

# Theory of electromagnetic fields at the nanoscale : scattering, Green tensor and local density of states

3

All kudos to Introduction to Nanophotonics (Benisty, Lalanne, Greffet), Chapter 12.

## 3.1 The Green tensor and integral formulation of electromagnetism

The most usual formulation of the scattering of electromagnetic fields is based on partial differential equations. The propagation equation in a linear, isotropic, inhomogeneous medium characterized by the relative permittivity  $\varepsilon_r(\mathbf{r})$  can be cast in the form

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) - \varepsilon_r(\mathbf{r})k_0^2 \mathbf{E}(\mathbf{r}) = i\omega\mu_0 \mathbf{j}_{\text{inc}}(\mathbf{r}), \quad (3.1)$$

where  $\mathbf{j}_{\text{inc}}$  stands for the current density in the sources generating an incident field. Here  $\varepsilon_r$  can be a function of both the position  $\mathbf{r}$  and the frequency for inhomogeneous and dispersive media. Note also that its imaginary part accounts for losses. The double curl operator can be reexpressed using :

$$\nabla \times \nabla \times \rightarrow \nabla(\nabla \cdot) - \Delta \quad (\overrightarrow{\text{grad}}(\text{div}) - \overrightarrow{\Delta})$$

When considering transverse solutions only (fields checking  $\text{div } \mathbf{E} = 0$ ), the propagation equation can be simplified into the Helmholtz equation (with source term) :

$$\Delta \mathbf{E}(\mathbf{r}) + \varepsilon_r(\mathbf{r})k_0^2 \mathbf{E}(\mathbf{r}) = -i\omega\mu_0 \mathbf{j}_{\text{inc}}(\mathbf{r}), \quad (3.2)$$

Once boundary conditions are specified, the problem is well posed, and the goal is to solve the equation to compute  $\mathbf{E}(\mathbf{r})$  in all space. This type of formulation is very practical for simple shapes such as planes or spheres.

For example, diffraction problems defines boundary conditions on the plane (of the diffracting object). This lead us to the plane wave expansion, defining the amplitude of each plane wave contained in the spectrum. A similar procedure can be used for spheres using spherical functions. The solution is known as Mie theory.

This procedure of calculation of  $\mathbf{E}$  from a propagation equation becomes intractable for complex geometries, as general solutions are difficult to find.

Instead, it is possible to reformulate the problem in terms of an integral equation which has a transparent physical meaning.

## The equivalence principle

In order to move to an integral formulation of electromagnetism, the basic idea is to consider that field propagation always occur in vacuum and that the physical impact of the presence of a material medium can be accounted for by introducing additional source terms. This picture is actually somewhat consistent with the microscopic picture of light propagation : a material medium is a collection of point-like sources placed in a rather empty space.

Let us proceed, by adding the term  $k_0^2[\epsilon_r(\mathbf{r}) - 1]\mathbf{E}$  on both sides of Eq. (3.2). This yields

$$\nabla \times \nabla \times \mathbf{E} - k_0^2 \mathbf{E} = k_0^2[\epsilon_r - 1]\mathbf{E} + i\omega\mu_0\mathbf{j}_{\text{inc}} = i\omega\mu_0\mathbf{j}_{\text{ind}} + i\omega\mu_0\mathbf{j}_{\text{inc}}, \quad (3.3)$$

where the induced current density is defined as

$$\mathbf{j}_{\text{ind}}(\mathbf{r}) = -i\omega\epsilon_0[\epsilon_r(\mathbf{r}) - 1]\mathbf{E}(\mathbf{r}). \quad (3.4)$$

We now have a propagation equation in vacuum with two source terms. The known source term  $\mathbf{j}_{\text{inc}}$  generates the incident field  $\mathbf{E}_{\text{inc}}(\mathbf{r})$ , and the (as yet unknown) induced source term  $\mathbf{j}_{\text{ind}}$  generates the scattered field  $\mathbf{E}_{\text{scat}}(\mathbf{r})$ . The total electric field  $\mathbf{E}(\mathbf{r})$  is the sum, therefore the interference, of the incident field and the scattered field.

We still want to compute  $\mathbf{E}(\mathbf{r})$ , but now, we have transformed a reflection or scattering problem into a radiation problem. This is known as the **equivalence principle**. This is still *not* an integral formulation of the problem, we are still dealing with a propagation equation.

The situation described by the equivalence principle remains quite complex : the scattered field is responsible for inducing source currents in space, that radiate to generate...the scattered field.

Let us rephrase this idea. Equation (3.2) considers that the field generated by the current density  $\mathbf{j}_{\text{inc}}$  is scattered by the medium described by  $\epsilon_r(\mathbf{r})$ , whereas Eq. (3.3) describes radiation in vacuum by two current density distributions,  $\mathbf{j}_{\text{inc}}$  and  $\mathbf{j}_{\text{ind}}$ . Yet, we still need to determine the induced sources  $\mathbf{j}_{\text{ind}}$ . As opposed to "simple" radiation problem, where the currents are assumed to be known, here the currents must be determined self-consistently from the incident field.

## The Green tensor

We rephrased the problem of propagation and scattering in a material environment in terms of radiation in vacuum by current elements. We want to compute the the electric field  $\mathbf{E}(\mathbf{r})$ . A perfect tool to achieve this task would be to get a linear operatir relating the vector current density  $\mathbf{j}_{\text{inc}}$  and  $\mathbf{j}_{\text{ind}}$  to the vector electric fields they radiate in vacuum  $\mathbf{E}_{\text{inc}}(\mathbf{r})$  and  $\mathbf{E}_{\text{scat}}(\mathbf{r})$ .

In general, these two vectors are **not** collinear. Indeed, it can be seen in the propagation equation that the operator  $\nabla \times \nabla \times$  couples the different components of the electric field to each component of the current density. A simpler way to express this fact is to note that the electric field radiated in the far field is perpendicular to the propagation direction

and therefore not always parallel to the current density : in the far field, the electric field radiated by a source is proportional to the transverse component of the current density.

The required operator is thus a **tensor** (also called a dyadic) connecting vector sources to the vector electric field. Hence, we define the **Green tensor**  $\overleftrightarrow{\mathbf{G}}_0$  by

### Definition of the Green's tensor

$$\mathbf{E}(\mathbf{r}) = i\omega\mu_0 \int \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') \mathbf{j}(\mathbf{r}') d^3\mathbf{r}'. \quad (3.5)$$

This relation expresses that  $\overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') \mathbf{j}(\mathbf{r}') d^3\mathbf{r}'$  is the electric field produced at position  $\mathbf{r}$  by the current source  $\mathbf{j}(\mathbf{r}') d^3\mathbf{r}'$  positioned at  $\mathbf{r}'$ . The total electric field is the sum of fields radiated by all source elements. We inject this expression of the electric field into the propagation equation :

$$\begin{aligned} \nabla \times \nabla \times i\omega\mu_0 \int \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') \mathbf{j}(\mathbf{r}') d^3\mathbf{r}' - k_0^2 i\omega\mu_0 \int \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') \mathbf{j}(\mathbf{r}') d^3\mathbf{r}' \\ = i\omega\mu_0 \int \overleftrightarrow{\mathbf{I}} \mathbf{j}(\mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') d^3\mathbf{r}' \\ \int \left[ \nabla \times \nabla \times \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') - k_0^2 \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') \right] \mathbf{j}(\mathbf{r}') d^3\mathbf{r}' = \int \left[ \overleftrightarrow{\mathbf{I}} \delta(\mathbf{r} - \mathbf{r}') \right] \mathbf{j}(\mathbf{r}') d^3\mathbf{r}' \end{aligned}$$

This leads to a general definition of the Green's tensor, as a solution of an operator equation

### Definition of Green's tensor (continued)

$$\nabla \times \nabla \times \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') - k_0^2 \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') = \overleftrightarrow{\mathbf{I}} \delta(\mathbf{r} - \mathbf{r}'), \quad (3.6)$$

where  $\overleftrightarrow{\mathbf{I}}$  is the unit dyadic. This indicates that the source can be a dipole with three independent orientations. This equation can be solved with radiation boundary conditions.

### Derivation of the Green tensor expression

In this section, we derive the integral equation obeyed by the electric field and we identify the explicit expression of the vacuum Green's tensor, as introduced in the previous section. To proceed, we start from the general expression of the field in terms of the electromagnetic potentials. The vector potential generated by a distribution of sources is given by the retarded potential expression

$$\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int \mathbf{j}(\mathbf{r}') \frac{e^{ik_0 R}}{R} d^3\mathbf{r}', \quad (3.7)$$

where  $R = |\mathbf{r} - \mathbf{r}'|$ . This solution assumes that the field decays at infinity. The currents can be either produced by an external source, or induced in the material medium. We do not need to make an explicit distinction so far for the derivation of Green's tensor.

Using the general relation between the electric field and the potentials, we obtain

$$\mathbf{E}(\mathbf{r}) = -\frac{\partial \mathbf{A}(\mathbf{r})}{\partial t} - \nabla V(\mathbf{r}). \quad (3.8)$$

The scalar potential can be derived from the vector potential using the Lorenz gauge condition,

$$\nabla \cdot \mathbf{A}(\mathbf{r}) - \frac{i\omega}{c^2} V(\mathbf{r}) = 0. \quad (3.9)$$

Inserting this expression for the scalar potential into Eq. (3.8) yields

$$\mathbf{E}(\mathbf{r}) = i\omega \left[ \mathbf{A}(\mathbf{r}) + \frac{1}{k_0^2} \nabla (\nabla \cdot \mathbf{A}(\mathbf{r})) \right]. \quad (3.10)$$

Using the explicit expression of the vector potential, we finally obtain

$$\begin{aligned} \mathbf{E}(\mathbf{r}) &= i\omega \frac{\mu_0}{4\pi} \int \left[ \frac{e^{ik_0 R}}{R} \mathbf{j}(\mathbf{r}') d^3 \mathbf{r}' \right] + i\omega \frac{\mu_0}{4\pi} \frac{1}{k_0^2} \int \left[ \nabla (\nabla \cdot \frac{e^{ik_0 R}}{R} \mathbf{j}(\mathbf{r}')) d^3 \mathbf{r}' \right] \\ &= i\omega \mu_0 \int \left[ \left( \overleftrightarrow{I} + \frac{1}{k_0^2} \nabla (\nabla \cdot) \right) \frac{e^{ik_0 R}}{4\pi R} \right] \mathbf{j}(\mathbf{r}') d^3 \mathbf{r}' \end{aligned}$$

From its definition, we identify the expression of Green's tensor, for  $\mathbf{r} \neq \mathbf{r}'$ , as

$$\overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') = \left( \overleftrightarrow{I} + \frac{1}{k_0^2} \nabla \nabla \right) \frac{e^{ik_0 R}}{4\pi R}, \quad R = |\mathbf{r} - \mathbf{r}'|. \quad (3.11)$$

This formula gives the electric field both inside and outside the sources. Its physical meaning is transparent : the field is the sum of the incident field produced by all currents element induced in the source volume  $V$ . It contains terms that vary as  $1/R$ ,  $1/R^2$ , and  $1/R^3$ , consistent with the electric field generated by an electric dipole. The Green tensor diverges when  $\mathbf{r} = \mathbf{r}'$ , when  $R \rightarrow 0$ , when evaluating the field at a point belonging to the sources. This point is addressed in the next section.

## Singularity of the Green tensor and integral equation

The field generated at a position  $\mathbf{r}$  is related to the integral of the Green's tensor over the source distribution. What is relevant is the investigation of singularities of  $\mathbf{E}(\mathbf{r}) = i\omega \mu_0 \int \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') \mathbf{j}(\mathbf{r}') d^3 \mathbf{r}'$ . when  $\mathbf{r}$  is located within the source volume.

The first term in the calculation of the field is given by

$$i\omega\mu_0 \int \overleftrightarrow{\mathbf{I}}(\mathbf{r}, \mathbf{r}') \frac{e^{ik_0 R}}{4\pi R} \mathbf{j}(\mathbf{r}') d^3 r'$$

thanks to the  $r'^2 dr'$  dependence of the volume element  $d^3 r'$ , this contribution never diverges.

The second term to consider is :

$$\int \left[ \nabla(\nabla \cdot \frac{e^{ik_0 R}}{R} \mathbf{j}(\mathbf{r}')) d^3 r' \right]$$

Taking the derivative  $\nabla(\nabla \cdot)$  of the vector integral in Eq. (??) does not introduce any difficulty provided that the field is evaluated at a point  $\mathbf{r}$  that does not belong to the current distribution. In that case,  $\mathbf{r} \neq \mathbf{r}'$  and the integrand is non-singular. By contrast, if the point  $\mathbf{r}$  belongs to the sources, the integral exhibits a singularity.

It arises from the second spatial derivative, which produces a term varying as  $1/r'^3$ . When combined with the  $r'^2 dr'$  dependence of the volume element  $d^3 r'$ , this leads to a  $1/R$  term and thus to a logarithmic divergence.

To avoid this difficulty, one introduces an exclusion volume  $\delta V$  around the observation point  $\mathbf{r}$ . In what follows, we choose a spherical exclusion volume and let its radius tend to zero.

The field produced by the "grad-div" term of Green's tensor can then be written as the sum of two contributions,

$$\lim_{\delta V \rightarrow 0} \frac{i\omega\mu_0}{4\pi k_0^2} \int \left[ \nabla(\nabla \cdot \frac{e^{ik_0 R}}{R} \mathbf{j}(\mathbf{r}')) d^3 r' \right] = \left[ \frac{1}{\epsilon_0} \lim_{\delta V \rightarrow 0} \nabla(\nabla \cdot) \int_{V-\delta V} \frac{\mathbf{j}(\mathbf{r}')}{-i\omega} \frac{e^{ik_0 R}}{4\pi R} d^3 r' \right] \quad (3.12)$$

$$+ \left[ \frac{1}{\epsilon_0} \lim_{\delta V \rightarrow 0} \nabla \nabla \int_{\delta V} \frac{\mathbf{j}(\mathbf{r}')}{-i\omega} \frac{e^{ik_0 R}}{4\pi R} d^3 r' \right] \quad (3.13)$$

$$(3.14)$$

where we can identify a polarization density vector defined as  $\mathbf{j}(\mathbf{r}') = (-i\omega)\mathbf{P}(\mathbf{r}')$ .

For the first term, the singularity has been removed, because the exclusion volume has been introduced and the order of differentiation and integration can be exchanged.

The second term requires special treatment, but can be obtained from a physical argument. When the exclusion volume is sufficiently small, we can consider that the volume of the sphere is uniformly polarized, and that all points in the volume of the sphere are in the near field region of any other point of the sphere : retardation effects are negligible and the electrostatic approximation applies.

In other words, the field generated by this spherical exclusion volume at its center is given by the answer to a textbook problem of electrostatics : the field produced inside a uniformly

polarized sphere is equal to  $-\mathbf{P}/(3\epsilon_0)$ . We thus obtain

$$\begin{aligned}
 & \lim_{\delta V \rightarrow 0} \frac{i\omega\mu_0}{4\pi k_0^2} \int \left[ \nabla(\nabla \cdot \frac{e^{ik_0 R}}{R} \mathbf{j}(\mathbf{r}') d^3 \mathbf{r}') \right] \\
 &= \left[ \frac{i\omega\mu_0}{k_0^2} \lim_{\delta V \rightarrow 0} \nabla(\nabla \cdot) \int_{V-\delta V} \mathbf{j}(\mathbf{r}') \frac{e^{ik_0 R}}{4\pi R} d^3 \mathbf{r}' \right] - \frac{\mathbf{P}}{3\epsilon_0} \\
 &= i\omega\mu_0 \left[ \lim_{\delta V \rightarrow 0} \int_{V-\delta V} \frac{1}{k_0^2} \nabla(\nabla \cdot \frac{e^{ik_0 R}}{R} \mathbf{j}(\mathbf{r}')) d^3 \mathbf{r}' \right] - \left[ \frac{1}{3\epsilon_0} \int_V \frac{\mathbf{j}(\mathbf{r}')}{-i\omega} \delta(\mathbf{r} - \mathbf{r}') d^3 \mathbf{r}' \right] \\
 &= i\omega\mu_0 \left[ \lim_{\delta V \rightarrow 0} \int_{V-\delta V} \frac{1}{k_0^2} \nabla(\nabla \cdot \frac{e^{ik_0 R}}{R} \mathbf{j}(\mathbf{r}')) d^3 \mathbf{r}' \right] - i\omega\mu_0 \left[ \int_V \frac{\overleftrightarrow{\mathbf{I}}}{3k_0^2} \delta(\mathbf{r} - \mathbf{r}') \mathbf{j}(\mathbf{r}') d^3 \mathbf{r}' \right]
 \end{aligned}$$

This result, combined with the previous calculated term, shows that the Green's tensor is an operator that can be expressed as :

#### Green's tensor in vacuum

$$\overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') = PV \left[ \left( \overleftrightarrow{\mathbf{I}} + \frac{1}{k_0^2} \nabla \nabla \right) \frac{e^{ik_0 R}}{4\pi R} \right] - \frac{\overleftrightarrow{\mathbf{I}}}{3k_0^2} \delta(\mathbf{r} - \mathbf{r}'), \quad (3.15)$$

PV denotes evaluation in the sense of the Cauchy principal value, which is, by definition, the value of an integral when introducing an exclusion volume around a singularity and letting it shrink to zero.

Here, calculation of the field is performed, when relevant, after exclusion from the integration volume of the singularity at  $\mathbf{r} = \mathbf{r}'$ , which is accounted for by the last term of the operator, which is specifically non-zero. By contrast, when  $\mathbf{r} \neq \mathbf{r}'$ , there is no divergence, and the last term of the operator is equal to zero, therefore introducing no irrelevant correction.

### Integral relation and integral equation

The dyadic Green tensor coincides with the electric field radiated by a dipole, except that the singularity at the origin has been explicitly identified and assigned a clear physical meaning. The integral equation shows that the field at any point is the sum of the incident field and the field radiated by all induced dipoles within the scattering object.

The electric field at any point  $\mathbf{r}$  can now be expressed in integral form as a superposition of the fields radiated by all current elements. Now, we explicitly make a difference between source currents related to the incident field and induced currents :

$$\mathbf{E}(\mathbf{r}) = i\omega\mu_0 \int \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') [\mathbf{j}_{\text{inc}}(\mathbf{r}') + \mathbf{j}_{\text{ind}}(\mathbf{r}')] d^3 \mathbf{r}'. \quad (3.16)$$

The physical content of this equation is transparent : the field at any point is the superposition of the fields radiated by all current elements in the system. Substituting the expression of the induced current density and identifying the incident and scattered fields yields

$$\begin{aligned} \mathbf{E}(\mathbf{r}) &= \mathbf{E}_{\text{inc}}(\mathbf{r}) + i\omega\mu_0 \int \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') \mathbf{j}_{\text{ind}}(\mathbf{r}') d^3\mathbf{r}' \\ &= \mathbf{E}_{\text{inc}}(\mathbf{r}) + k_0^2 \int \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') [\varepsilon_r(\mathbf{r}') - 1] \mathbf{E}(\mathbf{r}') d^3\mathbf{r}'. \end{aligned} \quad (3.17)$$

$$= \mathbf{E}_{\text{inc}}(\mathbf{r}) + \mathbf{E}_{\text{scat}}(\mathbf{r}) \quad (3.18)$$

The integral equation shows that the field at any point is the sum of the incident field and the field radiated by all induced dipoles within the scattering object. Each volume element  $d^3\mathbf{r}'$  carries a dipole moment  $\delta\mathbf{p} = \varepsilon_0[\varepsilon_r(\mathbf{r}') - 1]\mathbf{E}(\mathbf{r}')d^3\mathbf{r}'$  and radiates a field  $k_0^2 \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}')[\varepsilon_r(\mathbf{r}') - 1]\mathbf{E}(\mathbf{r}')d^3\mathbf{r}'$ . The resulting problem is therefore intrinsically a multiple-scattering problem. It should be emphasized once again that the Green tensor used here is the Green tensor in vacuum. A dipole embedded in a metal emits a wave that cannot propagate freely : the field is mostly evanescent. However, one can show that the attenuation of the field due to evanescence emerges naturally from the coherent superposition (in other words, interference) of all scattered fields produced by the induced currents in the medium, and that are propagating in vacuum.

### Lippmann-Schwinger equation for the electric field

Besides, Equation (3.18) shows that the field can be computed everywhere outside the scattering object, provided the field is known *inside* it. The key issue is therefore to determine the internal field. Restricting the integral relation to the volume  $V$  where  $\varepsilon_r(\mathbf{r}') \neq 1$  leads to the integral equation

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_{\text{inc}}(\mathbf{r}) + k_0^2 \int_V \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') [\varepsilon_r(\mathbf{r}') - 1] \mathbf{E}(\mathbf{r}') d^3\mathbf{r}', \quad \mathbf{r} \in V. \quad (3.19)$$

The unknown is the electric field, which appears both inside and outside the integral. This equation is known in physics as the *Lippmann-Schwinger equation* : it describes scattering problems. Here, we deal with scattering of light waves, while the Lippmann-Schwinger equation is usually seen in the context of quantum physics, where we treat scattering of wavefunctions. The structure of the physics underlying the equation is however strictly equivalent. This integral formulation provides a complete description of the scattering problem and is strictly equivalent to the differential formulation with boundary conditions.

The integral formalism has many useful properties. It provides physical insight into scattering processes, allows a clear distinction between single and multiple scattering, and facilitates the derivation of approximate solutions for small scatterers or weak dielectric contrast. It also provides a natural framework for introducing the scattering matrix and analyzing the far-field behavior of the scattered field.

## Multiple scattering

The integral equation provides a rigorous framework for defining single and multiple scattering. From a mathematical point of view, it can be solved by iteration. Introducing the simplified notation

$$[\varepsilon - 1]\mathbf{E} \rightarrow V\mathbf{E}, \quad k_0^2 \int \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}') \mathbf{X}(\mathbf{r}') d^3\mathbf{r}' \rightarrow \mathbf{G}_0 \mathbf{X}, \quad (3.20)$$

the integral equation becomes

$$\begin{aligned} \mathbf{E} &= \mathbf{E}_{\text{inc}} + \mathbf{G}_0 V \mathbf{E} \\ &= \mathbf{E}_{\text{inc}} + \mathbf{G}_0 V \mathbf{E}_{\text{inc}} + \mathbf{G}_0 V \mathbf{G}_0 V \mathbf{E} \\ &= [1 + \mathbf{G}_0 V + \mathbf{G}_0 V \mathbf{G}_0 V + \mathbf{G}_0 V \mathbf{G}_0 V \mathbf{G}_0 V + \dots] \mathbf{E}_{\text{inc}}. \end{aligned} \quad (3.21)$$

This series, known as the *Liouville expansion*, has a clear physical interpretation. The term proportional to  $\mathbf{G}_0 V$  corresponds to single scattering, while the term  $(\mathbf{G}_0 V)^n$  describes  $n$  successive scattering events. Multiple scattering introduces a nonlinear dependence of the scattered field on  $V$ , which lies at the heart of super-resolution reconstruction techniques.

## The Green's tensor in an arbitrary environment. Dyson equation

An alternative formulation consists in introducing a Green tensor that explicitly accounts for the environment. Instead of defining  $\overleftrightarrow{\mathbf{G}}_0$  as the field produced in vacuum by a dipole, we define a Green tensor  $\overleftrightarrow{\mathbf{G}}$  that describes propagation in the medium characterized by  $\varepsilon_r(\mathbf{r})$ . It obeys

$$\nabla \times \nabla \times \overleftrightarrow{\mathbf{G}}(\mathbf{r}, \mathbf{r}') - \varepsilon_r(\mathbf{r}) k_0^2 \overleftrightarrow{\mathbf{G}}(\mathbf{r}, \mathbf{r}') = \overleftrightarrow{\mathbf{I}} \delta(\mathbf{r} - \mathbf{r}'). \quad (3.22)$$

And now the permittivity describing the arbitrary environment is present in the equation of the Green's tensor. The electric field generated by an arbitrary current distribution is then

$$\mathbf{E}(\mathbf{r}) = i\omega\mu_0 \int \overleftrightarrow{\mathbf{G}}(\mathbf{r}, \mathbf{r}') \mathbf{j}_{\text{inc}}(\mathbf{r}') d^3\mathbf{r}'. \quad (3.23)$$

For a monochromatic electric dipole moment  $\mathbf{p}$  located at  $\mathbf{r}_0$ , corresponding to a current density  $-i\omega\mathbf{p}\delta(\mathbf{r} - \mathbf{r}_0)$ , the field reads

$$\mathbf{E}(\mathbf{r}) = \mu_0\omega^2 \overleftrightarrow{\mathbf{G}}(\mathbf{r}, \mathbf{r}_0) \mathbf{p}. \quad (3.24)$$

Deriving  $\overleftrightarrow{\mathbf{G}}$  analytically is generally difficult, but it can be achieved for simple geometries. The Green tensor for a planar interface is derived in Complement 12.B using a plane-wave expansion and Fresnel coefficients.

Finally, inserting Eq. (3.23) into Eq. (3.18), and noting that the relation holds for any current distribution, one obtains an integral equation for the Green tensor itself,

$$\overleftrightarrow{\mathbf{G}} = \overleftrightarrow{\mathbf{G}}_0 + \overleftrightarrow{\mathbf{G}}_0 V \overleftrightarrow{\mathbf{G}} + \dots \quad (3.25)$$

This equation is known as the *Dyson equation*.

## 3.2 Local Density of states

In the first section of this chapter, we introduced the Green's tensor as a quantity, purely classical in nature, that establishes a connection between sources and the field they produce in their environment; it is also simply the field produced by a point dipole in the same given environment. This field can be expanded over the basis of the available electromagnetic modes of the system. In that regard, the Green's tensor describes the way a point source is globally branched on the available modes of the system, and how it decays by emitting a field in these various modes.

In this new section, we start with a different point of view to discuss the same domain of ideas : how does a source radiate in its environment? In the context of Fermi Golden Rule, the answer to this question introduces the concept of the density of modes as a factor that impacts the spontaneous decay rate. Our goal is to demonstrate a relation between the Green's tensor and the Local Density of States, establishing a bridge between classical electrodynamics and the well-known problem of the coupling of a two-level system to surrounding vacuum in quantum physics.

### States and modes in wave physics

Before starting the discussion, we make a remark on semantics regarding the meaning of *state*, *mode*, and *eigenfunction*. The word “state” is usually used in the context of quantum mechanics or statistical physics, whereas the word “mode” is often used in wave theory. A state is an eigenfunction of a Hermitian operator for a given set of boundary conditions. Similarly, a mode of an acoustical or electromagnetic resonator is an eigenfunction of the homogeneous wave equation for a given geometry.

For electrons in a semiconductor in the term *density of states* (DOS) is used for a function  $g(E)$  such that  $g(E) dE$  is the number of electronic states (modes) with energy in the interval  $[E, E + dE]$ . Here, we aim to find the number of electromagnetic modes such that  $\rho(\omega) d\omega$  is the number of electromagnetic states in the interval  $[\omega, \omega + d\omega]$ .

To begin with, we briefly recall how to derive the density of electromagnetic states, or equivalently how to count the number of different solutions (plane waves) of Maxwell's equations in vacuum. A difficulty immediately arises, since this number is infinite. However, it is possible to define the number of modes per unit volume.

To proceed, it is convenient to introduce a perfectly conducting virtual cubic box of side length  $L$  and examine the limit as  $L$  tends to infinity. Perfectly conducting walls impose

finite boundary conditions. The modes are stationary waves with discrete wavevectors of the form

$$k_x = \frac{n\pi}{L}, \quad k_y = \frac{m\pi}{L}, \quad k_z = \frac{l\pi}{L}, \quad (3.26)$$

where  $n$ ,  $m$ , and  $l$  are positive integers. In  $\mathbf{k}$ -space, the volume occupied by one state is therefore  $(\pi/L)^3$ . As a consequence, the number of states in the volume element  $dk_x dk_y dk_z$  is

$$\frac{2L^3}{\pi^3} dk_x dk_y dk_z, \quad (3.27)$$

where the factor 2 accounts for the two possible polarizations of each electromagnetic state.

The number of modes increases as  $L^3$ , i.e. proportionally to the volume of the box. We now let the size of the box increase and divide by the volume  $V$  in order to obtain the number of modes per unit volume. In this limit, the influence of the boundaries becomes negligible, and we obtain a density of states per unit volume which is an intrinsic property of vacuum. The DOS in  $\mathbf{k}$ -space per unit volume is therefore equal to  $2/\pi^3$ .

Using the dispersion relation  $\omega = ck$ , we can now derive the vacuum DOS  $\rho_v(\omega)$ . The states with frequencies between  $\omega$  and  $\omega + d\omega$  occupy a volume  $\pi k^2 dk/2$  in  $\mathbf{k}$ -space, since only positive values of  $k_x$ ,  $k_y$ , and  $k_z$  are considered. Using  $k = \omega/c$ , we find

### Density of modes in vacuum

$$\rho_v(\omega) d\omega = \frac{\pi k^2 dk}{2} \frac{2}{\pi^3} = \frac{\omega^2}{\pi^2 c^3} d\omega. \quad (3.28)$$

So far, we have discussed stationary waves in a perfectly conducting box. An alternative approach consists in imposing periodic boundary conditions (the Born–von Karman conditions). In this case, the modes are propagating waves. The periodicity condition, for instance  $\exp[ik_x(x + L)] = \exp(ik_x x)$ , implies

$$k_x = \frac{2\pi n}{L}, \quad k_y = \frac{2\pi m}{L}, \quad k_z = \frac{2\pi l}{L}, \quad (3.29)$$

where  $n$ ,  $m$ , and  $l$  are positive or negative integers. The DOS in  $\mathbf{k}$ -space is then  $1/(4\pi^3)$ , but since both positive and negative components of the wavevector must be counted, the same result for the DOS is recovered.

Using the DOS, we can now compute the number of states  $N(\omega)$  available between 0 and  $\omega$  in a volume  $V$  :

$$N(\omega) = V \int_0^\omega \rho_v(\omega') d\omega' = V \frac{\omega^3}{3\pi^2 c^3} = \frac{8\pi}{3} \frac{V}{\lambda^3}. \quad (3.30)$$

This result provides a useful rule of thumb : the number of electromagnetic states with frequencies smaller than  $\omega$  is approximately equal to the volume divided by  $(\lambda/2)^3$ .

We now illustrate the importance of this concept using two examples : blackbody radiation and the spontaneous emission rate. Each electromagnetic mode carries a quantum of energy

$\hbar\omega$ , and its mean occupation number is given by the Bose–Einstein distribution

$$n_{\text{BE}}(\omega) = \frac{1}{\exp(\hbar\omega/k_B T) - 1}. \quad (3.31)$$

Multiplying these two quantities by the DOS yields the blackbody energy density :

$$u(\omega, T) = \frac{\omega^2}{\pi^2 c^3} \frac{\hbar\omega}{\exp(\hbar\omega/k_B T) - 1}. \quad (3.32)$$

The DOS therefore plays a central role in the thermodynamic properties of radiation, and in particular in energy and momentum transfer mediated by electromagnetic fields.

The DOS also plays a crucial role in the lifetime of an excited state of a two-level system. According to Fermi's golden rule, the decay rate is proportional to the number of available final states. When considering radiative relaxation, the spontaneous decay rate is therefore proportional to the number of electromagnetic states at the transition frequency. This can be seen by comparing the Einstein coefficients for stimulated and spontaneous emission. Their ratio is given by

$$\frac{A_{21}}{B_{21}\hbar\omega} = \frac{\omega^2}{\pi^2 c^3}, \quad (3.33)$$

which is precisely the vacuum DOS. In stimulated emission, only the mode of the incident photon is involved, whereas in spontaneous emission all electromagnetic modes contribute. Hence, the spontaneous emission coefficient is proportional to the DOS.

In summary, the concept of DOS is essential for understanding both the thermodynamic properties of electromagnetic radiation and the radiative decay of quantum emitters. In the following, we analyze why it is necessary to introduce a *local* density of states and how it can be related to the Green tensor.

## Introduction to the concept of local density of states

The purpose of this section is to motivate the introduction of a local density of states (LDOS) and to provide its general form. We begin with the case of electrons.

The number of states in the frequency interval  $[\omega, \omega + \delta\omega]$  is given by

$$dN(\omega) = g(\omega) \delta\omega. \quad (3.34)$$

If the spectrum is discrete, the DOS can be written as

$$g(\omega) = \sum_n \delta(\omega - \omega_n), \quad (3.35)$$

where the index  $n$  labels the states and allows for degeneracy.

To introduce spatial dependence, we define the LDOS  $g(\mathbf{r}, \omega)$ .

This is motivated by the fact that not all spatial points are equivalent unless the system is translationally invariant. For example, at a metal–vacuum interface, the electronic wavefunction decays into the vacuum and exhibits oscillations near the interface.

The probability of finding an electron in state  $\Psi_n$  within the volume element  $d\mathbf{r}$  is  $|\Psi_n(\mathbf{r})|^2 d\mathbf{r}$ . This naturally leads to the definition of the electronic LDOS :

$$g(\mathbf{r}, \omega) = \sum_n |\Psi_n(\mathbf{r})|^2 \delta(\omega - \omega_n). \quad (3.36)$$

Integrating the LDOS over space yields the total DOS. We now extend this concept to electromagnetic fields.

The need for an electromagnetic LDOS can be illustrated by two examples. First, the spontaneous emission rate of an atom depends on its position relative to the nodes and antinodes of the electromagnetic modes. Second, the blackbody energy density vanishes at a perfectly conducting surface, where the field is zero. Thus, while the DOS is uniform in vacuum, it becomes position dependent in structured environments.

To formalize this idea, we recall that the energy is proportional to the square of the field amplitude. For simplicity, we first consider a scalar field. Guided by Eq. (3.45), we define

$$\rho(\mathbf{r}, \omega) = \sum_n |\Psi_n(\mathbf{r})|^2 \delta(\omega - \omega_n), \quad (3.37)$$

where  $\Psi_n(\mathbf{r})$  satisfies the normalization condition

$$\int_V |\Psi_n(\mathbf{r})|^2 dV = 1. \quad (3.38)$$

It follows immediately that

$$\int_V \rho(\mathbf{r}, \omega) dV = \rho(\omega). \quad (3.39)$$

## Connecting the LDOS to the Green's tensor by a mode expansion

The LDOS is a quantity that allows to count for available modes in a given environment. The Green's tensor can be understood as the field produced by a single point source in a given environment. This field depends on the position of the dipole, because its coupling to the environment depends on its position. The generated field can be expanded over a basis of the modes of the system. In order to connect the Green's tensor to the LDOS, it is interesting to look for a way to expand the Green's tensor over a mode basis.

The general problem requires to deal with tensor quantities. For the sake of simplicity, we will illustrate the derivation using scalar quantities; the generalization of the result is tedious but straightforward.

In this scalar approach, we start by defining the Green function as the solution of the Helmholtz equation

$$\nabla^2 G(\mathbf{r}, \mathbf{r}', \omega) + \frac{\omega^2}{c^2} G(\mathbf{r}, \mathbf{r}', \omega) = -\delta(\mathbf{r} - \mathbf{r}'). \quad (3.40)$$

with the appropriate boundary conditions of the problem. We now consider the complete orthogonal set of modes  $\{\Psi_n\}$  of the problem. Here, they simply correspond to the modes of the Laplacian operator

$$\nabla^2 \Psi_n = -\frac{\omega_n^2}{c^2} \Psi_n, \quad (12.60)$$

with eigenvalues  $-\omega_n^2/c^2$ . We expand the Green function on this basis :

$$G(\mathbf{r}, \mathbf{r}', \omega) = \sum_n c_n(\mathbf{r}', \omega) \Psi_n(\mathbf{r}). \quad (12.61)$$

Inserting this expansion in the equation that defines  $G$ , we obtain :

$$\sum_n c_n(\mathbf{r}', \omega) \left( \frac{\omega^2}{c^2} - \frac{\omega_n^2}{c^2} \right) \Psi_n(\mathbf{r}) = -\delta(\mathbf{r} - \mathbf{r}'). \quad (3.41)$$

Since the  $\{\Psi_n\}$  form an orthonormal basis, we have

$$\int \Psi_n(\mathbf{r}) \Psi_m^*(\mathbf{r}) d^3r = \delta_{n,m}. \quad (3.42)$$

By multiplying the equation by  $\Psi_m^*(\mathbf{r})$  and integrating, we obtain :

$$c_m(\mathbf{r}', \omega) = -\frac{\Psi_m^*(\mathbf{r}')}{\frac{\omega^2}{c^2} - \frac{\omega_m^2}{c^2}}. \quad (12.64)$$

Finally, the Green function can be cast in the form

$$G(\mathbf{r}, \mathbf{r}', \omega) = -\sum_n \frac{c^2 \Psi_n(\mathbf{r}) \Psi_n^*(\mathbf{r}')}{\omega^2 - \omega_n^2}. \quad (3.43)$$

and more interestingly, we inspect the case  $\mathbf{r} = \mathbf{r}'$  :

### Expansion of the fields radiated by a source over the modes

$$G(\mathbf{r}, \mathbf{r}, \omega) = -\sum_n \frac{c^2 |\Psi_n(\mathbf{r})|^2}{\omega^2 - \omega_n^2}. \quad (3.44)$$

and we can already feel the connection with the LDOS

$$g(\mathbf{r},\omega) = \sum_n |\Psi_n(\mathbf{r})|^2 \delta(\omega - \omega_n). \quad (3.45)$$

Now the question is mostly the derivation of the connection to the Dirac distribution of modes.

A specific mathematical identity is involved at this point. We use the following identity, which can be demonstrated by contour integration in the complex plane (to be done in appendices...)

$$\lim_{\eta \rightarrow 0} \text{Im} \left[ \frac{1}{(\omega + i\eta)^2 - \omega_n^2} \right] = \frac{\pi}{2\omega_n} [\delta(\omega - \omega_n) - \delta(\omega + \omega_n)]. \quad (3.46)$$

This is a pure mathematical identity so far. We note that we deal exclusively with positive frequencies, so that the term  $\delta(\omega + \omega_n)$  can be dispelled. Only the first Dirac  $\delta(\omega - \omega_n)$  remains.

$$\lim_{\eta \rightarrow 0} \text{Im} [G(\mathbf{r},\mathbf{r},\omega + i\eta)] = \lim_{\eta \rightarrow 0} \text{Im} \sum_n \frac{c^2 |\Psi_n(\mathbf{r})|^2}{(\omega + i\eta)^2 - \omega_n^2} = \sum_n \frac{c^2 |\Psi_n(\mathbf{r})|^2 \pi}{2\omega_n} \delta(\omega - \omega_n) \quad (3.47)$$

At a given frequency  $\omega$ , only terms with  $\omega_n = \omega$  are non-zero. We can replace all occurrences of the different eigenfrequencies  $\omega_n$  with  $\omega$ . Finally, we get

### Connecting the LDOS to Green's tensor - scalar case

$$\rho(\mathbf{r},\omega) = \sum_n |\Psi_n(\mathbf{r})|^2 \delta(\omega - \omega_n) = \lim_{\eta \rightarrow 0} \frac{2\omega}{\pi c^2} \text{Im} [G(\mathbf{r},\mathbf{r},\omega + i\eta)]. \quad (3.48)$$

## Vector case

Let us now consider briefly the vector case for non-lossy systems. The Green tensor satisfies the propagation equation. Assuming that the field can be expanded over a set of orthogonal modes  $\mathbf{E}_m(\mathbf{r})$  satisfying

$$\int \mathbf{E}_m(\mathbf{r}) \cdot \mathbf{E}_n^*(\mathbf{r}) d^3r = \delta_{m,n}, \quad (3.49)$$

the Green tensor can be expanded as :

$$\overleftrightarrow{G}(\mathbf{r},\mathbf{r}',\omega) = \sum_m \frac{c^2 \mathbf{E}_m(\mathbf{r}) \mathbf{E}_m^*(\mathbf{r}')}{\omega_m^2 - \omega^2}. \quad (3.50)$$

It follows that the field  $\mathbf{E}(\mathbf{r})$  radiated by a current density  $\mathbf{j}(\mathbf{r})$  is given by

$$\mathbf{E}(\mathbf{r}) = \sum_m C_m \mathbf{E}_m(\mathbf{r}), \quad (3.51)$$

where the mode amplitude  $C_m$  is given by an overlap integral :

$$C_m = \frac{i\omega}{\varepsilon_0} \frac{1}{\omega_m^2 - \omega^2} \int \mathbf{E}_m^*(\mathbf{r}') \cdot \mathbf{j}(\mathbf{r}') d^3r'. \quad (3.52)$$

We can derive

$$\lim_{\eta \rightarrow 0} \text{Im} \left[ \overleftrightarrow{G}(\mathbf{r}, \mathbf{r}, \omega + i\eta) \right] = \sum_m \frac{\pi c^2}{2\omega} \mathbf{E}_m(\mathbf{r}) \mathbf{E}_m^*(\mathbf{r}) \delta(\omega - \omega_m). \quad (3.53)$$

It follows that

### Connecting the LDOS to Green's tensor - Vector case

$$\rho(\mathbf{r}, \omega) = \lim_{\eta \rightarrow 0} \frac{2\omega}{\pi c^2} \text{Tr} \left\{ \text{Im} \left[ \overleftrightarrow{G}(\mathbf{r}, \mathbf{r}, \omega + i\eta) \right] \right\}. \quad (3.54)$$

In most situations where we discuss spontaneous emission, we are dealing with dipoles with a given orientation. Such a dipole is not coupled to all modes available at its position, but only to the modes that share the same polarization. This means that only some components of the Green's tensor must be considered to account for the appropriate density of states.

### Partial LDOS (projected LDOS along $\mathbf{u}$ )

We introduce the partial LDOS as the LDOS projected along the dipole unit vector  $\mathbf{u}$  :

$$\rho_{\mathbf{u}}(\mathbf{r}, \omega) = \lim_{\eta \rightarrow 0} \frac{2\omega}{\pi c^2} \left\{ \text{Im} \left[ \mathbf{u} \cdot \overleftrightarrow{G}(\mathbf{r}, \mathbf{r}, \omega + i\eta) \cdot \mathbf{u} \right] \right\}. \quad (3.55)$$

We retrieve an expression similar to the scalar case. In vacuum (and more generally in all homogenous, isotropic media), the partial LDOS amounts to 1/3 of the "total" LDOS, as we have to consider dipoles with all possible orientations in  $(\mathbf{u}_x, \mathbf{u}_y, \mathbf{u}_z)$ .