tag{3.109}$$

Based on this expression, we now derive the expansion of a plane wave propagating along z axis with electric field

$$\mathbf{E} = (\mathbf{e}_x \pm i\mathbf{e}_y)\,e^{ikz} \equiv \mathbf{e}_+\,e^{ikz}\,, \tag{3.110}$$

$$\mathbf{H} = \mathbf{e}_z \times \mathbf{E} = \mp i\,\mathbf{E}\,. \tag{3.111}$$

Since vector spherical harmonics form a complete basis, and the field of a plane wave is regular in the coordinate origin, the general expression for expansion of this kind is

$$\mathbf{E} = \sum_{l=1}^{\infty}\sum_{m=-l}^{l}\left[\frac{i}{k}\,a_\pm(l,m)\;\mathrm{rot}\left[j_l(kr)\,\mathbf{X}_{lm}\right] - b_\pm(l,m)\,j_l(kr)\,\mathbf{X}_{lm}\right]\,, \tag{3.112}$$

$$\mathbf{H} = \sum_{l=1}^{\infty}\sum_{m=-l}^{l}\left[a_\pm(l,m)\,j_l(kr)\,\mathbf{X}_{lm} + \frac{i}{k}\,b_\pm(l,m)\;\mathrm{rot}\left[j_l(kr)\,\mathbf{X}_{lm}\right]\right]\,. \tag{3.113}$$

Since $\mathbf{H} = \mp i\mathbf{E}$, $a_\pm(l,m) = \pm i b_\pm(l,m)$. In turn, $b_\pm(l,m)$ can be calculated by projecting $\mathbf{E}$ onto the vector spherical harmonics:

$$\begin{aligned}
b_\pm(l,m)\,j_l(kr) &= -\int \mathbf{E}\cdot\mathbf{X}^*_{lm}\,d\Omega = -\int e^{ikz}\,(\mathbf{e}_x \pm i\mathbf{e}_y)\cdot\frac{\hat{\mathbf{L}}^*}{\sqrt{l\,(l+1)}}\,Y^*_{lm}\,d\Omega = \\
&= -\int e^{ikz}\,\frac{1}{\sqrt{l(l+1)}}\left(\hat{L}^*_x \pm i\hat{L}^*_y\right)\,Y^*_{lm}\,d\Omega = \\
&= -\frac{1}{\sqrt{l(l+1)}}\int e^{ikz}\,(\hat{L}_\mp Y_{lm})^*\,d\Omega =
\end{aligned}$$

$$= -\sqrt{\frac{(l \pm m)(l \mp m + 1)}{l(l+1)}} \int e^{ikr\,\cos\theta}\,(Y_{l,m\mp1})^*\,d\Omega \overset{(3.109)}{=} \tag{3.114}$$

$$= -\sqrt{\frac{(l \pm m)(l \mp m + 1)}{l(l+1)}}\,\delta_{m,\pm1}\,i^l\,\sqrt{4\pi\,(2l+1)}\,j_l(kr)\,. \tag{3.115}$$

This yields

$$b_\pm(l,m) = -\delta_{m,\pm1}\,i^l\,\sqrt{4\pi\,(2l+1)}\,, a_\pm(l,m) = \mp\delta_{m,\pm1}\,i^{l+1}\,\sqrt{4\pi\,(2l+1)}\,. \tag{3.116}$$

As a result, the decomposition of the incident plane wave into the spherical ones takes the form ($q = \omega/c$):

$$\mathbf{E}_0 = \sum_{l=1}^{\infty} i^l\,\sqrt{4\pi\,(2l+1)}\,\left\{\pm\frac{1}{q}\,\mathrm{rot}\,[j_l(qr)\,\mathbf{X}_{l,\pm1}] + j_l(qr)\,\mathbf{X}_{l,\pm1}\right\}\,,$$

$$\mathbf{H}_0 = \sum_{l=1}^{\infty} i^l\,\sqrt{4\pi\,(2l+1)}\,\left\{\mp i j_l(qr)\,\mathbf{X}_{l,\pm1} - \frac{i}{q}\,\mathrm{rot}\,[j_l(qr)\,\mathbf{X}_{l,\pm1}]\right\}\,. \tag{3.117}$$

Decomposition of the fields inside and outside the sphere

The field outside the sphere ($r > a$) $\mathbf{E}^{\text{out}} = \mathbf{E}_0 + \mathbf{E}_{\text{s}}$, where $\mathbf{E}_{\text{s}}$ denotes the scattered field, which can be also expanded into the spherical harmonics as follows:

$$\mathbf{E}_{\text{s}} = \sum_{l=1}^{\infty} i^l\,\sqrt{4\pi\,(2l+1)}\,\left[\mp\frac{a_\pm(l)}{q}\,\mathrm{rot}\,\left[h_l^{(1)}(qr)\,\mathbf{X}_{l,\pm1}\right] - b_\pm(l)\,h_l^{(1)}(qr)\,\mathbf{X}_{l,\pm1}\right]\,,$$

$$\mathbf{H}_{\text{s}} = \sum_{l=1}^{\infty} i^l\,\sqrt{4\pi\,(2l+1)}\,\left[\pm i\,a_\pm(l)\,h_l^{(1)}(qr)\,\mathbf{X}_{l,\pm1} + \frac{i b_\pm(l)}{q}\,\mathrm{rot}\,\left[h_l^{(1)}(qr)\,\mathbf{X}_{l,\pm1}\right]\right]\,, \tag{3.118}$$

where we introduce expansion coefficients $a_\pm(l)$ and $b_\pm(l)$ linked to the standard multipole coefficients as follows:

$$a_E(l,m) = \mp\,i^{l-1}\,\sqrt{4\,\pi\,(2l+1)}\,a_\pm(l)\,\delta_{m,\pm1}\,, \tag{3.119}$$

$$a_M(l,m) = -i^l\,\sqrt{4\,\pi\,(2l+1)}\,b_\pm(l)\,\delta_{m,\pm1}\,. \tag{3.120}$$

The fields inside the sphere ($r < a$, $k = q\,n$), according to Sec. 3.2, can be expanded as

$$\mathbf{E}^{\text{in}} = \frac{1}{n} \sum_{l=1}^{\infty} i^l \sqrt{4\pi\,(2l+1)} \left[\mp \frac{\tilde{a}_{\pm}(l)}{k} \,\text{rot}\left[j_l(kr)\,\mathbf{X}_{l,\pm1}\right] - \tilde{b}_{\pm}(l)\, j_l(kr)\,\mathbf{X}_{l,\pm1} \right] , \tag{3.121}$$

$$\mathbf{H}^{\text{in}} = \sum_{l=1}^{\infty} i^l \sqrt{4\pi\,(2l+1)} \left[\pm i\tilde{a}_{\pm}(l)\, j_l(kr)\,\mathbf{X}_{l,\pm1} + \frac{i\,\tilde{b}_{\pm}(l)}{k} \,\text{rot}\left[j_l(kr)\,\mathbf{X}_{l,\pm1}\right] \right] . \tag{3.122}$$

The boundary conditions (the continuity of the tangential components of the electric and magnetic fields) yield the following set of equations:

$$-\frac{1}{n}\,\tilde{b}_{\pm}(l)\, j_l(qna) = j_l(qa) - b_{\pm}(l)\, h_l^{(1)}(qa) \quad (\mathbf{E}, \mathbf{X}_{l,\pm1})\,, \tag{3.123}$$

$$\begin{aligned} \frac{i\,\tilde{b}_{\pm}(l)}{qna}\,\frac{d}{dr}\left[r\, j_l(qnr)\right]\Big|_{r=a} = &-\frac{i}{qa}\,\frac{d}{dr}\left[r j_l(qr)\right]\Big|_{r=a} + \\ &+ \frac{i\, b_{\pm}(l)}{qa}\,\frac{d}{dr}\left[r\, h_l^{(1)}(qr)\right]\Big|_{r=a} \quad (\mathbf{H}, \mathbf{Z}_{l,\pm1})\,, \end{aligned} \tag{3.124}$$

$$\pm i\tilde{a}_{\pm}(l)\, j_l(qna) = \mp\, i j_l(qa) \pm i a_{\pm}(l)\, h_l^{(1)}(qa) \quad (\mathbf{H}, \mathbf{X}_{l,\pm1})\,, \tag{3.125}$$

$$\begin{aligned} \pm\frac{\tilde{a}_{\pm}(l)}{qn^2\,a}\,\frac{d}{dr}\left[r\, j_l(qnr)\right]\Big|_{r=a} = &\pm \frac{1}{qa}\,\frac{d}{dr}\left[r\, j_l(qr)\right]\Big|_{r=a} \mp \\ &\mp \frac{a_{\pm}(l)}{qa}\left[r\, h_l^{(1)}(qr)\right]\Big|_{r=a} \quad (\mathbf{E}, \mathbf{Z}_{l,\pm1})\,. \end{aligned} \tag{3.126}$$

Hence, the *Mie coefficients* $a_{\pm}(l)$ and $b_{\pm}(l)$ are defined as follows:

$$\boxed{\begin{aligned} a_{\pm}(l) &= \frac{j_l(qa)\,[rj_l(qnr)]' - n^2\, j_l(qna)\,[rj_l(qr)]'}{h_l^{(1)}(qa)\,[rj_l(qnr)]' - n^2\, j_l(qna)\,[rh_l^{(1)}(qr)]'}\,, \\ b_{\pm}(l) &= \frac{j_l(qa)\,[rj_l(qnr)]' - j_l(qna)\,[rj_l(qr)]'}{h_l^{(1)}(qa)\,[rj_l(qnr)]' - j_l(qna)\,[rh_l^{(1)}(qr)]'}\,, \end{aligned}} \tag{3.127}$$

where the derivatives comprising this expression are evaluated for $r = a$. Note also that $a_{+}(l) = a_{-}(l)$ and $b_{+}(l) = b_{-}(l)$, therefore from now on we omit $\pm$ subscript. The coefficients $a(l)$ and $b(l)$ describe the contribution of electric and magnetic multipoles, respectively. Therefore, they have poles at complex frequencies corresponding to electric and magnetic multipolar modes, respectively [cf. Eqs. (3.106), (3.105)]. Note that these designations are consistent with those of Bohren-Huffman book.

Results for multipole radiation

Using the results from Sec. 3.4, we find the scattering pattern of the multipoles excited in the sphere:

$$\frac{dP_{l,\pm1}}{d\Omega} = \frac{c\,|\mathbf{E}|^2(2l+1)}{8\,q^2\,l(l+1)}\,\left[|a(l)|^2+|b(l)|^2\right]\,\left[l\,(l+1)\,|Y_{l0}|^2+2\,|Y_{l1}|^2+\right.$$
$$\left.+(l-1)\,(l+2)\,|Y_{l2}|^2\right]\,. \quad (3.128)$$

Total power scattered by the sphere

$$P_{\rm sc} = \frac{c\,|E|^2}{4\,q^2}\sum_{l=1}^{\infty}(2l+1)\,\left[|a(l)|^2+|b(l)|^2\right]\,. \quad (3.129)$$

The scattering cross-section defined as the ratio $P_{\rm sc}/S_{\rm in}$ reads:

$$\boxed{\sigma_{\rm sc} = \frac{2\,\pi}{q^2}\sum_{l=1}^{\infty}(2l+1)\,\left[|a(l)|^2+|b(l)|^2\right]\,.} \quad (3.130)$$

Additionally, it can be noticed that $a(l) = (1-e^{2i\delta_l})/2$ and $b(l) = (1-e^{2i\delta_l'})/2$, where the *phase shifts* δ_l and δ_l' are defined as

$$e^{2i\delta_l} = -\frac{h_l^{(2)}(qa)\,[rj_l(qnr)]' - n^2\,j_l(qna)\,[rh_l^{(2)}(qr)]'}{h_l^{(1)}(qa)[rj_l(qnr)]' - n^2\,j_l(qna)\,[rh_l^{(1)}(qr)]}\,, \quad (3.131)$$

$$e^{2i\delta_l'} = -\frac{h_l^{(2)}(qa)\,[rj_l(qnr)]' - j_l(qna)\,[rh_l^{(2)}(qr)]'}{h_l^{(1)}(qa)[rj_l(qnr)]' - j_l(qna)\,[rh_l^{(1)}(qr)]'}\,. \quad (3.132)$$

With such definitions, the scattering cross-section can be expressed via the phase shifts as follows:

$$\sigma_{\rm sc} = \frac{2\pi}{q^2}\sum_{l=1}^{\infty}(2l+1)\,\left[\sin^2\,\delta_l+\sin^2\,\delta_l'\right]\,, \quad (3.133)$$

which is analogous to the formula for the scattering cross-section in quantum mechanics.

Extinction cross-section

Above, we have evaluated the incident power scattered by the sphere and calculated the scattering cross-section. However, some part of the incident power can also be absorbed inside the particle. To take into account both of these mechanisms leading to the loss of incident energy, it is convenient to introduce *extinction* $P_{\rm ext} = P_{\rm abs} + P_{\rm sc}$.

Electric and magnetic fields are presented as a sum of the incident and scattered waves: $\mathbf{E} = \mathbf{E}_0 + \mathbf{E}_s$, $\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_s$. Hence, the time-averaged Poynting vector

$$\begin{aligned}\mathbf{S} &= \frac{c}{8\pi}\,\mathrm{Re}\,[\mathbf{E}\times\mathbf{H}^*] \\ &= \underbrace{\frac{c}{8\pi}\,\mathrm{Re}\,[\mathbf{E}_0\times\mathbf{H}_0^*]}_{\mathbf{S}_0} + \underbrace{\frac{c}{8\pi}\,\mathrm{Re}\,[\mathbf{E}_s\times\mathbf{H}_s^*]}_{\mathbf{S}_s} + \underbrace{\frac{c}{8\pi}\,\mathrm{Re}\,[\mathbf{E}_0\times\mathbf{H}_s^* + \mathbf{E}_s\times\mathbf{H}_0^*]}_{\mathbf{S}_{ext}}\ .\end{aligned} \tag{3.134}$$

Next we integrate Eq. (3.134) over the closed surface placed in the far field of the scattering object and surrounding it. Taking into account that the energy of the incident field is conserved without an object, i.e. $\oint \mathbf{S}_0\cdot\mathbf{n}\,df = 0$, we get

$$P_{\mathrm{abs}} \equiv -\oint \mathbf{S}\cdot\mathbf{n}\,df = \underbrace{-\oint \mathbf{S}_s\cdot\mathbf{n}\,df}_{-P_s} - \oint \mathbf{S}_{ext}\cdot\mathbf{n}\,df\ . \tag{3.135}$$

Identifying $-\oint \mathbf{S}\cdot\mathbf{n}\,df$ with absorbed power and $\oint \mathbf{S}_s\cdot\mathbf{n}\,df$ with the scattered power, we deduce that extinction is given by

$$P_{\mathrm{ext}} \equiv P_{\mathrm{abs}} + P_{\mathrm{sc}} = -\oint \mathbf{S}_{ext}\cdot\mathbf{n}\,df = -\oint \frac{c}{8\pi}\,\mathrm{Re}\,[\mathbf{E}_0\times\mathbf{H}_s^* + \mathbf{E}_s\times\mathbf{H}_0^*]\cdot\mathbf{n}\,df\ , \tag{3.136}$$

where, in our case, the incident field is given by Eq. (3.117), and the scattered field is given by Eq. (3.118). In these expressions, we apply Eq. (3.43) and omit the radial components of the fields, which are negligible in the far-field zone. In fact, we do not even need to use the far-field asymptotics for the spherical Bessel and Hankel functions, since

$$j_l(x)\,\left[x\,h_l^{(1)}(x)\right]' - h_l^{(1)}(x)\,\left[x\,j_l(x)\right]' = i \tag{3.137}$$

Using this identity and orthogonality of vector spherical harmonics, we deduce that

$$P_{\mathrm{ext}} = \frac{c}{2\,q^2}\sum_{l=1}^{\infty}(2l+1)\ \mathrm{Re}\ [a(l)+b(l)]\ , \tag{3.138}$$

and, since $\mathbf{S}_0 = c/(4\pi)$, the extinction cross-section is equal to

$$\boxed{\sigma_{\mathrm{ext}} = \frac{2\pi}{q^2}\sum_{l=1}(2l+1)\ \mathrm{Re}\ [a(l)+b(l)]\ .} \tag{3.139}$$

Clearly, in the lossless case the extinction cross-section is equal to the scattering cross-section, which yields an identity $\mathrm{Re}\,a(l) = |a(l)|^2$ or, equivalently, $\mathrm{Re}\ a^{-1}(l) = 1$, which is also straightforward to see from the expressions for Mie coefficients Eqs. (3.127).

Evaluation of sphere polarizability

Let's assume that the incident wave has polarization $\mathbf{E} = \mathbf{e}_x + i\,\mathbf{e}_y$. Then it would excite the dipole moment with $d_y = i\,d_x$ rotating in Oxy plane counter-clockwise, which is associated with the multipole coefficient $a_E(1,1) = -\sqrt{12\,\pi}\,a(1)$. On the other hand, the same multipole coefficient is defined via the dipole moment of the particle as follows [Eq. (3.64)]: $a_E(1,1) = iq^3\,\sqrt{4\pi/3}\,(d_x - i\,d_y) = 2iq^3\,\sqrt{4\pi/3}\,d_x$. Since the strength of the field E_x is equal to 1, d_x is equal to the particle polarizability. Thus, we derive the following result for the particle polarizabilities:

$$\boxed{\begin{aligned} \alpha_{\rm E} &= \frac{3i}{2\,q^3}\,a(1)\;, \\ \alpha_{\rm M} &= \frac{3i}{2\,q^3}\,b(1)\;. \end{aligned}} \tag{3.140}$$

This said, the polarizabilities of the sphere are related to $a(1)$ and $b(1)$ coefficients in Mie series. Clearly, the polarizability tensor of the sphere is isotropic, which is fully consistent with the symmetry of the particle.

Equation (3.140) yields an important identity for the imaginary part of inverse polarizability:

$$\alpha_{\rm E}^{-1} = -\frac{2iq^3}{3}\,a^{-1}(1) = -\frac{2iq^3}{3}\,\frac{h_l^{(1)}(qa)\,[rj_l(qnr)]' - n^2\,j_l(qna)\,[rh_l^{(1)}(qr)]'}{j_l(qa)\,[rj_l(qnr)]' - n^2\,j_l(qna)\,[rj_l(qr)]'}\,. \tag{3.141}$$

Here, $h_l^{(1)} = j_l + i\,n_l$, where both j_l and n_l are purely real functions. Hence, for any l $\mathrm{Re}\,a^{-1}(l) = 1$ and similarly $\mathrm{Re}\,b^{-1}(l) = 1$, and thus

$$\begin{aligned} \mathrm{Im}\;\alpha_{\rm E}^{-1} &= -\frac{2\,q^3}{3}\;, \\ \mathrm{Im}\;\alpha_{\rm M}^{-1} &= -\frac{2\,q^3}{3}\;. \end{aligned} \tag{3.142}$$

Equation (3.142) is known as Sipe-Kranendonk condition, and it is valid not only for spherical particles, but also for any lossless dipole scatterer. This imaginary correction to polarizability is associated with the radiation losses.

In turn, the real part of the inverse polarizability of a small dielectric particle can be expanded in series with respect to the parameter $\xi = qa$. The leading-order terms read:

$$\mathrm{Re}\;\alpha_{\rm E}^{-1} = \frac{1}{a^3}\,\frac{\varepsilon+2}{\varepsilon-1} - \frac{3\,\xi^2}{5\,a^3}\,\frac{\varepsilon-2}{\varepsilon-1}\,, \tag{3.143}$$

$$\mathrm{Re}\ \alpha_{\mathrm{M}}^{-1} = \frac{1}{\xi^2\, a^3}\,\frac{30}{\varepsilon - 1} - \frac{10}{7\, a^3}\,\frac{2\varepsilon - 5}{\varepsilon - 1}\,. \tag{3.144}$$

Quite obviously, in the low-frequency limit $\xi \ll 1$ only the electric polarizability remains, whereas the magnitude of the magnetic polarizability is proportional to the square of frequency.

Quadrupole polarizability of the sphere

In a similar way, we can also calculate the quadrupole moment of the sphere induced by the gradient of the external field. We define the quadrupole polarizability as

$$Q_{ij}^{\mathrm{E}} = \alpha_{\mathrm{EQ}}\ (\partial_i\, E_j + \partial_j\, E_i)\ , \tag{3.145}$$

$$Q_{ij}^{\mathrm{M}} = \alpha_{\mathrm{MQ}}\ (\partial_i\, H_j + \partial_j\, H_i)\ . \tag{3.146}$$

Scalar form of the quadrupole polarizability is dictated by the full rotational symmetry of the sphere. Note that quadrupole polarizability of a less symmetric object will have a more complicated tensorial form. The derivatives of the field here are calculated at the center of the sphere. Below, we calculate the electric quadrupole polarizability, whereas the calculation for the magnetic polarizability is fully analogous.

Assume that the incident wave has the field profile $\mathbf{E} = (\mathbf{e}_x + i\, \mathbf{e}_y)\ e^{iqz}$. Then the only nonzero components of the quadrupole moment are:

$$Q_{13}^{\mathrm{E}} = Q_{31}^{\mathrm{E}} = \alpha_{\mathrm{EQ}}\left(\frac{\partial E_x}{\partial z} + \frac{\partial E_z}{\partial x}\right) = iq\, \alpha_{\mathrm{EQ}}\ , \tag{3.147}$$

$$Q_{23}^{\mathrm{E}} = Q_{32}^{\mathrm{E}} = \alpha_{\mathrm{EQ}}\left(\frac{\partial E_y}{\partial z} + \frac{\partial E_z}{\partial y}\right) = i\, Q_{13}^{\mathrm{E}}\,. \tag{3.148}$$

On the other hand, we have the relation between the multipole coefficients and the multipole moments, Eq. (3.58):

$$\frac{i\,\sqrt{6}}{q^4}\sum_{m=-2}^{2} a_E(2,m)\, Y_{2m} = \frac{1}{2}\, Q_{ij}\, n_i\, n_j\ . \tag{3.149}$$

Next, due to the form of Mie solution Eq. (3.119), for the given wave polarization only $a_{\mathrm{E}}(2,1)$ is nonzero. Scalar spherical harmonic

$$Y_{21} = -\sqrt{\frac{15}{8\,\pi}}\ \sin\theta\ \cos\theta\, e^{i\varphi} = -\sqrt{\frac{15}{8\,\pi}}\, n_3\, (n_1 + i\, n_2)\ . \tag{3.150}$$

Therefore, Eq. (3.149) yields:

$$\frac{i\sqrt{6}}{q^4}\left(-i\sqrt{20\pi}\,a(2)\right)\left(-\sqrt{\frac{15}{8\pi}}\,n_3\,(n_1+i\,n_2)\right)=iq\,\alpha_{\rm EQ}\,n_3\,(n_1+i\,n_2)\,. \quad (3.151)$$

Finally, we derive:

$$\boxed{\begin{aligned}\alpha_{\rm EQ}&=\frac{15\,i}{q^5}\,a(2)\,,\\ \alpha_{\rm MQ}&=\frac{15\,i}{q^5}\,b(2)\,.\end{aligned}} \quad (3.152)$$

Since in the lossless case for all Mie coefficients $\mathrm{Re}\,a^{-1}(n)=\mathrm{Re}\,b^{-1}(n)=1$, imaginary correction to quadrupole polarizabilities reads:

$$\mathrm{Im}\ \alpha_{\rm EQ}^{-1}=\mathrm{Im}\ \alpha_{\rm MQ}^{-1}=-\frac{i\,q^5}{15}\,. \quad (3.153)$$

The latter condition can be associated with energy conservation for the quadrupole source. In the limit $q\,a\ll 1$, the quadrupole polarizabilities are given by

$$\begin{aligned}\alpha_{\rm EQ}&\approx\frac{\varepsilon-1}{2\varepsilon+3}\,a^5\,,\\ \alpha_{\rm MQ}&\approx\frac{\varepsilon-1}{105}\,q^2\,a^7\,.\end{aligned} \quad (3.154)$$

Note that Eq. (3.154) agrees with the solution of electrostatic problem for the sphere placed in the field of a point charge, see the book by Stratton for details.

Most importantly, even though the dipole and quadrupole polarizabilities were extracted from the Mie solution describing the scattering of a plane wave, they can be applied to *arbitrary* arrays of spheres interacting with each other via their near and far fields.

Literature

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