Resonant Scattering Characteristics of Homogeneous Dielectric Sphere

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Abstract—In the present article the classical problem of electromagnetic scattering by a single homogeneous sphere is revisited. Main focus is the study of the scattering behavior as a function of the material contrast and the size parameters for all electric and magnetic resonances of a dielectric sphere. Specifically, the Padé approximants are introduced and utilized as an alternative system expansion of the Mie coefficients. Low order Padé approximants can give compact and physically insightful expressions for the scattering system and the enabled dynamic mechanisms. Higher order approximants are used for predicting accurately the resonant pole spectrum. These results are summarized into general pole formulae, covering up to fifth order magnetic and forth order electric resonances of a small dielectric sphere. Additionally, the connection between the radiative damping process and the resonant linewidth is investigated. The results obtained reveal the fundamental connection of the radiative damping mechanism with the maximum width occurring for each resonance. Finally, the suggested system ansatz is used for studying the resonant absorption maximum through a circuit-inspired perspective.

Index Terms—Lorenz–Mie Theory; Light Scattering; Mie Coefficients; Padé Approximants; Radiative Damping

I. INTRODUCTION

A n over-centennial and, perhaps, one of the most studied canonical problem encountered in electromagnetics is the scattering of electromagnetic radiation by a single sphere [1]–[3]. Its importance still resonates between classical and modern disciplines, such as RF engineering and nanotechnology, continuously delivering novel engineering achievements for a broad range of applications [1], [4], [5]. This problem is widely used either as a testbed for different material and morphological induced effects [1], [4], [6] or for expanding our physical intuition about scattering aspects, such as non-radiating states, Fano resonances, and anomalous scattering, naming only a few [1], [7], [8]. All of the aforementioned occurring aspects become visible by the careful study and interpretation of the scattering processes on a simple sphere.

The electromagnetic resonant perspectives of a sphere can be described as a system for which the physical processes are encapsulated and described by the Mie coefficients. In order to reach a more complete picture regarding the resonant perspectives of a relatively small, homogeneous sphere, we revisit this problem, utilizing an alternative system ansatz for the Mie coefficients based on the recently introduced Padé approximant technique [9], [10].

The aim of this article is to propose and discuss a systematic way for studying the fundamental resonant scattering aspects caused by a subwavelength sphere. We concentrate our main efforts in exposing the resonant conditions and their size dependencies of the lowest multipole (dipole, quadrupole, etc.) magnetic and electric resonances. In parallel, the effects of the radiative damping mechanism on the scattering process are revealed, especially about the resonant width and the absorption maximum of each mode. These, non-trivial, aspects reinforce our understanding regarding the light scattering/absorptive characteristics of a sphere, being readily expandable for other canonical-shaped geometries.

This work is divided into four general parts. Section II discusses some observations derived directly from the analysis of the Mie coefficients. Section III presents compact expansions of the main coefficients in an attempt to extract physical intuition through the Padé approximants. Section IV discusses more accurate pole conditions, which utilize higher order Padé expansions; in addition, the accuracy of the proposed pole conditions and the widths of the Mie resonances are discussed. Finally, Section V presents a circuit-inspired analysis, revealing the importance of the radiative damping term to the overall scattering process. Conclusions and appendices complete the discussion about the proposed perspective. The reader who wishes to extract only the analytical pole conditions formulas regarding the electric and magnetic resonances of a dielectric sphere can skip the analysis sections and go directly to the tables provided in Section IV.

II. MIE–SCATTERING PRELIMINARIES

Let us begin by briefly introducing the mathematical model describing the electromagnetic scattering by a small homogeneous sphere of radius a illuminated by a monochromatic plane wave ($e^{-i\omega t}$); an extensive review can be found in [2]. It is well known that the scattered fields can be decomposed into set of spherical harmonics, whose complex amplitudes are given by the $a_n$ and $b_n$ Lorentz–Mie coefficients [1] viz.,

$$a_n = \frac{m^2 j_n(mx) j''_n(x) - \mu_c j_n(x) j'_n(mx)}{m^2 j_n(mx) [x h_n^{(1)}(x)]' - \mu_c j_n(mx) j'_n(mx)} \quad (1)$$

$$b_n = \frac{\mu_c j_n(mx) j''_n(x) - j_n(x) j'_n(mx)}{\mu_c j_n(mx) [x h_n^{(1)}(x)]' - h_n^{(1)}(x) [x j_n(mx)]'} \quad (2)$$

where $x = ka$ is the free space size parameter, $m = \frac{k}{\sqrt{\epsilon_c \mu_c}}$ is the material contrast, and $\epsilon_c = \epsilon_1/\epsilon$ and $\mu_c = \mu_1/\mu$ are the permittivity and permeability contrasts, respectively.
These $a_n$ and $b_n$ terms are generally complex and demonstrate the electric and magnetic multipole contributions to the overall scattering process [12]. Usually, most of the far field scattering processes are quantified through these two coefficients. Note that these coefficients can be found in the literature by many names, i.e., TM and TE modes, E-wave and H-wave coefficients [11], [12] etc. Here we will refer to them as electric ($a_n$) and magnetic ($b_n$) multipole terms, having for each value of $n = 1, 2, 3, \ldots$ names such as dipole ($n = 1$), quadrupole ($n = 2$) and so on. Similarly, the internal fields can be quantified through the $c_n$ and $d_n$ coefficients, viz.,

$$d_n = \frac{\mu_cm_j(x) \left[ xh_n^{(1)}(x) \right]'}{m^2j_n(mx) \left[ xh_n^{(1)}(x) \right]'} - \mu_cm_h^{(1)}(x) \left[ mxj_n(mx) \right]'$$

(3)

$$c_n = \frac{\mu_cm_j(x) \left[ xh_n^{(1)}(x) \right]'}{\mu_cm_j(mx) \left[ xh_n^{(1)}(x) \right]'} - h_n^{(1)}(x) \left[ mxj_n(mx) \right]'$$

(4)

where $d_n$ and $c_n$ corresponds to the electric and the magnetic multipole term, respectively.

All coefficients, i.e., Eqs. (1), (2), (3), and (4), can rigorously describe the material and size dependences of the scattering and internal fields. However their complex structure prevent us from obtaining a simple physical interpretation on their resonant behavior. Therefore, a question arises: how can we extract any physically intuitive information regarding their size- and material-dependent characteristics?

For the quasistatic limit ($x \rightarrow 0$) these terms are usually expanded in a Taylor (Maclaurin) series [12], revealing some interesting perspectives e.g., the Rayleigh scattering limit [11]. The series expansion of Eqs. (1) and (2) for small $x$ reads

$$a_1^T \approx -\frac{2}{3} \frac{\varepsilon_c - 1}{\varepsilon_c + 2} x^3 - i \frac{1}{5} \frac{\varepsilon_c^2(1 + \varepsilon_c) - 6\varepsilon_c + 4}{(\varepsilon_c + 2)^2} x^5 + O[x]^6$$

(5)

$$b_1^T \approx -\frac{2}{3} \frac{\mu_c - 1}{\mu_c + 2} x^3 - i \frac{1}{5} \frac{\mu_c^2(1 + \varepsilon_c) - 6\mu_c + 4}{(\mu_c + 2)^2} x^5 + O[x]^6$$

(6)

$$d_1^T \approx \frac{3 \varepsilon_c + 2}{10} + \frac{3}{10} \frac{\mu_c(\varepsilon_c^2 + 4\varepsilon_c) + 5\varepsilon_c - 10}{(\varepsilon_c + 2)^2} x^2 + O[x]^{5/2}$$

(7)

$$c_1^T \approx \frac{3\mu_c}{(\mu_c + 2)\sqrt{\mu_c\varepsilon_c}} + O[x]^{3/2}$$

(8)

Indeed, many intuitive results are visible in this simple system expansion, such as the electrostatic polarization enhancement condition ($\varepsilon_c = -2$), also known as Fröhlich frequency [11], [13]. The external coefficients suggests a dual behavior, i.e., invariance with respect to interchanging $\varepsilon_c$ and $\mu_c$. However, the same does not apply directly for the internal ones. For instance, the $c_n$ coefficient possesses two resonant conditions, $\mu_c = -2$ and $\varepsilon_c = 0$, while $d_n$ only for $\varepsilon_c = -2$.

In this work we focus on the resonant conditions and the physical mechanisms for a small, magnetically inert ($\mu_c = 1$), homogeneous sphere. Fig. 1 depicts the resonant scattering extinction spectrum of a lossless sphere as a function of the material and size parameters. Several resonances occur for both positive and negative permittivity values. Note that the scattering efficiency depends on $a_n$ and $b_n$, i.e., $\sigma^2_\text{ext} \propto \sum_{n=1}^{\infty} (\Re\{a_n\} + \Re\{b_n\})$. Based on the values of permittivity we categorize the resonances as plasmonic ($\varepsilon(\omega) < 0$), and dielectric ($\varepsilon(\omega) > 0$). As we can see in Fig. 1 the scattering spectrum reveals a wealth of resonances in both regions with several qualitative differences. For example the plasmonic resonances may appear even for very small spheres.

As a reference, Fig. 2 depicts the real and imaginary values of both external and internal Mie coefficients for a given size parameter ($x = 0.75$). One observes that both external and internal coefficients exhibit maximum values in both negative and positive permittivity regions. Although the external coefficients are bounded, i.e., they reach a maximum unity amplitude for the lossless case, the internal coefficient are unbounded to a specific value. Hence they may exhibit a qualitatively different resonant lineshape than the external ones.

A usual treatment for extracting the resonant conditions is derived by observing that Eq. (1) and (2) can be decomposed in a rational form $\frac{a_n}{\varepsilon_c + s_n}$, where $r_n$, $s_n$ are real functions for the lossless case [14]. The approach in [8], [15] is that each $r_n$ and $s_n$ term is expanded in a Taylor series, enabling in such a way a pole condition study. However, the Taylor expansions might suffer from a slow convergence, especially near the poles of the system. Similar rational expansions were given in [16] for a quick numerical evaluation of the Mie coefficients for small spheres. Furthermore, for the case of optically large spheres several asymptotic formulas have been also derived in [17].

In order to find a suitable coefficient expansion with which

Fig. 1. The scattering efficiency of a lossless dielectric sphere, as a function of the material permittivity and the size parameter. There are two visible regions: the plasmonic region for $\varepsilon < 0$ and the dielectric region ($\varepsilon_c > 0$). In both regions vibrational resonances occur. The dielectric resonances are geometrical induced resonances, of either magnetic or electric origin, respectively. The plasmonic resonances are due to the free oscillating charges, thus characterized as electric. The inset image depicts (only a few of) the main plasmonic resonances residing in region $-3 < \varepsilon(\omega) < -1$. 


Fig. 2. The external scattering coefficients \( a_1 \) and \( b_1 \) (up), and the internal coefficients \( d_1 \) and \( c_1 \) for \( x = 0.75 \) as a function of the permittivity (lossless case). The absolute value of the external coefficients cannot exceed unity due to passivity while the amplitude of the internal coefficients is not bounded.

to unlock the material and size dependencies we utilize an alternative approximative perspective based on the Padé approximants for the Mie coefficients, recently introduced in [10]. Earlier, Padé-like expansions have been given for certain of the scattering characteristics, e.g., fixed material parameters [18] or small spheres [19], [20]. There, however, the focus was not in identifying neither the resonant conditions nor the physical processes.

The Padé approximants are a special type of rational (approximative) expressions constructed by expressing a function in a rational form and expanding each of the rational terms to the pole condition up to the fifth order, we obtain

\[
\varepsilon_c = -2 - \frac{12}{5} x^2 (1 + 3 x^2) - 2 i x^3 (1 + \frac{7}{5} x^2) + \ldots
\]  

(11)

In a similar manner each term to the pole condition can be recognized, i.e., static (\(-2\)), dynamic (\(-\frac{12}{5} x^2\)), and damping term (\(-2 i x^3\)), respectively. Notice that a similar but somewhat less accurate condition can be readily found in \[11\] Ch.12, p.329.

As for the magnetic coefficient, the \([5/5]\) Padé \( b_1 \) expansion is

\[
b_1^p \approx -i \frac{\varepsilon_c - 1}{45} \varepsilon_c^5 \left( 1 + \frac{1}{25} (5 - 2 \varepsilon_c) x^2 + |x|^4 - i \frac{1}{45} (\varepsilon_c - 1) x^5 \right)
\]

(12)

with the truncated term to be

\[
|x|^4 = -\frac{2 \varepsilon_c^2 + 100 \varepsilon_c - 125}{2205} x^4
\]

(13)

Expression (12) gives a resonant condition yielding to the value

\[
\varepsilon_c = -2.07 + \frac{10.02}{x^2} + 1.42 x^2 - 2 i x (1.06 - 0.77 x^2)
\]

(14)

with accuracy up to the second decimal. However, not every pole of the Padé expansions correspond to an observed pole [9]. This is happening for three reasons. The Mie terms are described by a set of complex functions, hence all the poles exist \textit{a-priori} in the complex plane. These complex poles, known also as \textit{natural frequencies} [12], may exhibit large imaginary parts. Thus their physical observation is extremely difficult. Secondly, the Padé approximants can give some intrinsic, non-existent poles [24] to the system. Finally, some of the poles can be mutually canceled by system’s zeros, and therefore cannot be observed. For the above reasons we will restrict our analysis only to physically observable poles, verified by the Mie spectrum.

The condition described in Eq. (14) reveals certain interesting phenomena regarding the nature of the magnetic resonances enabled on a dielectric sphere. First, there is an inverse square dependence, showing that the magnetic resonance for small spheres can be reached only for huge contrast materials, making very difficult its observation for very small spheres. Secondly, there is a constant term, slightly regulating the real part of the pole condition. Lastly, the radiative damping process of a magnetic dipole does not follow the same volume dependence \((x^3)\) observed in the previous electric dipole case (Eq. (11)), but rather a linear \(x\) dependence. Actually, a closer look reveals that this dependence in not exactly linear, exposing a plateau for size parameters around 0.5 [10].
The Padé expansions $[0/3]$ and $[0/5]$ of the internal coefficients read
\[
d_1^P \approx \frac{3}{(\varepsilon_c + 2) \left( 1 - \frac{1}{10} \varepsilon_c^2 + 9 \varepsilon_c - 10 \varepsilon_c^2 - \frac{1}{3} \varepsilon_c + 1 \varepsilon_c^2 \right)}
\]
(15)
\[
e_1^P \approx \frac{1}{\sqrt{\varepsilon_c} \left( 1 + \frac{1}{6} (1 - \varepsilon_c^2) x^2 + |x^4| - i \frac{1}{10} (\varepsilon_c - 1)^2 x^2 \right)}
\]
(16)
where $|x^4| = \frac{1}{120} (\varepsilon_c^2 - 6 \varepsilon_c + 5) x^4$. Following the same pole analysis as above we obtain two resonances for the $d_1$ coefficient, one of which follows exactly the value of Eq. (11) for the external $a_1$ coefficient, while the other reads
\[
\varepsilon_c = -7 + \frac{10}{x^2}
\]
(17)
This condition is a very rough approximation for the electric resonances for $\varepsilon_c > 0$. The accurate evaluation of this pole requires a higher order Padé expansion and its form will be extracted in Section V. Notice that also this pole exhibits an inverse square size resonant condition, similar to the magnetic resonances.

Expression (16) gives three poles, two of which are spurious, while the remaining one is at $\varepsilon_c = 0$. This pole condition exists for every $c_n$ coefficient, since in every expansion there is a term of the form $\frac{1}{\varepsilon_c^n}$, where $n$ is the order of the coefficient. In other words the $c_n$ coefficient experiences a epsilon-near-zero (ENZ) resonance for every multipole term. ENZ behavior is closely related to what it is called perfect magnetic conductor (PMC), and it is conceptually used for light trapping [6] and shape-invariant resonant cavities [25]. Surprisingly, this is not true for the mu-near-zero case, since the $d_n$ coefficients are not dual to $c_n$ in terms of the material parameters ($a_n$ and $b_n$ are dual, as seen from the expansion Eqs. (5) and (6)).

**Electric resonances for $\varepsilon_c > 0$**

The above analysis made clear that small-order Padé expansions provide us with simple expressions for all dipole $a_1$, $b_1$, $d_1$, and $c_1$ Mie coefficients and their corresponding pole conditions. The Padé approximants are able to predict the zeros and the poles of this system. In order to obtain more system poles for $a_1$ in the $\varepsilon_c > 0$ regime, higher order approximants should be used. However, the Padé expressions of these expansions are lengthy, hence will be omitted.

To start with, the $[7/2]$ expansion of the $a_1$ coefficient gives in total four poles, one corresponding to the plasmonic case, two non-observable double complex roots, and a fourth yielding the following expression
\[
\varepsilon_c^{[7/2]} = -14.5 + \frac{22.5}{x^2} + i \frac{77.778}{x} + ...
\]
(18)
where the superscript indicates the order of the used Padé approximant.

This first, very rough pole condition, exhibits the same inverse square size dependence observed in Eq. (17). Here the radiative damping term is extremely large, an indication that a more accurate, higher order expansion is needed. To do so we increase the order of the numerator, keeping the denominator order as low as possible. By this, straightforward, and numerically convenient heuristic method we are able to identify more accurately any of the pole conditions. After several iterations a quite accurate pole condition for the electric resonance occurs from a $[19/2]$ Padé expansion, converging to the value
\[
\varepsilon_c^{[19/2]} = -1.99546 + \frac{20.193}{x^2} - 2.05137 x^2 + ...
\]
(19)
An interesting remark can be drawn here; the estimated radiative damping term (afflicting the absorption maximum, see Section V) gives both an $x$ and $x^3$ dependence. However the first linear term is a numerical artifact, converging quickly to a close-to-zero value. The the $x^3$ term converges close to two, resembling the plasmonic radiative damping term. This is a reasonable result since both resonances are of electric dipole nature. Eq. (19) exhibits a linear imaginary term, two orders of magnitude smaller than the magnetic, demonstrating some fundamental differences between the electric and the magnetic dipole resonances on a sphere.

**Resonant Lineshape**

By plotting the compact expressions given by Eqs. (9) and (12) versus the Mie coefficients $a_1$ and $b_1$ (Fig. 3), one observes that even for relatively large spheres ($x = 0.75$) the resonant lineshape almost coincides with the exact one obtained by the full Mie solution. The Padé approximants can be used instead the complex Mie terms to emulate the exact physical behavior of the scattering sphere. This is an attractive
feature where simple and physically intuitive models are needed, e.g., homogenization models for composite materials and surfaces [4].

IV. POLE CONDITIONS WITH INCREASED ACCURACY

Throughout the aforementioned analysis it has become clear that low order Padé approximants can be used for extracting intuition regarding the physical mechanisms of the system. By using higher order approximants and applying the same heuristic method described above, more accurate pole conditions can be extracted for all resonances. However, these approximants are lengthy and will be omitted. Details about the pole conditions can be found in Appendix B. Table I contains the converged formulas of the first resonances for the first five \((n = 1, 2, 3, 4, 5)\) magnetic \(b_n\) coefficients, and the first four electric \(a_n\) coefficients for the dielectric case with parametric values listed in Table II.

The above generalized conditions give the value of the complex permittivity value required for the system to resonate. These expressions can be readily used as design rule-of-thumb equations. The pole conditions of the electric resonances, found in Table II, second equation and Eq. (20), reveal a similar but not identical imaginary part; only the \(a_1\) (dipole resonance) exhibits the same \(x^3\) imaginary part dependency. This minor point describes that the behavior of the electric resonances in the plasmonic and dielectric region is close but not completely identical. Note that the \(p_n\) coefficients correspond to the first root of the \(n\)-th spherical Bessel function of the first kind \((J_n(p_n) = 0)\). The dots in Table II denote that the higher order \(t_n\) values can be extracted in a similar way for resonances above \(n = 4\).

TABLE I

POLAR FORMULAE OF THE DIELECTRIC RESONANCES FOR \(n = 1, 2, 3, \ldots\)

\[
\varepsilon_p[n] = - \frac{2}{n^2 - 1} + \left( \frac{p_n}{x} \right)^2 - i \frac{2}{(2n - 1)!} x^{2n - 1} (1 - t_n x^2)
\]

\[
\varepsilon_{an}^\text{dielectric} = - \frac{2}{n} + \left( \frac{p_{n+1}}{x} \right)^2 - i \frac{2}{(n(2n - 1)!!)} x^{2n + 1} \left( 1 - \frac{t_{n+1} x^2}{2} \right)
\]

TABLE II

VALUES OF USES PARAMETERS FOR THE \(b_n\) AND \(a_n\) POLE RESONANCES

\begin{tabular}{cccccc}
\(n\) & 1 & 2 & 3 & 4 & 5 \\
p_n & \(\pi\) & 4.4934 & 5.7634 & 6.9879 & 8.1428 \\
t_n & 0.6960 & 0.2508 & 0.1560 & 0.1166 & \ldots \\
t_n' & 0.0040 & 0.0954 & 0.3461 & 1.3923
\end{tabular}

Finally, a general resonant condition for the plasmonic resonances \((\varepsilon(\omega) < 0)\) reads

\[
\varepsilon_{\text{plasm}}^{\text{an}} = \frac{n}{n + 1} + \frac{2(n+1)(n+1)}{n^2(2n-1)(2n+3)} x^2 - i \frac{n}{n(2n-1)!!} x^{2n+1}, \ n = 1, 2, \ldots 
\] (20)

Error analysis

The accuracy of the obtained formulas with respect to the full Mie resonant position is depicted in Fig. 4 for the first electric resonances in the plasmonic and dielectric case. Specifically, an pole condition with more than 1% accuracy can be achieved up to \(x \approx 0.6\) for the plasmonic case. This value is obtained by considering only the real part of Eq. (20). By introducing the imaginary part and evaluating the absolute value of Eq. (20) the accuracy is increased; the error reach a 3% value for \(x \approx 0.7\) and drops, expanding the accurate region up to \(x \approx 0.95\).

For the dielectric case the second order term gives accurate predictions for sizes up to \(x \approx 0.8\). Similar results regarding the magnetic coefficient can be found in [10], where the pole condition (Table I first equation) exhibits less than 1% the error for size parameters up to 0.6.

Width of the resonances

The proposed Padé expansion can also provide information about the linewidth of the resonances. As we can see in Fig. 3 the approximated line shape can be very close to the analytical one even for relatively large particles, i.e., up to \(x = 0.75\). This feature can be particularly useful for evaluating the linewidth of the scattering process. It is known that the full width half maximum (FWHM) scattering linewidth, i.e., \(|\alpha_1|^2 = \frac{1}{2}\) for the electric dipole, is restricted by the intrinsic material losses [27], [28].

The partial extinction efficiency of each electric and magnetic term is proportional to the real part of each coefficient, i.e., \(\sigma_e^{\text{ext}} \propto \Re\{\alpha_n\}\) and \(\sigma_m^{\text{ext}} \propto \Re\{b_n\}\). Let us simplify the analysis by considering only the first electric extinction cross section. For the lossless case the extinction linewidth reads

\[
\Delta \varepsilon(\omega) = 4x^3
\] (21)
revealing that the linewidth is twice the radiative damping term, explaining in a way the fact that radiative damping affects the scattering strength, linewidth and, consequently, the radiative decay rates \((29)\). This result can be generalized for every multipole term through the imaginary part of conditions in Table 1 and \((20)\), respectively. For example the width of the first three plasmonic resonances is of the order \(x^3, x^3\), and \(x^3\), respectively. Note that higher order modes experience a very narrow bandwidth, and hence are very difficult to be tracked, as also seen in Fig. 1.

The previous result has a fundamental connection with the bandwidth bounds derived for an electrically small resonator, namely with the quality factor of an electrically small antenna (ESA), expressed as \(Q_{ESA} \approx \frac{1}{\sigma_{ext}} + \frac{1}{\epsilon} \) \([30]\). This bound is derived from the decomposition of the antenna secondary field into a set of spherical harmonics \([31]-[33]\). In our analysis, the linewidth (BW) of a very small plasmonic scatterer is of the order of \(x^3\), since only the electric dipole term is present. Similarly, for a small dielectric resonator (magnetic dipole) the linewidth is \(x\). Assuming \(Q \approx BW\), the \(Q_{ESA}\) value can be reached qualitatively from the combination of the first electric and the first magnetic resonance. Consequently, the decomposition of the secondary scattering field by an arbitrary shaped scatterer into spherical harmonics can give a straightforward hint about its resonant bandwidth.

Let us now assume material losses, i.e., \(\varepsilon(\omega) = \varepsilon'(\omega) + i\varepsilon''(\omega)\). In this case the extinction linewidth is a function of both real and imaginary part of permittivity. The maximum value of the extinction cross section as a function of \(\varepsilon'\) can be found by evaluating the position on which the first partial derivative is zero, i.e., \(\partial\sigma_{ext}/\partial\varepsilon' = 0\). This procedure gives that the resonant linewidth, with respect to the \(\varepsilon'\) is

\[
\Delta\varepsilon' = 2\varepsilon'' + 4x^3
\]

(22)
demonstrating that total linewidth is a superposition between the material losses and the radiative damping. Obviously for zero material losses Eq. (22) yields to the lossless case of Eq. (21).

These material-model independent results demonstrate that not only the material losses but the radiative damping mechanism is responsible of the width of the scattering spectrum. Note that the absorptive linewidth exhibits a more complex behavior as a function of the material losses. Hence, in the following section we will study how the scattering and material losses affect the overall absorptive characteristics.

V. CIRCUIT-INSPIRED ANALYSIS OF THE SCATTERING PROCESS: MAXIMIZING ABSORPTION EFFICIENCY

To this point, the Padé-expanded Mie coefficients exhibit reduced complexity, revealing a set qualitative characteristics about the underlying physical mechanisms. In other words we exchanged mathematical exactness for physical intuition. In this section the aim is to exploit further the Padé expansions for finding the necessary conditions that maximize the absorption efficiency of a small homogeneous sphere.

By carefully examining the approximated Mie coefficients, one can rewrite them in the following simple form e.g.,

\[
d_1 = \frac{Z_R}{Z_R + Z_L} = \frac{1}{1 + \frac{2i}{\varepsilon''}}
\]

(23)

where the impedances are

\[
Z_R = 2\varepsilon''x^3 - 2i(\varepsilon' - 1)x^3 = R_R + iX_R
\]

(24)

and

\[
Z_L = 3(\varepsilon' + 2) - \frac{9}{5}(\varepsilon' - 2)x^2 + i3\varepsilon''\left(1 - \frac{3}{5}x^2\right)
\]

(25)

Arguably, \(Z_L\) possesses a non-passive character (\(R_L < 0\)) for certain size and material combinations, a fact that has been identified in \([34]\). The quantity \(\frac{Z_L}{Z_R}\) yields to the value of \(iX_L\), known also as reactance \([14]\). In this section we try to extract the necessary conditions for maximizing the absorption achieved for each coefficient.

In the case of a small plasmonic sphere \((\varepsilon' < 0, \varepsilon'' > 0)\), the electric dipole resonance is dominating, leading to the following expressions for the partial extinction, scattering, and absorption efficiency

\[
\sigma_{ext} = \frac{6}{x^2} \frac{R_R(R_R + R_L) + X_R(X_R + X_L)}{(R_R + R_L)^2 + (X_R + X_L)^2}
\]

(26)

\[
\sigma_{sca} = \frac{6}{x^2} \frac{R_R^2 + X_R^2}{(R_R + R_L)^2 + (X_R + X_L)^2}
\]

(27)

\[
\sigma_{ext} - \sigma_{sca} = \sigma_{abs} = \frac{6}{x^2} \frac{R_R R_L + X_R X_L}{(R_R + R_L)^2 + (X_R + X_L)^2}
\]

(28)

Similar to circuit theory, the absorption efficiency is maximized when the partial derivatives with respect to \(R_R\) and \(X_R\) are simultaneously zero. Alternatively,

\[
\frac{\partial\sigma_{abs}(R_L, X_L)}{\partial R_L} = 0, \text{ and } \frac{\partial\sigma_{abs}(R_L, X_L)}{\partial X_L} = 0
\]

(29)

After some algebra, the above expressions are mutually satisfied when

\[
R_R = R_L, \text{ and } X_R = X_L
\]

(30)

Since \(Z_R\) is primarily attributed to radiative damping mechanisms \((x^3)\) and \(Z_L\) incorporate constant (static) and dynamic \((x^3)\) terms it is clear that the absorption maximum takes place when the two internal mechanisms are matched \([35]\). For \(Z_R = Z_L\) both impedances are equivalent and Eq. (23) yields to the real value of \(\sigma^1 = \frac{1}{2}\), hence this is the amplitude for which the absorption efficiency is maximized for every coefficient. This value stresses the fact that the absorbed power can be \(\propto |\sigma^1|^2 = \frac{1}{4}\) on its maximum value \([36]\).

By solving the above matching condition we obtain

\[
\varepsilon' = -2 - \frac{12}{5}x^2 + ...
\]

(31)

\[
\varepsilon'' = 2x^3 + ...
\]

(32)

Surprisingly, condition \((31)\) fits exactly the pole condition (real part of Eq. (11)) for the first electric Mie coefficient,
while condition (22) coincides with the radiative damping term (imaginary part of Eq. (11)).

The same analysis can be followed for any multipole term e.g., the absorption maximum occurring for the first magnetic coefficient is approximately at 2x; the radiative damping mechanism affects not only the width of the resonances but also the amount of losses required for maximum resonant absorption. This fact can be exploited for inverse-scattering purposes, where the determination of the level of losses can be extracted by the level of the absorption efficiency, since the maximum of the latter occurs for losses matching the radiative damping.

VI. Summary

This article presented the use of Padé approximants as an alternative system ansatz for the Mie coefficients. This perspective provides insights into the scattering mechanisms, i.e., static, dynamic, and radiative damping processes. Additionally, the higher order Padé approximants are used for the extraction of accurate pole condition formulas for every resonance. The accuracy of the proposed formulas is relatively high for size parameters up to 0.5 for all cases.

It has been proved that the overall scattering characteristics, such as the resonant linewidth and the absorption maximum, are affected by the radiative damping and dissipative mechanisms. The intrinsic resonant absorption limitations were obtained utilizing a simple, circuit-inspired analogy; the position and strength of the optimum absorption is a manifestation of the matching between the radiative and absorptive processes.

We foresee that a similar, Padé-based analysis can be implemented for various canonical problems, such as cylinders and core-shell spheres, where simple resonant scattering conditions may facilitate a deeper and more physically intuitive interpretation of their response. Similarly, the existence of analytical resonant conditions may also support the reverse material engineering process, where natural or artificial materials can be optimally used for the design of simple or complex light controlling concepts and applications.

APPENDIX A

Simple Padé Expansions of spherical Bessel, Hankel, and Riccati–Bessel/Hankel Functions

In this section we give the simple Padé expansions of some necessary functions, such as the spherical Bessel functions and their derivatives. These terms can be readily used for a simple estimation of the a_j and b_j coefficients. Notice that the Maclaurin expansion of each numerator and denominator term of a rational expression is not always equivalent with the Padé expansion of the same function.

Alternative series expansions for the same functions can be found in classical textbooks ([12] Ch.7.4) and [31] Ch.9.1). In these expansion at least one pole and one zero is visible. Also similar expressions were given by Wiscombe [16] as a computationally efficient way of evaluating the Mie coefficients for small size parameters. Note that the spherical Bessel and Riccati–Bessel functions are purely real for the approximated terms, while Hankel and Riccati–Hankel are complex functions. A physical interpretation can be given to the above expressions, since spherical Bessel functions are real and resemble a standing wave behavior, while Hankel functions are generally complex, representing traveling waves [37].

APPENDIX B

Accurate Poles for the b_n and a_n coefficients

In this section the numerical values obtained by the heuristic method described above will be presented with accuracy up to the 4th decimal digit. The subscript denotes the Mie coefficient for which the pole is extracted, e.g., b_1, b_2, etc. The superscript denotes the order of the Padé approximant used. Tables IV and V present the pole conditions of the first five b_n, and the first four a_n coefficients, respectively.

| TABLE II | Padé approximants of j_n or h^{(1)} and their derivatives |
|-----------|----------------------------------------------------------|
| j_1(x) ≈ x/3 (1 + x^2) | j_2(x) ≈ x^2/15 (1 + x^2) |
| h_1^{(1)}(x) ≈ −i(1 + 1/2 + x^2) | h_2^{(1)}(x) ≈ −i(1 + 1/2 + x^2) |

|x_j1(x)|' ≈ 2x/3 (1 + x^2) | [x_j2(x)]' ≈ x^2/5 (1 + 5/4 + x^2) |

| TABLE III | Pole conditions of the first five b_n coefficients |
|-----------|----------------------------------------------------------|
| b_1^{[27/2]} = −2 + (17/6) x^2 + 1.6960x^2 − 1.1232x^4 + ... |
| b_2^{[29/2]} = −2 + (4.4934/3) x^2 + 0.2497x^2 + 0.1289x^4 + ... |
| b_3^{[31/2]} = −2 + (5.7634/3) x^2 − 0.0351x^2 − 0.0119x^4 + ... |
| b_4^{[33/2]} = −2 + (6.9879/7) x^2 − 0.0119x^2 − 0.0010x^4 + ... |
| b_5^{[35/2]} = −2 + (8.1827/9) x^2 − 0.0055x^2 − 0.0002x^4 + ... |

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