Electromagnetic density of modes for a finite-size three-dimensional structure

Giuseppe D'Aguanno,[1,2,3,*] Nadia Mattiucci,[1,2,4] Marco Centini,[2,3] Michael Scalora,[2] and Mark J. Bloemer[2]
[1]*Time Domain Corporation, Cummings Research Park, 7057 Old Madison Pike, Huntsville, Alabama 35806, USA*
[2]*Weapons Sciences Directorate, Research Development and Engineering Center, U.S. Army Aviation & Missile Command, Building 7804, Redstone Arsenal, Alabama 35898-5000, USA*
[3]*INFM at Dipartimento di Energetica, Università di Roma "La Sapienza," Via A. Scarpa 16, I-00161 Rome, Italy*
[4]*Università "RomaTre," Dipartimento di Fisica "E. Amaldi," Via Della Vasca Navale 84, I-00146 Rome, Italy*
(Received 29 September 2003; published 24 May 2004)

The concept of the density of modes has been lacking a precise mathematical definition for a finite-size structure. With the explosive growth in the fabrication of photonic crystals and nanostructures, which are inherently finite in size, a workable definition is imperative. We give a simple and physically intuitive definition of the electromagnetic density of modes based on the Green's function for a generic three-dimensional open cavity filled with a linear, isotropic, dielectric material.

DOI: 10.1103/PhysRevE.69.057601 PACS number(s): 42.70.Qs, 41.20.−q

Several attempts have been made to generalize the notion of the local density of modes (LDOM)—or local density of states—and the density of modes (DOM)—or density of states—to the case of open cavities—i.e., structure of finite size where electromagnetic energy can flow in and out of the volume bounded by the surface S of the cavity [1–6]. Quite surprisingly, the concept of the density of states for a finite-size structure still lacks a simple, concise definition. In the words of Felbacq and Smaali, "*Such notions as that of the density of states or local density of states, which are crucial in the description of the coupling between field and matter, cannot be straightforwardly defined for finite structures*" [5]. In our estimation, the most likely reason why the concepts of the LDOM and DOM have not yet found straightforward extensions to the case of three-dimensional (3D), finite structures is probably due to the fact that most approaches have focused on the mathematical rather than the basic physical aspects of the problem. Furthermore, due to their basic simplicity, 1D and 2D open cavities filled with nonabsorbing materials remain the subject of choice of most researchers.

If we have a closed cavity such that the field vanishes at the edges or a cavity where periodic boundary conditions can be applied (such as a multilayer stack of infinite length), filled with a nonabsorbing medium, we can expect that the electromagnetic energy will be conserved inside the cavity, and the problem in Hermitian. In this case, the LDOM stands for the number of eigenmodes per unit volume and unit frequency at a point $\vec{r}$ inside the cavity. If the electromagnetic field can be specified by a single field component (TE or TM polarization), then the scalar Green's function can be expanded in terms of the eigenmodes of the cavity and the LDOM can be calculated through the imaginary part of the scalar Green's function: $\rho_\omega(\vec{r}) \propto -\mathrm{Im}[G_\omega(\vec{r},\vec{r})]$ [4,7,8]. The DOM is then defined as the average LDOM inside the volume V of the cavity. So we ask (i) what happens if the cavity is open, such that electromagnetic energy can flow in and out of the volume bounded by the surface S of the cavity? (ii) What happens if the cavity is filled with an absorbing material? These questions have no easy answers fundamentally because the electromagnetic problem is no longer Hermitian and the cavity does not admit eigenmodes in the usual sense of the word. As a consequence, the Green's function does not admit a straightforward expansion in terms the cavity modes [7,9] and the very notion of the LDOM would seem to lose its validity. In other words, can a LDOM still be defined when the problem is not Hermitian (the case of open cavity or material absorption), and what is its physical meaning in this case [10]?

To answer these deceptively simple but crucial questions we go back to the usual starting place—that is, Maxwell's equations, which we write in MKSA units, in the frequency domain, assuming a harmonic time dependence of the type $e^{(-i\omega t)}$ and nonmagnetic materials ($\mu_r \cong 1$):

$$\vec{\nabla} \times \vec{E}_\omega = i\omega \vec{B}_\omega, \tag{1a}$$

$$\vec{\nabla} \times \vec{B}_\omega = \mu_0 \vec{J}_\omega(\vec{r}) - i\frac{\omega}{c^2}\varepsilon_\omega(\vec{r})\vec{E}_\omega, \tag{1b}$$

where $\vec{J}_\omega(\vec{r})$ is a complex current density, $\varepsilon_\omega(\vec{r})$ is the spatially dependent, relative, complex dielectric function of the material, and $\varepsilon_\omega(\vec{r}) = \varepsilon^R_\omega(\vec{r}) + i\varepsilon^I_\omega(\vec{r})$. Note that we use a generic, linear, and isotropic dielectric material. Equations (1) describe the steady-state case; i.e., we assume that both the electromagnetic field and the source $\vec{J}_\omega(\vec{r})$ oscillate with a harmonic time dependence. Taking the curl of Eq. (1a) and using Eq. (1b), we arrive at the following equation for the electric field:

$$-\vec{\nabla} \times \vec{\nabla} \times \vec{E}_\omega + \frac{\omega^2}{c^2}\varepsilon_\omega(\vec{r})\vec{E}_\omega = -i\omega\mu_0\vec{J}_\omega. \tag{2}$$

Let us now consider a cavity of volume V and surface S filled with a dielectric material of dielectric function $\varepsilon_\omega(\vec{r})$, where a known current density $\vec{J}_\omega(\vec{r})$ is present. Multiplying Eq. (2) by $\vec{E}^*_\omega$, integrating over the volume V, using the vector analog of Green's first identity [11], and using Eq. (1a), we arrive at the equation

*Electronic address: giuseppe.daguanno@timedomain.com

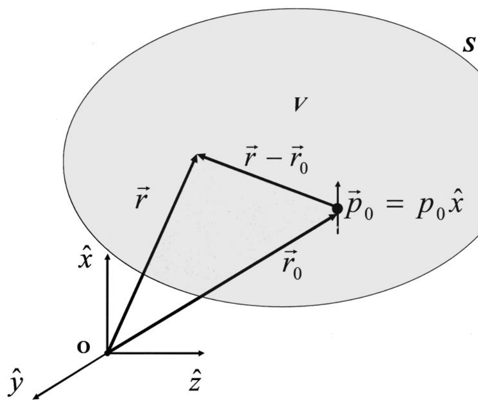

FIG. 1. Schematic representation of a point dipole embedded in a cavity of volume V and surface S filled with a generic linear and isotropic dielectric material.

$$-\frac{1}{2}\mathrm{Re}\int_V \vec{J}_\omega \cdot \vec{E}^*_\omega dV = \frac{1}{2}\omega\varepsilon_0\int_V \varepsilon^I_\omega|\vec{E}_\omega|^2 dV + \frac{1}{2}\mathrm{Re}\int_S\left[\frac{\vec{E}^*_\omega\times\vec{B}_\omega}{\mu_0}\right]\cdot\hat{n}dS. \quad (3)$$

Equation (3) makes a statement about energy conservation. It says that the mean electromagnetic power emitted (or in any case lost) by the source $\vec{J}_\omega$ (left-hand side) is equal to the mean power dissipated in the volume V (first term on right-hand side), plus the mean power flowing through the surface S (second term on right-hand side) or

$$\overline{W}_{\text{emitted}} = \overline{W}_{\text{dissipated in } V} + \overline{W}_{\text{flowing through } S}. \quad (4)$$

The assumption of a steady state implies the presence of a generator, or forcing term, in order to maintain the current density under harmonic oscillation. In short, this means that $\overline{W}_{\text{emitted}} = -1/2\ \mathrm{Re}\int_V \vec{J}_\omega\cdot\vec{E}^*_\omega dV = \eta\overline{W}_{\text{generator}}$, where $0<\eta<1$ is the efficiency of the generator.

Let us now suppose that the source of the electromagnetic radiation is located in a very small region inside the cavity and that it is centered near the point $\vec{r}_0$. We emphasize that we are not discussing an extended source, but a very well localized one. Let us also suppose that the source is a simple electric dipole of moment $\vec{p}_0$. It follows that $\vec{J}_\omega(\vec{r}) = -i\omega\vec{p}_0\delta(\vec{r}-\vec{r}_0)$ (point dipole), a situation which is depicted in Fig. 1. The mean power emitted by the dipole can be calculated by using Eq. (3) and by exploiting the properties of Dirac's δ function:

$$\overline{W}_{\text{emitted}}(\vec{r}_0) = -\frac{\omega^3\mu_0|\vec{p}_0|^2}{2}\mathrm{Im}[G_{\omega,\hat{x}\hat{x}}(\vec{r}_0,\vec{r}_0)], \quad (5)$$

where $G_{\omega,\hat{x}\hat{x}}(\vec{r}_0,\vec{r}_0)$ is the $\hat{x}\hat{x}$ component of the dyadic Green's function $\overline{\overline{G}}_\omega(\vec{r},\vec{r}_0)$ calculated at $\vec{r}=\vec{r}_0$, where $\hat{x}$ is the unit vector along which the dipole is oriented. The dyadic Green's function satisfies the equation

$$-\vec{\nabla}\times\vec{\nabla}\times\overline{\overline{G}}_\omega(\vec{r},\vec{r}_0) + \frac{\omega^2}{c^2}\varepsilon_\omega(\vec{r})\overline{\overline{G}}_\omega(\vec{r},\vec{r}_0) = \overline{\overline{I}}\delta(\vec{r}-\vec{r}_0), \quad (6)$$

where

$$\varepsilon_\omega(\vec{r}) = \begin{cases}\varepsilon^R_\omega(\vec{r}) + i\varepsilon^I_\omega(\vec{r}) & \text{in } V,\\ \varepsilon_{\text{out}} & \text{outside } V,\end{cases}$$

and ε_{out} is the real dielectric constant of the homogeneous medium that surrounds the cavity. The appropriate boundary conditions that apply in our case are those of an outgoing wave; i.e., no electromagnetic energy is flowing from outside into the cavity through the surface S. Here $\overline{\overline{I}}$ is the unit dyadic. As a particular case, from Eq. (5) we can calculate the power emitted by a point dipole in free space. In that case and for the boundary conditions just described, the dyadic Green's function solution of Eq. (6) is [12,13]

$$G^{\text{free space}}_{\omega,\hat{\alpha}\hat{\beta}}(\vec{r},\vec{r}_0) = -\frac{1}{4\pi}\left[\delta_{\alpha\beta} + \frac{1}{k_0^2}\frac{\partial^2}{\partial\alpha\,\partial\beta}\right]\frac{\exp[ik_0|\vec{r}-\vec{r}_0|]}{|\vec{r}-\vec{r}_0|},$$

$$(\alpha,\beta) = x,y,z, \quad (7)$$

where $k_0=\omega/c$ is the vacuum wave vector and $\delta_{\alpha\beta}$ is Kronecker's delta. From Eqs. (5) and (7) we obtain

$$\overline{W}_{\text{emitted,free space}} = \frac{\omega^4\mu_0|\vec{p}_0|^2}{12\pi c}. \quad (8)$$

This is the power emitted, or lost, by an electric dipole in free space, and it is the classical result we are all familiar with [14]. Now, from Eq. (5) and (8), we obtain

$$\frac{\overline{W}_{\text{emitted}}(\vec{r})}{\overline{W}_{\text{emitted,free space}}} = -\frac{6\pi c}{\omega}\mathrm{Im}[G_{\omega,\hat{x}\hat{x}}(\vec{r},\vec{r})]. \quad (9)$$

From Eq. (9) we deduce that the mean power emitted by a harmonically driven oscillating electric dipole oriented along $\hat{x}$ and located at a position $\vec{r}$ inside a generic, 3D cavity of volume V, filled with a generic linear and isotropic dielectric material, is modified with respect to the power emitted by the same dipole in free space by a factor proportional to the imaginary part of the $\hat{x}\hat{x}$ component of the dyadic Green's function. Note that this factor does not depend on the strength of the dipole moment $|\vec{p}_0|$, but still depends on its orientation, a fact that is often neglected, or unneeded, in lower-dimensional systems.

What one should generally require from the LDOM is that (i) it account for the modification of dipole emission rates with respect to emission rates in vacuum and (ii) it give the correct limiting value for the DOM of free space when calculated for an empty cavity whose dimensions go to infinity. The simplest way to satisfy these two requirements is to write the LDOM as

$$\rho_\omega(\vec{r}) \equiv \rho_{\omega,\text{free space}} \frac{\overline{W}_{\text{emitted}}(\vec{r})}{\overline{W}_{\text{emitted,free space}}}$$
$$= -\frac{6\pi c}{\omega}\rho_{\omega,\text{free space}}\text{Im}[G_{\omega,\hat{x}\hat{x}}(\vec{r},\vec{r})]. \tag{10}$$

Consequently, the DOM will be

$$\rho_\omega \equiv \rho_{\omega,\text{free space}} \frac{\langle \overline{W}_{\text{emitted}}(\vec{r})\rangle}{\overline{W}_{\text{emitted,free space}}}$$
$$= -\frac{6\pi c}{\omega}\rho_{\omega,\text{free space}}\,\langle \text{Im}[G_{\omega,\hat{x}\hat{x}}(\vec{r},\vec{r})]\rangle, \tag{11}$$

where the symbol $\langle\ \rangle$ denotes a spatial average over the volume V of the cavity. We note that for a closed cavity filled with a nonabsorbing material $\overline{W}_{\text{flowing through } S}\cong 0$, and $\overline{W}_{\text{dissipated in } V}\cong 0$. From Eqs. (4) and (10) it follows that $\rho_\omega(\vec{r})\cong 0$; i.e., dipole emission rates are inhibited [15]. In this regard, we note that the quantum spontaneous emission rate of an atom embedded in a dielectric microcavity is proportional to the total classical radiation energy of a corresponding dipole current in the same dielectric microcavity [16,17].

In the case of an open cavity filled with a nonabsorbing material we arrive at an *operational definition of the LDOM*. From Eq. (4), in the case of no absorption, we have $\overline{W}_{\text{emitted}}=\overline{W}_{\text{flowing through } S}$, and the LDOM is directly proportional to the mean power radiated by a harmonically driven point dipole:

$$\rho_\omega(\vec{r}) \equiv \rho_{\omega,\text{free space}} \frac{\overline{W}(\vec{r})_{\text{flowing through } S}}{\overline{W}_{\text{emitted,free space}}},$$

where $\overline{W}(\vec{r})_{\text{flowing through } S}$ *is a physical quantity that can be directly measured in an experiment*.

Our discussion shows that despite the prevailing view, concepts of the LDOM and DOM can easily be defined and understood for a finite, 3D, open cavity filled with a generic linear and isotropic dielectric material in terms of the *emission rates of a single-point dipole*, and not extended sources, as is normally done in lower-dimensional systems, where the symmetry of the source is usually exploited to reduce the complexity of the problem. By extended source here we mean a dipole layer that may be found inside 1D multilayer stacks [1–3,6] or a dipole current that runs along an infinitely long wire in the so-called “forest of rods” [4,5]. In this latter context, Fussell *et al.* [18] have recently calculated the Green’s dyadic for a 2D photonic crystal composed of a finite cluster of circular cylinders having infinite length, in the presence of a pointlike source. Although this represents remarkable progress from a computational point of view, the potential to obtain strong inhibition of the dipole emission in this class of photonic crystals is limited by the absence of a complete 3D photonic band gap. While the absence of a second and/or third dimension can certainly render the problem easier to be solved analytically or numerically, some caution should be exercised in extending the meaning of intrinsically three-dimensional quantities, such as the LDOM, to lower-dimensional problems. We will expand on this subject separately. Finally, when the dielectric is nonabsorbing, both the LDOM and DOM become directly measurable physical quantities by monitoring the power radiated by a point dipole outside the surface S.

Finally, a note about electric multipole and magnetic dipole sources. In this work we have explicitly referred to the case of a simple point electric dipole. Should the source consist of an electric quadrupole (dipole forbidden), for example, or even a magnetic dipole, things then appear to become more complex from a computational point of view. Conceptually, however, the problem retains its simplicity. In fact, our results suggest that the LDOM may be generally defined as

$$\rho_\omega(\vec{r}) \equiv \rho_{\omega,\text{free space}} \frac{\overline{W}_{\text{emitted}}(\vec{r})}{\overline{W}_{\text{emitted,free space}}}$$

where $\overline{W}_{\text{emitted}}(\vec{r})$ is the mean power emitted by the point source, regardless of its specific nature. What is also remarkable is that while in the case of an electric dipole the LDOM can be directly linked to the imaginary part of the Green’s dyadic [see Eq. (10)], in other cases the connection with the Green’s dyadic is not obvious, and its application should be explored on a case-by-case basis, depending on the particular nature of the source. Of course, whether a connection to a Green function can be made or not is only relevant from a mathematical point of view. Such a connection, or lack thereof, would take nothing away from the simplicity of the concept that we advance here: that for finite, 3D structures the LDOM can always be thought as being proportional to the ratio between the power emitted by a point source located inside the cavity and the power emitted by the same point source in free space.

In conclusion, we have shown that the physical concepts of the LDOM and DOM can be extended to 3D structures of finite size without conceptual difficulties. The results suggest that the LDOM is directly linked to the power emitted by a *point* source inside the cavity, regardless of the particular nature of the source. On the other hand, while the extension to 3D presents us with few conceptual obstacles, calculation of the Green’s dyadic function found in Eq. (6) for the electric-dipole case or the calculation of the power emitted by the point source in the most general case is a task that can only be accomplished numerically, an undertaking that takes nothing away from the simplicity of the underlying concepts of the DOM and LDOM.

ACKNOWLEDGMENTS

G.D. thanks the Army Research Laboratory-European Research Office for partial financial support (Contract No. N62558-03-M-0019). M.C. also thanks Army Research Laboratory-European Research Office for partial financial support.

[1] P. T. Leung, S. Y. Liu, and K. Young, Phys. Rev. A **49**, 3057 (1994).
[2] J. M. Bendickson, J. P. Dowling, and M. Scalora, Phys. Rev. E **53**, 4107 (1996).
[3] G. D'Aguanno *et al.*, Phys. Rev. E **64**, 016609 (2001).
[4] A. A. Asatryan *et al.*, Phys. Rev. E **63**, 046612 (2001).
[5] D. Felbacq and R. Smaali, Phys. Rev. B **67**, 085105 (2003).
[6] A. Settimi *et al.*, Phys. Rev. E **68**, 026614 (2003).
[7] E. N. Economou, *Green's Functions in Quantum Physics* (Springer-Verlag, Berlin, 1983).
[8] P. Sheng, *Introduction to Wave Scattering, Localization, and Mesoscopic Phenomena* (Academic, San Diego, 1995).
[9] P. Dennery and A. Krzywicki, *Mathematics for Physicist* (Dover, New York, 1967).
[10] It is out of the scope of this work to propose a "noncanonical" expansion of the Green's function over the cavity "modes." This approach has been followed, for example, in Refs. [1,6] for 1D systems. Our aim is to link the notions of the LDOM and DOM to physically measurable quantities.
[11] Let V be a closed region of space bounded by a regular surface S and let $\vec{P}$ and $\vec{Q}$ be two vectors functions of position which together with their first and second derivatives are continuous throughout V and on the surface S; the vector analog of Green's first identity is $\int_V(\vec{\nabla}\times\vec{P}\cdot\vec{\nabla}\times\vec{Q}-\vec{P}\cdot\vec{\nabla}\times\vec{\nabla}\times\vec{Q})dV =\int_S(\vec{P}\times\vec{\nabla}\times\vec{Q})\cdot\hat{n}dS$, where $\hat{n}$ is the unit normal to dS oriented outward respect to the close surface S.
[12] Kevin G. Sullivan and Dennis G. Hall, J. Opt. Soc. Am. B **14**, 1149 (1997).
[13] W. C. Chew, *Waves and Fields in Inhomogeneous Media* (Van Nostrand Reinhold, New York 1990).
[14] J. A. Stratton, *Electromagnetic Theory* (McGraw-Hill, New York, 1941).
[15] E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).
[16] Yong Xu, Reginald K. Lee, and Ammon Yariv, Phys. Rev. A **61**, 033807 (2000).
[17] Christian Hermann and Ortwin Hess, J. Opt. Soc. Am. B **19**, 3013 (2002).
[18] D. P. Fussel *et al.*, Phys. Rev. E **67**, 045601 (2003).