All spectrum identities for periodic metamaterials

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***Abstract*—In this paper, the forward scattering sum rule is used to investigate scattering and absorption of electromagnetic energy in periodic metamaterials. The sum rule is valid for arbitrary structures composed of linear and passive materials and it shows that the all spectrum interaction between the structure and the electromagnetic field is proportional to the polarizability of the structure. The theoretical results are illustrated with numerical examples for nano-spheres.**

1. Introduction

The forward scattering sum rule shows that the all-spectrum interaction between the electromagnetic field and an object is proportional to the (static) polarizability of the object [1], [2]. This identity is useful since it provides physical insight of the total dynamic interaction over a bandwidth from a relatively simple static problem. It also gives physical limitations on the total cross section bandwidth product expressed in the polarizability of the object. The sum rule has recently been used to derive an antenna identity and several physical bounds on antennas [3]. It has also been used to show bounds on metamaterial scatterers [4] and extraordinary transmission [5].

Here, the forward scattering sum rule is investigated for structures periodic in a plane but finite in the normal direction [6]. This version of the optical theorem shows that the scattered and absorbed power from an incident plane wave is proportional to $\mathrm{Im}\, h(k)$, where $h(k) = \mathrm{i}2\big(1 - T(k)\big)A$ is a Herglotz function [7], A denotes the cross section area of the unit cell, T the co-polarized part of the lowest order transmission coefficient, and k the wavenumber. The low-frequency asymptotic expansion of $h(k)$ is used to derive the forward scattering sum rule according to the general procedure in [7]. The derivation is based on the assumptions that the periodic structure does not support global currents in the low-frequency limit and that the microstructure is made of linear, passive, and time-translational invariant materials. The results are illustrated with numerical simulations for the scattering and absorption of single and periodic arrays of gold and silver nano-spheres [8], [9].

2. Optical theorem for periodic structures

The optical theorem for periodic structures is based on energy conservation [6]. The incident power per unit cell is $P_\mathrm{i} = A|E_0|^2/(2\eta_0)$, where A is the cross section area of the unit cell, $\boldsymbol{E}^{(\mathrm{i})}(\boldsymbol{r}) = \boldsymbol{E}_0\mathrm{e}^{\mathrm{i}k\hat{\boldsymbol{k}}\cdot\boldsymbol{r}}$ the incident field, k the wavenumber, and η_0 the free space impedance. Let P_r denote the reflected power. The corresponding transmitted power, $P_\mathrm{t} = |T|^2P_\mathrm{i} + P_\mathrm{t1}$, is decomposed into the contributions from the co-polarized part of the lowest order mode, $|T|^2P_\mathrm{i}$, and from the remaining modes, P_t1. The scattered power, P_s, is the sum of the reflected power, P_r, and the power in the scattered part of the transmitted field. This scattered power consists of the power in the co-polarized forward scattered field, i.e. the difference between the total field and the incident field, $|1-T|^2P_\mathrm{i}$, and transmitted power in the remaining modes, P_t1, *i.e.*, $P_\mathrm{s} = P_\mathrm{r} + |1-T|^2P_\mathrm{i} + P_\mathrm{t1}$. The absorbed power, P_a, is the difference between the incident and the sum of the reflected and transmitted powers, *i.e.*, $P_\mathrm{a} = P_\mathrm{i} - P_\mathrm{r} - P_\mathrm{t} = P_\mathrm{i} - P_\mathrm{r} - |T|^2P_\mathrm{i} - P_\mathrm{t1}$. The sum of the absorbed and scattered powers is

$$\begin{aligned}P_\mathrm{tot} &= P_\mathrm{a} + P_\mathrm{s}\\ &= P_\mathrm{i} - P_\mathrm{r} - |T|^2P_\mathrm{i} - P_\mathrm{t1} + P_\mathrm{r} + |1-T|^2P_\mathrm{i} + P_\mathrm{t1}\\ &= 2\,\mathrm{Re}\{1-T\}P_\mathrm{i}\end{aligned} \quad (1)$$

which after normalization with the incident power flux, $|E_0|^2/(2\eta_0)$, gives the total (or extinction) cross section

$$\sigma_\mathrm{tot} = \sigma_\mathrm{a} + \sigma_\mathrm{s} = 2\,\mathrm{Re}\{1-T\}A. \quad (2)$$

This is the optical theorem for the periodic structure.

3. Forward scattering sum rule

Causality and passivity of the transmission coefficient $T(k)$ is used to define a Herglotz function and construct sum rules. Causality implies that the transmission coefficient $T(k)$ is holomorphic in k for $\mathrm{Im}\, k > 0$ and passivity implies that it is bounded in magnitude by unity, *i.e.*, $|T| \leq 1$. We use the form of the total cross section (2) to construct the Herglotz function

$$h(k) = \mathrm{i}2\big(1-T(k)\big)A \quad \text{such that } \sigma_\mathrm{tot}(k) = \mathrm{Im}\{h(k)\}. \quad (3)$$

This is a Herglotz function [7], [10], *i.e.*, $h(k)$ is holomorphic and $\mathrm{Im}\{h(k)\} \geq 0$ for $\mathrm{Im}\, k > 0$.

Sum rules are equations stating that the sum or integral of a certain quantity has a given value. Many sum rules can be derived from Herglotz functions [7], where the integrand is the imaginary part of the Herglotz function weighted by some function of k. Moreover, the integral is related to the low- and high frequency asymptotic expansions of the function. In the case (3), we have the low- and high-frequency expansion

$$h(k) \sim \begin{cases} k\gamma = k(\hat{\boldsymbol{e}}\cdot\boldsymbol{\gamma}_{\mathrm{e}}\cdot\hat{\boldsymbol{e}} + (\hat{\boldsymbol{k}}\times\hat{\boldsymbol{e}})\cdot\boldsymbol{\gamma}_{\mathrm{m}}\cdot(\hat{\boldsymbol{k}}\times\hat{\boldsymbol{e}})) & \text{as } k\to 0 \\ \mathcal{O}(1) \quad \text{as } k\to\infty, \end{cases} \tag{4}$$

where $\boldsymbol{\gamma}_{\mathrm{e}}$ and $\boldsymbol{\gamma}_{\mathrm{m}}$ denote the electric and magnetic polarizability dyadics, respectively and $\boldsymbol{E}^{(\mathrm{i})} = \hat{\boldsymbol{e}}E_0$. The pertinent sum rule is [7]

$$\frac{2}{\pi}\int_0^\infty \frac{\sigma_{\mathrm{tot}}(k;\hat{\boldsymbol{k}},\hat{\boldsymbol{e}})}{k^2}\,\mathrm{d}k = \hat{\boldsymbol{e}}\cdot\boldsymbol{\gamma}_{\mathrm{e}}\cdot\hat{\boldsymbol{e}}+(\hat{\boldsymbol{k}}\times\hat{\boldsymbol{e}})\cdot\boldsymbol{\gamma}_{\mathrm{m}}\cdot(\hat{\boldsymbol{k}}\times\hat{\boldsymbol{e}}), \tag{5}$$

where $\sigma_{\mathrm{tot}} = \operatorname{Im} h$ is used and $\hat{\boldsymbol{e}}$ is the linear polarization (real valued). It is convenient to rewrite the sum rule as a function of the wavelength, $\lambda = 2\pi/k$, that transforms the sum rule (5) into

$$\frac{1}{\pi^2}\int_0^\infty \sigma_{\mathrm{tot}}(\lambda;\hat{\boldsymbol{k}},\hat{\boldsymbol{e}})\,\mathrm{d}\lambda = \hat{\boldsymbol{e}}\cdot\boldsymbol{\gamma}_{\mathrm{e}}\cdot\hat{\boldsymbol{e}}+(\hat{\boldsymbol{k}}\times\hat{\boldsymbol{e}})\cdot\boldsymbol{\gamma}_{\mathrm{m}}\cdot(\hat{\boldsymbol{k}}\times\hat{\boldsymbol{e}}), \tag{6}$$

where the symbol $\sigma_{\mathrm{tot}}(\lambda;\hat{\boldsymbol{k}},\hat{\boldsymbol{e}})$ is reused as the total cross section as a function of the wavelength. It is observed that (5) and (6) are identical to the forward scattering sum rule with σ_{tot} being the total (extinction) cross section for an object in free space [1], [2], [11], [12].

4. Numerical example

We illustrate the sum rule (6) with gold (Au) and silver (Ag) spheres of radius $a = 60\,\mathrm{nm}$ and the permittivity models [13], see Fig. 1. The total cross sections normalized with the geometrical cross sections are depicted on top and bottom in Fig. 1 for single spheres [2] and periodic arrays of spheres, respectively. The polarizabilities in the right hand side of (6) are identical for all (non-magnetic) metals. Consequently, the areas under the curves σ_{tot} are the same for the gold and silver objects. The (plasmonic) resonances can hence only shift the interaction between different wavelengths but not change the all spectrum interaction. The polarizability is $\gamma = 4\pi a^3$ for single spheres giving $4\cdot 60\pi^2 \approx 2369 \approx 3\cdot 790$ as the area under the curves $\sigma_{\mathrm{tot}}/\pi a^2$ and the corresponding area of the dashed rectangle in the left part of Fig. 1, note the x-axis in $\lambda/\,\mathrm{nm}$. The corresponding polarizability is computed to $\gamma \approx 1.2\cdot 4\pi a^3$ for the periodic structure with unit cell length $\ell_{\mathrm{x}} = \ell_{\mathrm{y}} = 3a$ using Comsol multiphysics [6] giving the area 2842.

5. Conclusion

The forward scattering sum rule shows that the all spectrum interaction between metallic objects and electromagnetic waves is independent of the specific metal and only depends on the shape of the objects. The results are illustrated numerically for gold and silver nano-spheres.

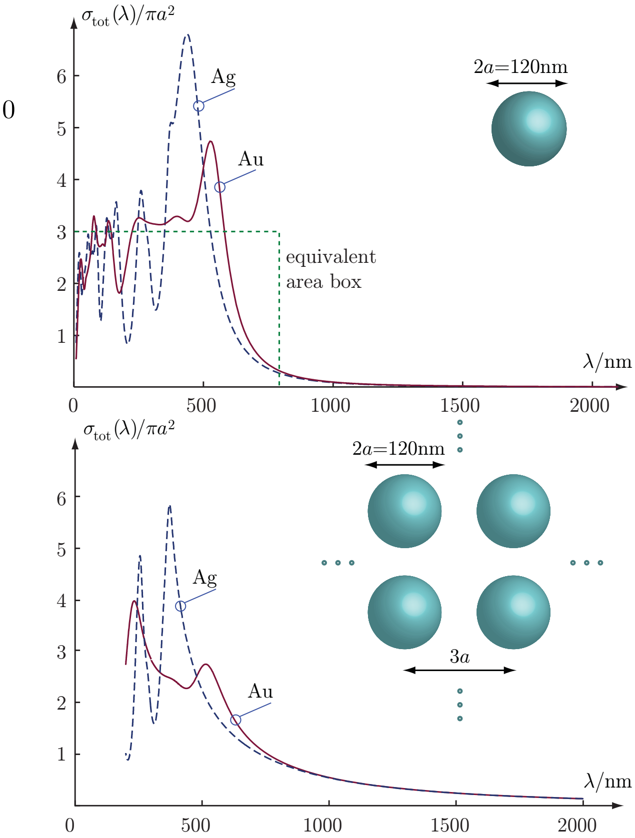

Fig. 1. Total cross sections for gold (Au) and silver (Ag) spheres with radius $a = 60\,\mathrm{nm}$. Top: single sphere. Bottom: periodic array of spheres with spacing (unit cell length) $\ell_{\mathrm{x}} = \ell_{\mathrm{y}} = 3a$.

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