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Electromagnetic Scattering by Bianisotropic Spheres

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Abstract: Electromagnetic fields in bulk bianisotropic media contain plane waves whose k-vectors can be found using the method of the index of refraction's operator and belong to the Fresnel wave surfaces that fall into one of the five hyperbolic classes of the Durach et al. taxonomy of bianisotropic media. Linear combinations of vector spherical harmonics can be used as a set of solutions of vector Helmholtz equations in gyrotropic media to develop Mie's theory of scattering by anisotropic spheres as accomplished by Lin et al. and Li et al. In this study, we introduced electromagnetic orbitals for bianisotropic media as linear combinations of vector spherical harmonics, which represent solutions of Maxwell's equations in bianisotropic media. Using these bianisotropic orbitals, we developed a theory of the scattering of electromagnetic radiation by bianisotropic spheres with arbitrary effective material parameters and sizes. As a by-product, we obtained a simple expression for the expansion of a vector plane wave over vector spherical harmonics in a more compact form than the frequently used by Sarkar et al. We obtained the polarizability expressions in the Rayleigh limit in agreement with the results of the electrostatic approximation of Lakhtahia and Sihvola.

Keywords: Mie scattering; Rayleigh scattering; bianisotropic and anisotropic media

1. Introduction

Electromagnetism occupies the crowning role in physics, science, and modern technology. As in the cases of the Second and the Third Industrial Revolutions, research into electromagnetism is driving the ongoing Fourth Industrial Revolution [1] related to the transition to renewable energy, telecommunications in the 5G and 6G standards [2], advanced micro-/nanofabrication for novel electronic devices [3], bioelectromagnetics [4], information and electronic warfare [5], machine learning, material training [6,7], and in other realms. The slide towards scientific and technological unification of the physical, chemical, biological, and digital worlds brought by the Fourth Industrial Revolution is due to the inalienable electromagnetic nature of these phenomena, based on the rule of the underlying laws of Coulomb, Gauss, Biot-Savart, Ampere, Kirchhoff, Faraday, and Maxwell [8–10]. We, the researchers of modern electromagnetism, are devoted to the development of the new electromagnetic materials collectively called composite artificial materials or metamaterials [11–17]. Metamaterials are made of arrays of subwavelength scatterers designed to exhibit the desired electromagnetic properties. In many important cases, metamaterials can be described as bianisotropic media [13–17]. In bianisotropic media, both the electric and magnetic responses depend on both the electric and magnetic fields of the external radiation [18,19].

The studies of bianisotropic materials are almost as old as electromagnetism itself, persisting through the 19th and 20th centuries in the work of scientists such as Roentgen, Wilson, Landau, Lifshitz, Dzyaloshinskii, Cheng, and Kong [18–24]. In the 21st century the field of bianisotropic optical materials has received the name of bianisotropics [25–27] and is closely related to the research on electromagnetic metamaterials, since, typically, the desired properties of metamaterials depend on them being anisotropic and bianisotropic media [13–19]. Despite all these efforts and the rich history of research into bianisotropics until recently, very few general properties of bianisotropic media were established due to

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the complexity of these media [14,18,28–35]. The bianisotropic media are the most general case of local linear media [18,19,25,36,37], with the effective material parameters combined into a 6 × 6 matrix of material parameters $\hat{M}$, which characterizes the electric displacement field $\boldsymbol{D}$ and magnetic field $\boldsymbol{B}$ in terms of the fields $\boldsymbol{E}$ and $\boldsymbol{H}$:

$$\begin{pmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{pmatrix} = \hat{M}\begin{pmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{pmatrix} = \begin{pmatrix} \hat{\epsilon} & \hat{X} \\ \hat{Y} & \hat{\mu} \end{pmatrix}\begin{pmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{pmatrix} \tag{1}$$

The 3 × 3 matrices $\hat{\epsilon}$, $\hat{\mu}$, $\hat{X}$, $\hat{Y}$ are dielectric permittivity, magnetic permeability, and two magnetoelectric coupling matrices respectively. The inverse relationship can also be formulated:

$$\begin{pmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{pmatrix} = \begin{bmatrix} \hat{\epsilon} & \hat{X} \\ \hat{Y} & \hat{\mu} \end{bmatrix}^{-1}\begin{pmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{pmatrix} = \begin{bmatrix} \hat{\alpha}_{ED} & \hat{\alpha}_{EB} \\ \hat{\alpha}_{HB} & \hat{\alpha}_{HD} \end{bmatrix}\begin{pmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{pmatrix} \tag{2}$$

The relationships in Equations (1) and (2) mean that, unlike in many naturally occurring isotropic media, the electrical polarization and magnetization vectors in bianisotropic media are not directed in the same direction as the electric and magnetic fields. Such differences in the isotropic media can be achieved in engineered metamaterial structures [13–17].

One of the jewels in the crown of electromagnetism is Mie's theory of scattering by spheres. Originally, Mie's theory was introduced to describe scattering by isotropic spheres [38,39], but later, it was extended to describe scattering by bi-isotropic [40], rotationally symmetric and anisotropic [41], orthorhombic and dielectric–magnetic [42], magneto- and electro-gyrotropic [43–45], and spherically-symmetric bianisotropic [46] spheres. Despite this activity, the theory of scattering by a generic bianisotropic sphere has not yet been constituted [47].

The plane waves which can propagate in bianisotropic media belong to Fresnel wave surfaces, which can be characterized using the method of the index of refraction's operator [31–33]. The Fresnel wave surfaces in bianisotropic media follow quartic dispersion equations, and, therefore, can be classified using the taxonomy of Durach et al. [31–33], which includes the five hyperbolic classes: non-, mono-, bi-, tri-, and tetra-hyperbolic materials [31–33,48–59]. The prefix in the name of each topological class indicates the number of double cones that the iso-frequency's k-surface has in its high-k limit. Note that hyperbolic metamaterials, which are already known for their applications in optical imaging, hyperlensing, and emission rate and directivity control, utilize the diverging optical density of high-k states [51–59]. In Figure 1a, we show an example of an iso-frequency Fresnel wave surface for a tetra-hyperbolic bianisotropic medium with the effective material parameter matrix $\hat{M}$ color-coded in Figure 1b.

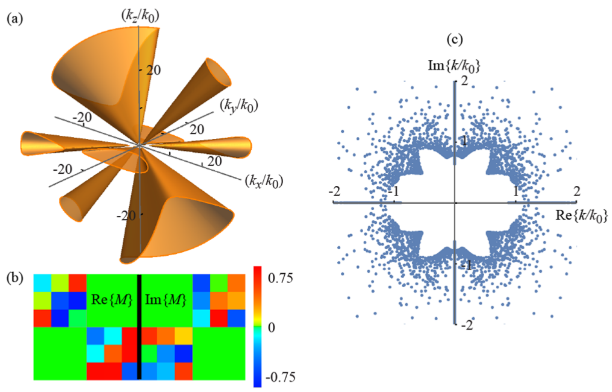

Figure 1. (**a**) Iso-frequency Fresnel wave surface for a tetra-hyperbolic bianisotropic medium with the effective material parameters matrix $\hat{M}$ color-coded in (**b**); (**c**) eigenvalues of the index of refraction's operator [31–33] in a complex plane for the same material.

The Fresnel wave surfaces only include the plane waves with real wave vectors $\boldsymbol{k}$. Nevertheless, the inhomogeneous plane waves with an imaginary $\boldsymbol{k}$ are also important. In Figure 1c, we plot the eigenvalues of the index of refraction's operator [31–33] in a complex plane for the material color-coded in Figure 1b for plane waves propagating in directions spanning the entire solid angle with steps in the angles $\Delta\theta = \pi/40$ and $\Delta\phi = 2\pi/40$. Note that in Figure 1c, only the eigenvalues on the horizontal axis $\mathrm{Re}\{k/k_0\}$ correspond to the real wave vectors belonging to the Fresnel wave surfaces depicted in Figure 1a.

In unbounded homogeneous bianisotropic media, plane waves represent the set of solutions of Maxwell's equations which is typically used, but to consider the scattering of electromagnetic waves by bianisotropic spheres, it is more convenient to express the electromagnetic fields inside such spheres in terms of vector spherical harmonics. In this study, we proposed a theory of scattering by bianisotropic spheres with arbitrary effective media parameters $\hat{M}$. To accomplish this, we introduced bianisotropic orbitals composed of vector spherical harmonics.

2. Results

2.1. Bianisotropic Orbitals

The plane waves whose k-vectors belong to Fresnel's wave surfaces represent a complete set of solutions of Maxwell's equations in the bulk bianisotropic media. A different set of solutions can be found as expansion of vector spherical harmonics. Recently, the close connection between the multipole composition of electromagnetic fields and bianisotropy has been revealed [60].

Due to the solenoidal nature of D- and B-fields, namely $\nabla\cdot\mathrm{D} = 0$ and $\nabla\cdot\mathrm{B} = 0$, we can express them as an expansion over the vector spherical harmonics $\boldsymbol{M}^1_{lm}$, $\boldsymbol{N}^1_{lm}$ found from solutions of the scalar Helmholtz equations [61–63]

$$\psi^{(j)}_{lm} = -\frac{1}{i\sqrt{l(l+1)}} z^{(j)}_l(kr) Y_{lm}, \;\; \psi^{(j)}_{00} = i z^{(j)}_0(kr) Y_{00} \tag{3}$$

according to

$$\boldsymbol{L}^{(j)}_{lm} = \frac{1}{k}\nabla\psi^{(j)}_{lm}, \;\; \boldsymbol{M}^{(j)}_{lm} = \nabla\times\left(\boldsymbol{r}\psi^{(j)}_{lm}\right), \;\; \boldsymbol{N}^{(j)}_{lm} = \frac{1}{k}\nabla\times\boldsymbol{M}^{(j)}_{lm} \tag{4}$$

Detailed definitions of the vector spherical harmonics used in this study are in Appendix A. We represent the D- and B-fields of a bianisotropic orbital with a wave number k_q as

$$\boldsymbol{D}_q = \sum_{lm}\left\{ f^{DM}_{qlm}\boldsymbol{M}^1_{lm}(k_q) + f^{DN}_{qlm}\boldsymbol{N}^1_{lm}(k_q)\right\} \tag{5}$$

$$\boldsymbol{B}_q = \sum_{lm}\left\{ f^{BM}_{qlm}\boldsymbol{M}^1_{lm}(k_q) + f^{BN}_{qlm}\boldsymbol{N}^1_{lm}(k_q)\right\} \tag{6}$$

The corresponding E- and H-fields can be expressed using Equation (2) as

$$\begin{aligned}\boldsymbol{E}_q &= \sum_{uv}\left(\mu^{eq}_{uv}\boldsymbol{M}^{1q}_{uv} + \nu^{eq}_{uv}\boldsymbol{N}^{1q}_{uv} + \lambda^{eq}_{uv}\boldsymbol{L}^{1q}_{uv}\right) = \hat{\alpha}_{ED}\boldsymbol{D}_q + \hat{\alpha}_{EB}\boldsymbol{B}_q \\ &= \sum_{lm}\left\{ f^{DM}_{qlm}\left(\hat{\alpha}_{ED}\boldsymbol{M}^{1q}_{lm}\right) + f^{DN}_{qlm}\left(\hat{\alpha}_{ED}\boldsymbol{N}^{1q}_{lm}\right)\right\} + \sum_{lm}\left\{ f^{BM}_{qlm}\left(\hat{\alpha}_{EB}\boldsymbol{M}^{1q}_{lm}\right) + f^{BN}_{qlm}\left(\hat{\alpha}_{EB}\boldsymbol{N}^{1q}_{lm}\right)\right\} \\ &= \sum_{lm,uv}\left(\boldsymbol{M}^{1q}_{uv}, \boldsymbol{N}^{1q}_{uv}, \boldsymbol{L}^{1q}_{uv}\right)\cdot\begin{pmatrix} g^{\alpha ED}_{MM} & g^{\alpha ED}_{NM} & g^{\alpha EB}_{MM} & g^{\alpha EB}_{NM} \\ g^{\alpha ED}_{MN} & g^{\alpha ED}_{NN} & g^{\alpha EB}_{MN} & g^{\alpha EB}_{NN} \\ g^{\alpha ED}_{ML} & g^{\alpha ED}_{NL} & g^{\alpha EB}_{ML} & g^{\alpha EB}_{NL}\end{pmatrix}_{lm,uv}\cdot\begin{pmatrix} f^{DM}_{qlm} \\ f^{DN}_{qlm} \\ f^{BM}_{qlm} \\ f^{BN}_{qlm}\end{pmatrix}\end{aligned} \tag{7}$$

$$\begin{aligned} \boldsymbol{H}_q &= \sum_{uv}\left(\mu_{uv}^{hq}\boldsymbol{M}_{uv}^{1q} + \nu_{uv}^{hq}\boldsymbol{N}_{uv}^{1q} + \lambda_{uv}^{hq}\boldsymbol{L}_{uv}^{1q}\right) = \hat{\alpha}_{HD}\boldsymbol{D}_q + \hat{\alpha}_{HB}\boldsymbol{B}_q \\ &= \sum_{lm}\left\{f_{qlm}^{DM}\left(\hat{\alpha}_{HD}\boldsymbol{M}_{lm}^{1q}\right) + f_{qlm}^{DN}\left(\hat{\alpha}_{HD}\boldsymbol{N}_{lm}^{1q}\right)\right\} + \sum_{lm}\left\{f_{qlm}^{BM}\left(\hat{\alpha}_{HB}\boldsymbol{M}_{lm}^{1q}\right) + f_{qlm}^{BN}\left(\hat{\alpha}_{HB}\boldsymbol{N}_{lm}^{1q}\right)\right\} \\ &= \sum_{lm,uv}\left(\boldsymbol{M}_{uv}^{1q}, \boldsymbol{N}_{uv}^{1q}, \boldsymbol{L}_{uv}^{1q}\right) \cdot \begin{pmatrix} g_{MM}^{\alpha HD} & g_{NM}^{\alpha HD} & g_{MM}^{\alpha HB} & g_{NM}^{\alpha HB} \\ g_{MN}^{\alpha HD} & g_{NN}^{\alpha HD} & g_{MN}^{\alpha HB} & g_{NN}^{\alpha HB} \\ g_{ML}^{\alpha HD} & g_{NL}^{\alpha HD} & g_{ML}^{\alpha HB} & g_{NL}^{\alpha HB} \end{pmatrix}_{lm,uv} \cdot \begin{pmatrix} f_{qlm}^{DM} \\ f_{qlm}^{DN} \\ f_{qlm}^{BM} \\ f_{qlm}^{BN} \end{pmatrix} \end{aligned} \tag{8}$$

where the coefficients g is found using $\{\boldsymbol{U}|\hat{\alpha}|\boldsymbol{V}\} = \int_0^\infty \int_0^{2\pi} \int_0^\pi \boldsymbol{U} \cdot \hat{\alpha} \cdot \boldsymbol{V} r^2 \sin\theta dr\, d\theta\, d\varphi$, $\int Y_{uv}^*(\hat{\boldsymbol{r}}) Y_{lm}(\hat{\boldsymbol{r}}) d\Omega = \delta_{ul}\delta_{vm}$, and $\int_0^\infty j_u(k'r) j_l(kr) r^2 dr = \frac{\pi}{2k^2}\delta(k-k')$ as:

$$\begin{aligned} &\begin{pmatrix} \{\boldsymbol{M}_{uv}^\star|\hat{\alpha}|\boldsymbol{M}_{lm}\} & \{\boldsymbol{N}_{uv}^\star|\hat{\alpha}|\boldsymbol{M}_{lm}\} & \{\boldsymbol{L}_{uv}^\star|\hat{\alpha}|\boldsymbol{M}_{lm}\} \\ \{\boldsymbol{M}_{uv}^\star|\hat{\alpha}|\boldsymbol{N}_{lm}\} & \{\boldsymbol{N}_{uv}^\star|\hat{\alpha}|\boldsymbol{N}_{lm}\} & \{\boldsymbol{L}_{uv}^\star|\hat{\alpha}|\boldsymbol{N}_{lm}\} \\ \{\boldsymbol{M}_{uv}^\star|\hat{\alpha}|\boldsymbol{L}_{lm}\} & \{\boldsymbol{N}_{uv}^\star|\hat{\alpha}|\boldsymbol{L}_{lm}\} & \{\boldsymbol{L}_{uv}^\star|\hat{\alpha}|\boldsymbol{L}_{lm}\} \end{pmatrix} \\ &= \begin{pmatrix} g_{MM}^{\alpha} & g_{MN}^{\alpha} & g_{ML}^{\alpha} \\ g_{NM}^{\alpha} & g_{NN}^{\alpha} & g_{NL}^{\alpha} \\ g_{LM}^{\alpha} & g_{LN}^{\alpha} & g_{LL}^{\alpha} \end{pmatrix}_{lm,uv} \begin{pmatrix} \{\boldsymbol{M}_{uv}^\star|\boldsymbol{M}_{uv}\} = 1 & 0 & 0 \\ 0 & \{\boldsymbol{N}_{uv}^\star|\boldsymbol{N}_{uv}\} = 1 & 0 \\ 0 & 0 & \{\boldsymbol{L}_{uv}^\star|\boldsymbol{L}_{uv}\} \end{pmatrix} \end{aligned} \tag{9}$$

Please note that, while the D- and B-fields are divergence-free, as indicated by Equations (5) and (6), the E- and H-fields include the longitudinal vector spherical harmonic $\boldsymbol{L}$, as was previously shown for anisotropic media as well [43–45].

The bianisotropic orbitals with the radial quantum numbers k_q represent the solutions of Maxwell's equations in homogeneous bianisotropic media if the expansion coefficients f_{qlm} satisfy the following eigenproblem:

$$\sum_{lm}\begin{pmatrix} -g_{MN}^{\alpha HD} & -g_{NN}^{\alpha HD} & -g_{MN}^{\alpha HB} & -g_{NN}^{\alpha HB} \\ -g_{MM}^{\alpha HD} & -g_{NM}^{\alpha HD} & -g_{MM}^{\alpha HB} & -g_{NM}^{\alpha HB} \\ g_{MN}^{\alpha ED} & g_{NN}^{\alpha ED} & g_{MN}^{\alpha EB} & g_{NN}^{\alpha EB} \\ g_{MM}^{\alpha ED} & g_{NM}^{\alpha ED} & g_{MM}^{\alpha EB} & g_{NM}^{\alpha EB} \end{pmatrix}_{lm,uv} \begin{pmatrix} f_{qlm}^{DM} \\ f_{qlm}^{DN} \\ f_{qlm}^{BM} \\ f_{qlm}^{BN} \end{pmatrix} = i\left(\frac{k_0}{k_q}\right) \begin{pmatrix} f_{quv}^{DM} \\ f_{quv}^{DN} \\ f_{quv}^{BM} \\ f_{quv}^{BN} \end{pmatrix} \tag{10}$$

Note that the eigenproblem of Equation (10) differs from the eigenproblems formulated for the anisotropic media, which stem from the vector Helmholtz equations [43–45]. Such eigenproblems could not be used in the case of the bianisotropic media considered here and we used the pair of Maxwell's equations composed of Faraday's and Maxwell-Ampere's equations instead to obtain Equation (10).

The bianisotropic orbitals provided by the solutions of Equation (10) can be represented as expansions over plane wave solutions of the method of the index of refraction's operator [31–33] with the indexes of refraction $n = k_q/k_0$ (Appendix B). In Figure 2a, we show the inverse eigenvalues k_q/k_0 of Equation (10) for the eigenproblems which are truncated and have $l = 4$ (black dots), 10 (red), and 40 (green). Note the direct correspondence of the eigenvalues of Equation (10) in Figure 2a with the eigenvalues of the index of refraction's operator plotted in Figure 1b.

In other words, the inclusion of higher multipoles in the bianisotropic orbitals corresponds to higher angular resolution in the Fourier expansion of the fields in bianisotropic materials with a smaller $\Delta\theta$ and $\Delta\phi$ with the inclusion of both the real wave vectors belonging to the Fresnel wave surface, as well as the complex eigenvalues k/k_0 of the index of refractioná operator.

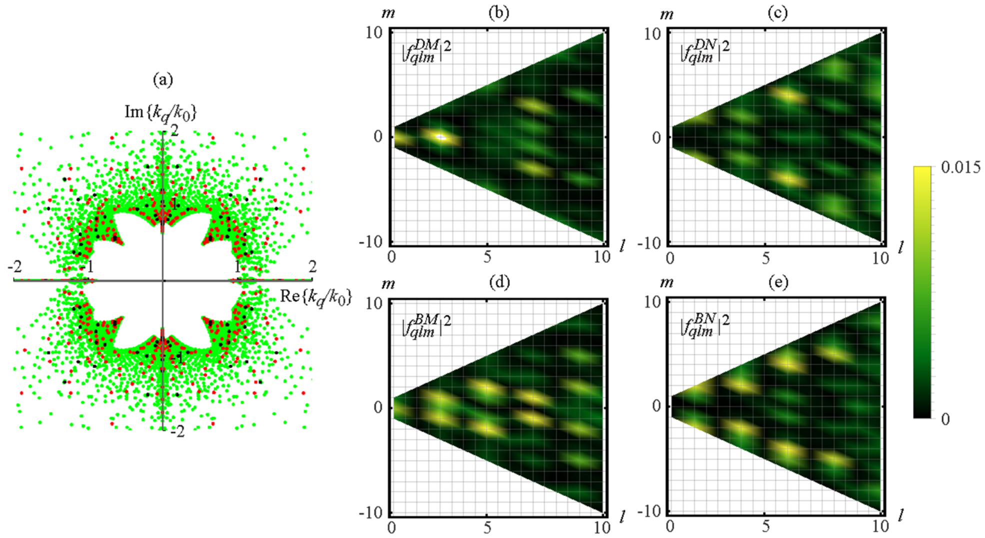

Figure 2. (**a**) Inverse eigenvalues k_q/k_0 of the eigenproblem in Equation (10) truncated at $l = 4$ (black dots), 10 (red dots), and 40 (green dots). Note the correspondence with the eigenvalues of the index of refraction's operator plotted in Figure 1b; (**b**–**e**) eigenvector components $\left|f_{qlm}\right|^2$ of the eigenproblem in Equation (10) for a bianisotropic orbital with $k_q/k_0 = 2.2$ in the angular momentum space *l*-*m*.

This correspondence between the plane waves and the bianisotropic orbitals introduced in this study shows the relationship between the solution of the scattering problem presented in this study with the method of plane wave expansion proposed for the scattering by the uniaxial anisotropic spheres [64,65]. In Figure 2b–e, we plot the components $\left|f_{qlm}\right|^2$ of the eigenproblem of Equation (10) for a bianisotropic orbital with $k_q/k_0 = 2.2$ in the angular momentum space *l*-*m*.

2.2. Scattering Cross-Section of Bianisotropic Spheres in a Vacuum

The bianisotropic orbitals can be used to solve a large range of problems with spherically shaped bianisotropic media from spheres and spherical shells, to spherical voids, combinations of such geometries, and so forth. Here, we considered a bianisotropic sphere with the arbitrary effective material parameters $\hat{M}$ with a radius R. We studied the scattering of an electromagnetic plane wave by such a sphere. The field of the plane wave is given by

$$\boldsymbol{E}_{in} = \boldsymbol{\epsilon}(\boldsymbol{k})e^{i\boldsymbol{kr}} = \sum_{lm}\left(q_{lm}\boldsymbol{M}^1_{lm} + p_{lm}\boldsymbol{N}^1_{lm}\right) \tag{11}$$

$$\boldsymbol{H}_{in} = \boldsymbol{h}(\boldsymbol{k})e^{i\boldsymbol{kr}} = \frac{1}{i}\sum_{lm}\left(p_{lm}\boldsymbol{M}^1_{lm} + q_{lm}\boldsymbol{N}^1_{lm}\right), \;\; \boldsymbol{h} = \hat{\boldsymbol{k}} \times \boldsymbol{\epsilon} \tag{12}$$

We defined the orientation of the incident electric and magnetic fields with the polarization angle α in the spherical coordinates with respect to the direction of incidence $\hat{\boldsymbol{k}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, $\boldsymbol{\epsilon}(\boldsymbol{k}) = (\sin\alpha\hat{\boldsymbol{\theta}} - \cos\alpha\hat{\boldsymbol{\phi}})$, $\boldsymbol{h}(\boldsymbol{k}) = (\cos\alpha\hat{\boldsymbol{\theta}} + \sin\alpha\hat{\boldsymbol{\phi}})$, where $\hat{\boldsymbol{\theta}} = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta)$, $\hat{\boldsymbol{\phi}} = (-\sin\phi, \cos\phi)$.

Expansions of the vector plane wave over vector spherical harmonics exist in the literature [43,66]. Nevertheless, we derived a compact expansion of a vector plane wave for our work (Appendix C):

$$\boldsymbol{a}e^{i\boldsymbol{kr}} = 4\pi\sum_{lm} i^l\left(-\sqrt{l(l+1)}\left\{\boldsymbol{a}\cdot\boldsymbol{Y}^{(-1)*}_{lm}(\hat{\boldsymbol{k}})\right\}\boldsymbol{L}^{(1)}_{lm} + \left\{\boldsymbol{a}\cdot\boldsymbol{Y}^{l*}_{lm}(\hat{\boldsymbol{k}})\right\}\boldsymbol{M}^{(1)}_{lm} - \left\{\boldsymbol{a}\cdot\boldsymbol{Y}^{(+1)*}_{lm}(\hat{\boldsymbol{k}})\right\}\boldsymbol{N}^{(1)}_{lm}\right)$$

Correspondingly, the coefficients in the expansions Equations (11) and (12) are

$$q_{lm} = 4\pi i^l \left\{ \boldsymbol{\epsilon}(\boldsymbol{k}) \cdot \boldsymbol{Y}^{l*}_{lm}(\hat{\boldsymbol{k}}) \right\}, \;\; p_{lm} = 4\pi i^{l+1} \left\{ \boldsymbol{h}(\boldsymbol{k}) \cdot \boldsymbol{Y}^{l*}_{lm}(\hat{\boldsymbol{k}}) \right\} \tag{13}$$

The scattered fields outside of the sphere are given by

$$\boldsymbol{E}_{sc} = \sum_{lm} \left(b_{lm} \boldsymbol{M}^3_{lm} + a_{lm} \boldsymbol{N}^3_{lm} \right) \tag{14}$$

$$\boldsymbol{H}_{sc} = \frac{1}{i} \sum_{lm} \left(a_{lm} \boldsymbol{M}^3_{lm} + b_{lm} \boldsymbol{N}^3_{lm} \right) \tag{15}$$

The scattered fields consist only of the outgoing vector spherical harmonics containing the spherical Hankel functions $h^{(1)}_l$.

We represent the field inside the bianisotropic sphere as a linear combination of the bianisotropic orbitals described by Equation (10).

$$\boldsymbol{E}_{sph} = \sum_q A_q \boldsymbol{E}_q, \;\; \boldsymbol{H}_{sph} = \sum_q A_q \boldsymbol{H}_q, \tag{16}$$

Please note that for reciprocal media, the eigenvalues of Equation (10) come in pairs with the radial wavenumber $\pm k_q$, and the corresponding modes in Equation (16) are equivalent. Therefore, among the orbitals with a real k_q, we only included the modes with a positive k_q. For the orbitals with a complex k_q, we only included the modes with Im $k_q > 0$. Note, however, that in non-reciprocal media, the symmetry of the reciprocity between the modes is broken, and all the bianisotropic orbitals of Equation (10) should be included into Equation (16). Correspondingly, additional boundary conditions (ABC) are needed, as described in [34].

The continuity of the tangential components of the E- and H-fields at the surface of the sphere lead to the following boundary conditions, expressed in terms of the Riccati–Bessel functions $\psi_l(x) = x j_l(x)$ and $\xi_l(x) = x h^{(1)}_l(x)$, where $j_l(x)$ and $h^{(1)}_l(x)$ are spherical Bessel functions of the first and third kinds, and the parameters $x = k_0 R$ and $x_q = k_q R$:

$$E_{in\theta} + E_{sc\theta} = E_{sph\theta}, \; q_{lm} + b_{lm} \left(\frac{\xi_l(x)}{\psi_l(x)} \right) = \sum_q A_q \left(\frac{x}{x_q} \right) \mu^{eq}_{lm} \left(\frac{\psi_l(x_q)}{\psi_l(x)} \right) \tag{17}$$

$$H_{in\theta} + H_{sc\theta} = H_{sph\theta}, \; p_{lm} + a_{lm} \left(\frac{\xi_l(x)}{\psi_l(x)} \right) = i \sum_q A_q \left(\frac{x}{x_q} \right) \mu^{hq}_{lm} \left(\frac{\psi_l(x_q)}{\psi_l(x)} \right) \tag{18}$$

$$E_{in\phi} + E_{sc\phi} = E_{sph\phi}, \;\; p_{lm} + a_{lm} \left(\frac{\xi'_l(x)}{\psi'_l(x)} \right) = \sum_q A_q \left(\frac{x}{x_q} \right) \left\{ \nu^{eq}_{lm} \left(\frac{\psi'_l(x_q)}{\psi'_l(x)} \right) + \lambda^{eq}_{lm} \left(\frac{j_l(x_q)}{\psi'_l(x)} \right) \right\} \tag{19}$$

$$H_{in\phi} + H_{sc\phi} = H_{sph\phi}, \;\; q_{lm} + b_{lm} \left(\frac{\xi'_l(x)}{\psi'_l(x)} \right) = i \sum_q A_q \left(\frac{x}{x_q} \right) \left\{ \nu^{hq}_{lm} \left(\frac{\psi'_l(x_q)}{\psi'_l(x)} \right) + \lambda^{hq}_{lm} \left(\frac{j_l(x_q)}{\psi'_l(x)} \right) \right\} \tag{20}$$

The boundary Equations (17)–(20) can be represented in the matrix form as

$$\hat{M}_\psi \vec{A} - \hat{\Psi}(ab) = (pq) \tag{21}$$

$$\hat{N}_\psi \vec{A} - \hat{\Phi}(ab) = (pq) \tag{22}$$

where $\vec{A}$ is the column of the amplitudes of the bianisotropic orbitals A_q inside the sphere, and (ab) and (pq) include the amplitudes of the scattered vector spherical harmonics and the known incident amplitudes of Equation (13).

The matrices $\hat{\Psi}$, $\hat{\Phi}$, are diagonal and contain the functions $\left(\frac{\xi_l(x)}{\psi_l(x)}\right)$ and $\left(\frac{\xi_l'(x)}{\psi_l'(x)}\right)$, while the matrices $\hat{M}_\psi$, $\hat{N}_\psi$ represent the coupling between different multipoles due to the bianisotropy in the bianisotropic orbitals, and correspond to the sums on the right-hand sides of Equations (17)–(20).

Excluding the coefficients (pq), we obtained the relationship between (ab) and $\vec{A}$

$$(ab) = \hat{\Omega}\vec{A},\ \hat{\Omega} = \left\{\hat{\Psi} - \hat{\Phi}\right\}^{-1}\left\{\hat{M}_\psi - \hat{N}_\psi\right\} \tag{23}$$

The amplitudes of the bianisotropic orbitals A_q were found from Equations (21) and (23) as follows

$$\vec{A} = \hat{\Xi}(pq) = \left\{\hat{M}_\psi - \hat{\Psi}\hat{\Omega}\right\}^{-1}(pq) \tag{24}$$

Substituting the amplitudes A_q from Equation (24) into Equation (23), we obtained the T-matrix for a bianisotropic sphere with arbitrary effective medium parameters and the scattering amplitudes (ab) in terms of the parameters of the incident wave (pq) as

$$(ab) = \hat{T}(pq),\ \hat{T} = \hat{\Omega}\hat{\Xi} \tag{25}$$

The scattering cross-section Q_s can be found from the scattering amplitudes as

$$Q_s = \frac{1}{k_0^2}\sum_{lm}\left(|a_{lm}|^2 + |b_{lm}|^2\right) \tag{26}$$

To validate our formulas and codes and check the accuracy of the numerical results obtained, in Figure 3, we compare our results with the published results of Lin et al. and Li et al. [43,45]. In Figure 3a, we show the scattering cross-section $Q_s/\left(\pi R^2\right)$ as a function of the angles θ for the anisotropic sphere with $\hat{\varepsilon} = 1$ and $\hat{\mu} = \hat{1} + (\mu_s - 1)\hat{\boldsymbol{z}}\hat{\boldsymbol{z}}$ for various values of μ_s in linear polarization for $\alpha = 0$. In Figure 3b, we show the scattering cross-section $Q_s/\left(\pi R^2\right)$ as a function of the angles θ for the gyromagnetic sphere with $\hat{\varepsilon} = 1$ and $\hat{\mu} = \hat{1} - i\mu_g(\hat{\boldsymbol{x}}\hat{\boldsymbol{y}} - \hat{\boldsymbol{y}}\hat{\boldsymbol{x}})$ for various values of μ_g in left- and right-handed circular polarizations. Figure 3 is an exact match with the results obtained in Figure 2 of Ref. [43] and Figures 2 and 3 of Ref. [45].

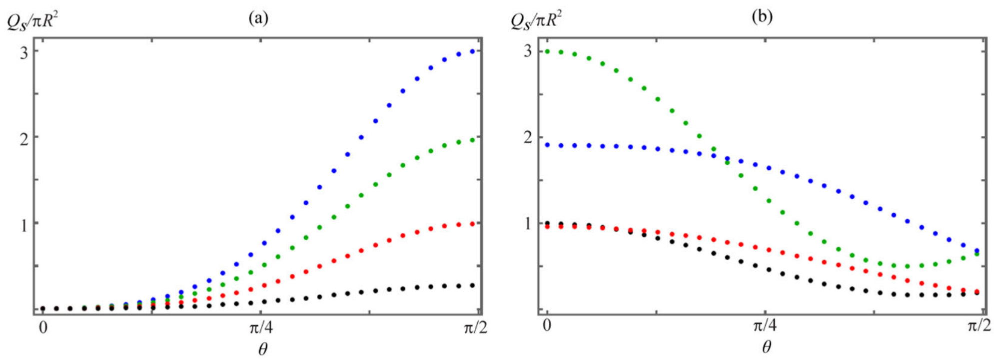

Figure 3. (**a**) Reduced scattering cross-section $Q_s/\left(\pi R^2\right)$ for all angles θ in response to the linear polarization $\alpha = 0$ for an anisotropic sphere with the values $\mu_s = 1.2$ (black), 1.4 (red), 1.6 (green), 1.8 (blue), and $x = k_0R = 4$. (**b**) Reduced scattering cross-section $Q_s/\left(\pi R^2\right)$ for all angles θ for an anisotropic sphere with $\mu_g = 0.4$ (black—LCP, red—RCP), 0.8 (green—LCP, blue—RCP), and $x = k_0R = 4$.

In Figure 4a,b, we plot the dependence of the reduced scattering cross-section $Q_s/\left(\pi R^2\right)$ for all incidence angles θ and ϕ for a bianisotropic sphere with the effective material parameters color-coded in Figure 1b and with $x = k_0R = 1$. Please note that to emphasize that our method is applicable to arbitrary bianisotropic materials, the effective parameters matrix $\hat{M}$ color-coded in the bottom of panel Figure 1b corresponds to a reciprocal material with effective parameters randomly generated in the range between -5 and 5. This material features anisotropic dielectric permittivity, magnetic permeability, and chirality tensors, which can be engineered by combining split-ring, helix, omega, fishnet, parallel-plate, and wire metaatoms [16,17].

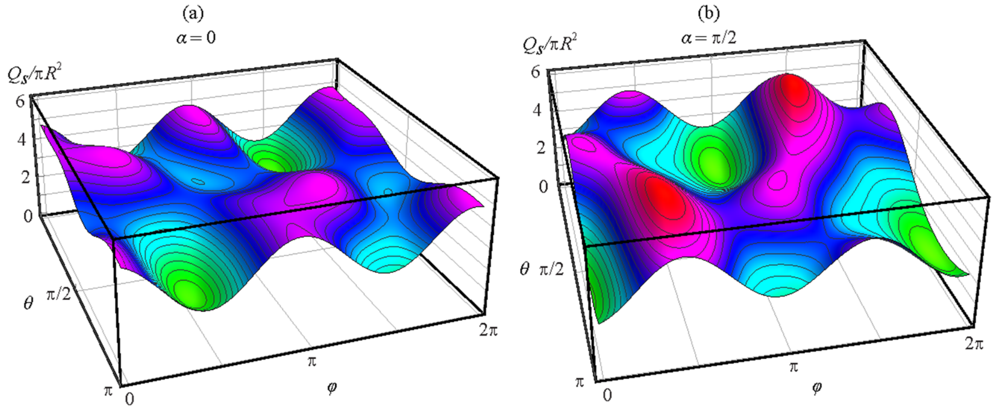

Figure 4. Reduced scattering cross-section $Q_s/(\pi R^2)$ for all incidence angles θ and ϕ for a bianisotropic sphere with the effective material parameters color-coded in Figure 1b and with $x = k_0R = 1$; In panel (**a**), the incidence polarization angle is $\alpha = 0$; in (**b**) $\alpha = \pi/2$. The color of the surface corresponds to the magnitude of $Q_s/(\pi R^2)$.

Figure 4a corresponds to the incidence polarization angle $\alpha = 0$, while in Figure 4b, the polarization angle is $\alpha = \pi/2$.

In Figure 4, one can see the strong dependence of scattering by the bianisotropic spheres in the incidence direction and polarization.

2.3. Expressions of Polarizability in the Rayleigh Limit

In the Rayleigh limit of electromagnetically small spheres $x \ll 1$, only the dipole terms of Mie's theory are retained. For $l,\ u = 1$, $g^{\alpha}_{MN} = g^{\alpha}_{ML} = g^{\alpha}_{NM} = 0$ and the E- and H-fields, Equations (7) and (8) can be written as

$$\boldsymbol{E} = \sum_{mv} \boldsymbol{M}^1_{1v}\left(g^{\alpha ED}_{MM}, g^{\alpha EB}_{MM}\right)_{m,v}\begin{pmatrix} f^{DM}_{1m} \\ f^{BM}_{1m}\end{pmatrix} + \sum_{mv} \boldsymbol{N}^1_{1v}\left(g^{\alpha ED}_{NN}, g^{\alpha EB}_{NN}\right)_{m,v}\begin{pmatrix} f^{DN}_{1m} \\ f^{BN}_{1m}\end{pmatrix} + \sum_{mv} \boldsymbol{L}^1_{1v}\left(g^{\alpha ED}_{NL}, g^{\alpha EB}_{NL}\right)_{m,v}\begin{pmatrix} f^{DN}_{1m} \\ f^{BN}_{1m}\end{pmatrix} \tag{27}$$

$$\boldsymbol{H} = \sum_{mv} \boldsymbol{M}^1_{1v}\left(g^{\alpha HD}_{MM}, g^{\alpha HB}_{MM}\right)_{m,v}\begin{pmatrix} f^{DM}_{1m} \\ f^{BM}_{1m}\end{pmatrix} + \sum_{mv} \boldsymbol{N}^1_{1v}\left(g^{\alpha HD}_{NN}, g^{\alpha HB}_{NN}\right)_{m,v}\begin{pmatrix} f^{DN}_{1m} \\ f^{BN}_{1m}\end{pmatrix} + \sum_{mv} \boldsymbol{L}^1_{1v}\left(g^{\alpha HD}_{NL}, g^{\alpha HB}_{NL}\right)_{m,v}\begin{pmatrix} f^{DN}_{1m} \\ f^{BN}_{1m}\end{pmatrix} \tag{28}$$

Applying Maxwell's equation to the E- and H-fields of Equations (20) and (21), we can obtain

$$-\boldsymbol{i}(\boldsymbol{k}_0/\boldsymbol{k})\boldsymbol{D} = \sum_{\boldsymbol{1m,1v}} \boldsymbol{N}^{\boldsymbol{1}}_{\boldsymbol{1v}} \cdot \left(g^{\alpha HD}_{MM}, g^{\alpha HB}_{MM}\right)_{m,v} \cdot \begin{pmatrix} \boldsymbol{f}^{\boldsymbol{DM}}_{\boldsymbol{1m}} \\ \boldsymbol{f}^{\boldsymbol{BM}}_{\boldsymbol{1m}}\end{pmatrix} + \sum_{\boldsymbol{1m,1v}} \boldsymbol{M}^{\boldsymbol{1}}_{\boldsymbol{1v}} \cdot \left(g^{\alpha HD}_{NN}, g^{\alpha HB}_{NN}\right)_{m,v} \cdot \begin{pmatrix} \boldsymbol{f}^{\boldsymbol{DN}}_{\boldsymbol{1m}} \\ \boldsymbol{f}^{\boldsymbol{BN}}_{\boldsymbol{1m}}\end{pmatrix}$$

$$\boldsymbol{i}(\boldsymbol{k}_0/\boldsymbol{k})\boldsymbol{B} = \sum_{\boldsymbol{1m,1v}} \boldsymbol{N}^{\boldsymbol{1}}_{\boldsymbol{1v}} \cdot \left(g^{\alpha ED}_{MM}, g^{\alpha EB}_{MM}\right)_{m,v} \cdot \begin{pmatrix} \boldsymbol{f}^{\boldsymbol{DM}}_{\boldsymbol{1m}} \\ \boldsymbol{f}^{\boldsymbol{BM}}_{\boldsymbol{1m}}\end{pmatrix} + \sum_{\boldsymbol{1m,1v}} \boldsymbol{M}^{\boldsymbol{1}}_{\boldsymbol{1v}} \cdot \left(g^{\alpha ED}_{NN}, g^{\alpha EB}_{NN}\right)_{m,v} \cdot \begin{pmatrix} \boldsymbol{f}^{\boldsymbol{DN}}_{\boldsymbol{1m}} \\ \boldsymbol{f}^{\boldsymbol{BN}}_{\boldsymbol{1m}}\end{pmatrix}$$

This translates into a system of equations

$$\hat{G}_M F_{Mq} = i(k_0/k_q)\hat{U}F_{Nq} \tag{29}$$

$$\hat{G}_N F_{Nq} = i(k_0/k_q)\hat{V}F_{Mq} \tag{30}$$

where $F_{Mq} = \left(f^{DM}_{1-1q}, f^{BM}_{1-1q}, f^{DM}_{10q}, f^{BM}_{10q}, f^{DM}_{11q}, f^{BM}_{11q}\right)^T$, $F_{Mq} = (f^{DN}_{1-1q}, f^{BN}_{1-1q}, f^{DN}_{10q}, f^{BN}_{10q}, f^{DN}_{11q}, f^{BN}_{11q})^T$, and the matrices $\hat{G}_M$ and $\hat{G}_N$ are composed of the coefficients g_{MM} and g_{NN}

$$\hat{G}_M = \begin{pmatrix} g^{\alpha HD}_{MM--} & g^{\alpha HB}_{MM--} & g^{\alpha HD}_{MM0-} & g^{\alpha HB}_{MM0-} & g^{\alpha HD}_{MM+-} & g^{\alpha HB}_{MM+-} \\ g^{\alpha ED}_{MM--} & g^{\alpha EB}_{MM--} & g^{\alpha ED}_{MM0-} & g^{\alpha EB}_{MM0-} & g^{\alpha ED}_{MM+-} & g^{\alpha EB}_{MM+-} \\ g^{\alpha HD}_{MM-0} & g^{\alpha HB}_{MM-0} & g^{\alpha HD}_{MM00} & g^{\alpha HB}_{MM00} & g^{\alpha HD}_{MM+0} & g^{\alpha HB}_{MM+0} \\ g^{\alpha ED}_{MM-0} & g^{\alpha EB}_{MM-0} & g^{\alpha ED}_{MM00} & g^{\alpha EB}_{MM00} & g^{\alpha ED}_{MM+0} & g^{\alpha EB}_{MM+0} \\ g^{\alpha HD}_{MM-+} & g^{\alpha HB}_{MM-+} & g^{\alpha HD}_{MM0+} & g^{\alpha HB}_{MM0+} & g^{\alpha HD}_{MM++} & g^{\alpha HB}_{MM++} \\ g^{\alpha ED}_{MM-+} & g^{\alpha EB}_{MM-+} & g^{\alpha ED}_{MM0+} & g^{\alpha EB}_{MM0+} & g^{\alpha ED}_{MM++} & g^{\alpha EB}_{MM++} \end{pmatrix}$$

$$\hat{G}_N = \begin{pmatrix} g^{\alpha ED}_{NN--} & g^{\alpha EB}_{NN--} & g^{\alpha ED}_{NN0-} & g^{\alpha EB}_{NN0-} & g^{\alpha ED}_{NN+-} & g^{\alpha EB}_{NN+-} \\ g^{\alpha HD}_{NN--} & g^{\alpha HB}_{NN--} & g^{\alpha HD}_{NN0-} & g^{\alpha HB}_{NN0-} & g^{\alpha HD}_{NN+-} & g^{\alpha HB}_{NN+-} \\ g^{\alpha ED}_{NN-0} & g^{\alpha EB}_{NN-0} & g^{\alpha ED}_{NN00} & g^{\alpha EB}_{NN00} & g^{\alpha ED}_{NN+0} & g^{\alpha EB}_{NN+0} \\ g^{\alpha HD}_{NN-0} & g^{\alpha HB}_{NN-0} & g^{\alpha HD}_{NN00} & g^{\alpha HB}_{NN00} & g^{\alpha HD}_{NN+0} & g^{\alpha HB}_{NN+0} \\ g^{\alpha ED}_{NN-+} & g^{\alpha EB}_{NN-+} & g^{\alpha ED}_{NN0+} & g^{\alpha EB}_{NN0+} & g^{\alpha ED}_{NN++} & g^{\alpha EB}_{NN++} \\ g^{\alpha HD}_{NN-+} & g^{\alpha HB}_{NN-+} & g^{\alpha HD}_{NN0+} & g^{\alpha HB}_{NN0+} & g^{\alpha HD}_{NN++} & g^{\alpha HB}_{NN++} \end{pmatrix}$$

while $\hat{U} = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$, $\hat{V} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix}$.

Excluding $F_{Mq} = i(k_q/k_0)\hat{V}\hat{G}_N F_{Nq}$ from the system Equations (29) and (30), we obtained an eigenproblem for F_{Nq}, which corresponded to six bianisotropic orbitals in the Rayleigh limit

$$(\hat{U}\hat{G}_M\hat{V}\hat{G}_N)F_{Nq} = (k_0/k_q)^2 F_{Nq} \tag{31}$$

The boundary conditions of Equations (17)–(20) turn into

$$j_1(k_0R)\ (pq) + h_1(k_0R)(ab) = \sum_q A_q j_1(k_qR)\, diag\{i,1,i,1,i,1\}\hat{G}_M F_{Mq} \tag{32}$$

$$\begin{gathered} \tfrac{\partial}{\partial r}[r\, j_1(k_0r)]_{r=R}\ (pq) + \tfrac{\partial}{\partial r}[r\, h_1(k_0r)]_{r=R}(ab) \\ = \sum_q A_q\left(\tfrac{k_0}{k_q}\right) diag\{1,i,1,i,1,i\} \times \left(\tfrac{\partial}{\partial r}\left[r\, j_1(k_qr)\right]_{r=R}\hat{G}_N F_{Nq} + j_1(k_qR)\hat{G}_L F_{Nq}\right) \end{gathered} \tag{33}$$

where $\hat{G}_L$ is composed of the coefficients g_{NL}, similar to the matrix $\hat{G}_N$ provided above, $(pq) = (p_{1-1}, q_{1-1}, p_{10}, q_{10}, p_{11}, q_{11})^T$, and $(ab) = (a_{1-1}, b_{1-1}, a_{10}, b_{10}, a_{11}, b_{11})^T$.

Taking the limit of $k_qR, k_0R \to 0$ in the spherical Bessel functions, and excluding the scattered amplitudes (ab), and substituting Equation (29) for $\hat{G}_M F_{Mq}$, we obtained

$$3(pq) = diag\{1,i,1,i,1,i\}\left(\hat{1} + 2\hat{G}_N + \hat{G}_L\right)\hat{F}_N\vec{A} \tag{34}$$

Equation (34) can be re-written using $\begin{pmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{pmatrix} = \frac{1}{\sqrt{3\pi}}\hat{T}^{-1}\hat{F}_N\vec{A}$, $(pq) = \sqrt{3\pi}\hat{T}\begin{pmatrix} \boldsymbol{\epsilon} \\ \boldsymbol{h} \end{pmatrix}$, and the matrix $\hat{T}$ given by $\hat{T} = \begin{pmatrix} -i & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & +i & 0 \\ 0 & 0 & -i\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{2} \\ i & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +i & 0 \end{pmatrix}$.

In accordance with Equation (34), $(\hat{1} + 2\hat{G}_N + \hat{G}_L) = \hat{T}(\hat{1} + 2\hat{M}^{-1})\hat{T}^{-1}$, or $3\hat{T}^{-1}(\hat{1} + 2\hat{G}_N + \hat{G}_L)^{-1}\hat{T} = 3\hat{M}(\hat{M} + 2\hat{1})^{-1}$. This resulted in

$$\begin{pmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{pmatrix} = 3\hat{M}(\hat{M} + 2\hat{1})^{-1}\begin{pmatrix} \boldsymbol{\epsilon} \\ \boldsymbol{h} \end{pmatrix} \tag{35}$$

Considering that $\begin{pmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{pmatrix} = \begin{pmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{pmatrix} + 4\pi\begin{pmatrix} \boldsymbol{P} \\ \boldsymbol{M} \end{pmatrix} = \hat{M}^{-1}\begin{pmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{pmatrix} + 4\pi\begin{pmatrix} \boldsymbol{P} \\ \boldsymbol{M} \end{pmatrix}$, we found $\begin{pmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{pmatrix} = 4\pi(\hat{1} - \hat{M}^{-1})^{-1}\begin{pmatrix} \boldsymbol{P} \\ \boldsymbol{M} \end{pmatrix}$,

$$\begin{pmatrix} \boldsymbol{P} \\ \boldsymbol{M} \end{pmatrix} = \frac{3}{4\pi}(\hat{M} - \hat{1})(\hat{M} + 2\hat{1})^{-1}\begin{pmatrix} \boldsymbol{\epsilon} \\ \boldsymbol{h} \end{pmatrix} \tag{36}$$

From this, we obtained the polarizability $\hat{\alpha}$ of the sphere of volume V in the Rayleigh approximation

$$\begin{pmatrix} \boldsymbol{p} \\ \boldsymbol{m} \end{pmatrix} = V\begin{pmatrix} \boldsymbol{P} \\ \boldsymbol{M} \end{pmatrix} = \hat{\alpha}\begin{pmatrix} \boldsymbol{\epsilon} \\ \boldsymbol{h} \end{pmatrix} = \frac{3V}{4\pi}(\hat{M} - \hat{1})(\hat{M} + 2\hat{1})^{-1}\begin{pmatrix} \boldsymbol{\epsilon} \\ \boldsymbol{h} \end{pmatrix}$$

This agrees with the polarizability of the bianisotropic spheres obtained previously in electrostatic approximations [67–69].

3. Discussion and Conclusions

Mie's theory of electromagnetic scattering by spheres is a very important part of electromagnetism. In the existing literature, it has been extended from the original results of Mie to bi-isotropic spheres by Bohren [40], and, recently, to anisotropic spheres by Lin et al. and Li et al. [43–45]. Nevertheless, there is no existing theory of scattering by bianisotropic spheres, and the methods used to find the scattering for isotropic or anisotropic spheres are not applicable to bianisotropic spheres.

The extension of our approach to other geometries could be very promising. For example, recently much attention has been paid to the Mie resonances in nanocylinder systems [70–72], and we believe that this opens a broad avenue for application.

To conclude, in this study, we introduced the bianisotropic orbitals and presented a theory of the scattering by bianisotropic spheres with arbitrary effective media parameters and sizes. In the Rayleigh limit, we obtained the results known from the electrostatic approximation approach.

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Conflicts of Interest: The author declares no conflict of interest.

Appendix A

We used a definition of vector spherical harmonics (VSH) that built upon the definitions of Stratton [61], Jackson [62], and Varshalovich et al. [63]. The starting point was the solution of the scalar Helmholtz equation $\nabla^2\psi + k^2\psi = 0$

$$\psi_{lm}^{(j)} = -\frac{1}{i\sqrt{l(l+1)}} z_l^{(j)}(kr)Y_{lm},\ \psi_{00}^{(j)} = iz_0^{(j)}(kr)Y_{00},$$

where the scalar spherical harmonic is $Y_{lm}(\hat{\boldsymbol{r}}) = \sqrt{\frac{2l+1}{4\pi}\cdot\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\varphi}$.

The VSH are derived from $\psi_{lm}^{(j)}$, analogous to the definitions of Stratton [61], as

$$\boldsymbol{L}_{lm}^{(j)} = \frac{1}{k}\nabla\psi_{lm}^{(j)},\ \boldsymbol{M}_{lm}^{(j)} = \nabla\times\left(\boldsymbol{r}\psi_{lm}^{(j)}\right),\ \boldsymbol{N}_{lm}^{(j)} = \frac{1}{k}\nabla\times\boldsymbol{M}_{lm}^{(j)}$$

$$\boldsymbol{L}_{00}^{(j)} = \frac{1}{k}\nabla\psi_{00}^{(j)},\ \boldsymbol{M}_{00}^{(j)} = 0,\ \boldsymbol{N}_{00}^{(j)} = 0$$

In spherical coordinates, these VSH can be expressed as

$$\boldsymbol{L}_{lm}^{(j)} = \frac{1}{k}\nabla\psi_{lm}^{(j)} = \frac{1}{k}\frac{\partial\psi_{lm}^{(j)}}{\partial r}\hat{\boldsymbol{r}} + \frac{1}{kr}\frac{\partial\psi_{lm}^{(j)}}{\partial\theta}\hat{\boldsymbol{\theta}} + \frac{1}{kr}\frac{im}{\sin\theta}\psi_{lm}^{(j)}\hat{\boldsymbol{\varphi}}$$

$$\boldsymbol{M}_{lm}^{(j)} = \nabla\times\left(\boldsymbol{r}\psi_{lm}^{(j)}\right) = \frac{im}{\sin\theta}\psi_{lm}^{(j)}\hat{\boldsymbol{\theta}} - \frac{\partial\psi_{lm}^{(j)}}{\partial\theta}\hat{\boldsymbol{\varphi}}$$

$$\boldsymbol{N}_{lm}^{(j)} = \frac{1}{k}\nabla\times\boldsymbol{M}_{lm}^{(j)} = \frac{l(l+1)}{kr}\psi_{lm}^{(j)}\hat{\boldsymbol{r}} + \frac{1}{kr}\frac{\partial^2}{\partial r\partial\theta}\left[r\psi_{lm}^{(j)}\right]\hat{\boldsymbol{\theta}} + \frac{1}{kr}\frac{im}{\sin\theta}\frac{\partial}{\partial r}\left[r\psi_{lm}^{(j)}\right]\hat{\boldsymbol{\varphi}}$$

These harmonics are directly related to the harmonics of Jackson [62]

$$\boldsymbol{X}_{lm}(\hat{\boldsymbol{r}}) = \frac{1}{\sqrt{l(l+1)}}\boldsymbol{L}Y_{lm},\ \hat{\boldsymbol{r}}Y_{lm},\ \hat{\boldsymbol{r}}\times\boldsymbol{X}_{lm},$$

where $\boldsymbol{L} = -i(\boldsymbol{r}\times\nabla)$ is the angular momentum operator

$$\boldsymbol{M}_{lm}^{(j)} = \frac{z_l^{(j)}(kr)}{i\sqrt{l(l+1)}}\boldsymbol{r}\times\nabla Y_{lm} = z_l^{(j)}(kr)\boldsymbol{X}_{lm}(\hat{\boldsymbol{r}})$$

$$\boldsymbol{N}_{lm}^{(j)} = \frac{1}{k}\nabla\times\left(z_l^{(j)}(kr)\boldsymbol{X}_{lm}(\hat{\boldsymbol{r}})\right) = \frac{i\sqrt{l(l+1)}}{kr}z_l^{(j)}(kr)\hat{\boldsymbol{r}}Y_{lm} + \frac{1}{kr}\frac{\partial}{\partial r}\left(rz_l^{(j)}(kr)\right)\hat{\boldsymbol{r}}\times\boldsymbol{X}_{lm}$$

The vector spherical harmonics $\boldsymbol{L}_{lm}^{(j)}$, $\boldsymbol{N}_{lm}^{(j)}$, $\boldsymbol{M}_{lm}^{(j)}$ can be expressed using the harmonics $\boldsymbol{Y}_{jm}^{l}(\hat{\boldsymbol{r}})$ of Varshalovich et al. [63].

$$\begin{pmatrix}\boldsymbol{L}_{lm}^{(j)}\\ \boldsymbol{M}_{lm}^{(j)}\\ \boldsymbol{N}_{lm}^{(j)}\end{pmatrix} = \begin{pmatrix}\frac{iz_{l-1}^{(j)}(kr)}{\sqrt{(l+1)(2l+1)}} & 0 & \frac{iz_{l+1}^{(j)}}{\sqrt{l(2l+1)}}\\ 0 & z_l^{(j)} & 0\\ i\sqrt{\frac{l+1}{2l+1}}z_{l-1}^{(j)} & 0 & -i\sqrt{\frac{l}{2l+1}}z_{l+1}^{(j)}\end{pmatrix}\begin{pmatrix}\boldsymbol{Y}_{lm}^{l-1}\\ \boldsymbol{Y}_{lm}^{l}\\ \boldsymbol{Y}_{lm}^{l+1}\end{pmatrix} \tag{A1}$$

According to the quantum theory of angular momentum, the vector spherical harmonics of Varshalovich et al. [63] can be expressed on a spherical basis by using Clebsch–Gordan coefficients.

$$\boldsymbol{Y}^{l}_{jm}(\hat{\boldsymbol{r}}) = \sum_{m',\sigma} lm'1\sigma|jmY_{lm'}(\hat{\boldsymbol{r}})\boldsymbol{e}_{\sigma} = \sum_{m',\sigma} C^{jm}_{lm',1\sigma} Y_{lm'}\boldsymbol{e}_{\sigma}$$

where the spherical basis vectors are the eigenstates of the spin operators S^2 and S_z.

$$\boldsymbol{e}_{\pm 1} = \mp\frac{1}{\sqrt{2}}(\hat{\boldsymbol{x}} \pm i\hat{\boldsymbol{y}}),\ \boldsymbol{e}_0 = \hat{\boldsymbol{z}}$$

Appendix B

The bianisotropic orbitals provided by the solutions of Equation (10) can be represented as an expansion over the plane wave solutions of method of the index of refraction's operator [31–33], with the indexes of refraction related to the radial quantum number k_q given by $n = k_q/k_0$. This can be understood by inspecting the expansion of the scalar spherical harmonics $\psi^{(1)}_{lm}$.

$$\psi^{(1)}_{lm}(k_q;r) = -\frac{1}{i\sqrt{l(l+1)}} j_l(k_q r) Y_{lm}(\hat{\boldsymbol{r}}) = \int \psi^{(1)}_{lm}(k_q;\boldsymbol{k})\ e^{i\boldsymbol{kr}} \frac{d^3k}{(2\pi)^3}$$

According to [63],

$$\psi^{(1)}_{lm}(k_q;\boldsymbol{k}) = \int \psi^{(1)}_{lm}(k_q;\boldsymbol{r})\ e^{-i\boldsymbol{kr}}\ dV = -\frac{(-1)^l}{i\sqrt{l(l+1)}} 2\pi^2 i^l \frac{\delta(k_q - k)}{k_q^2} Y_{lm}(\hat{\boldsymbol{k}})$$

which means that all scalar spherical harmonics contain only the plane waves with the wavenumbers k_q as follows

$$\psi^{(1)}_{lm}(k_q;\boldsymbol{r}) = -\frac{(-1)^l}{i\sqrt{l(l+1)}} \pi i^l \int e^{ik_q\hat{\boldsymbol{k}}\boldsymbol{r}}\ Y_{lm}(\hat{\boldsymbol{k}}) \frac{d^2\Omega_{\boldsymbol{k}}}{(2\pi)^2}$$

Correspondingly, the vector spherical harmonics are

$$\boldsymbol{L}^{(1)}_{lm} = \frac{1}{k_q}\nabla\psi^{(1)}_{lm} = -\frac{(-1)^l}{i\sqrt{l(l+1)}} \pi i^l \int e^{ik_q\hat{\boldsymbol{k}}\boldsymbol{r}}\ \hat{\boldsymbol{k}} Y_{lm}(\hat{\boldsymbol{k}}) \frac{d^2\Omega_{\boldsymbol{k}}}{(2\pi)^2}$$

$$\begin{aligned}\boldsymbol{M}^{(1)}_{lm} &= \nabla\times\left(\boldsymbol{r}\psi^{(1)}_{lm}\right) = j_l(k_q r)\boldsymbol{X}_{lm}(\hat{\boldsymbol{r}}) = \tfrac{j_l(k_q r)}{\sqrt{l(l+1)}}\hat{\boldsymbol{L}}Y_{lm} \\ &= -\tfrac{(-1)^l}{i\sqrt{l(l+1)}}\pi i^l \int e^{ik_q\hat{\boldsymbol{k}}\boldsymbol{r}}\ \hat{\boldsymbol{L}}_{\boldsymbol{k}} Y_{lm}(\hat{\boldsymbol{k}}) \tfrac{d^2\Omega_{\boldsymbol{k}}}{(2\pi)^2}\end{aligned}$$

$$\begin{aligned}\boldsymbol{N}^{(1)}_{lm} &= \tfrac{1}{k_q}\nabla\times\boldsymbol{M}^{(1)}_{lm} = \tfrac{1}{k_q}\nabla\times\left(j_l(k_q r)\boldsymbol{X}_{lm}(\hat{\boldsymbol{r}})\right) \\ &= -\tfrac{(-1)^l}{i\sqrt{l(l+1)}}\pi i^{l-1} \int e^{ik_q\hat{\boldsymbol{k}}r}\ \left[\hat{\boldsymbol{k}}\times\hat{\boldsymbol{L}}_{\boldsymbol{k}}\right] Y_{lm}(\hat{\boldsymbol{k}}) \tfrac{d^2\Omega_{\boldsymbol{k}}}{(2\pi)^2}\end{aligned}$$

Appendix C

According to [63],

$$\begin{aligned}\boldsymbol{a}e^{i\boldsymbol{kr}} &= 4\pi \sum_{lm}\sum_{q=l-1}^{l+1} i^q \left\{\boldsymbol{a}\cdot\boldsymbol{Y}^{q*}_{lm}(\hat{\boldsymbol{k}})\right\} j_q(kr)\boldsymbol{Y}^{q}_{lm}(\hat{\boldsymbol{r}}) \\ &= 4\pi \sum_{lm}\Big(i^{l-1}\left\{\boldsymbol{a}\cdot\boldsymbol{Y}^{l-1*}_{lm}(\hat{\boldsymbol{k}})\right\} j_{l-1}(kr)\boldsymbol{Y}^{l-1}_{lm}(\hat{\boldsymbol{r}}) \\ &+ i^l\left\{\boldsymbol{a}\cdot\boldsymbol{Y}^{l*}_{lm}(\hat{\boldsymbol{k}})\right\} j_l(kr)\boldsymbol{Y}^{l}_{lm}(\hat{\boldsymbol{r}}) + i^{l+1}\left\{\boldsymbol{a}\cdot\boldsymbol{Y}^{l+1*}_{lm}(\hat{\boldsymbol{k}})\right\} j_{l+1}(kr)\boldsymbol{Y}^{l+1}_{lm}(\hat{\boldsymbol{r}})\Big)\end{aligned}$$

From Equation (A1),

$$\begin{pmatrix} z_{l-1}^{(j)}\boldsymbol{Y}_{lm}^{l-1} \\ z_{l}^{(j)}\boldsymbol{Y}_{lm}^{l} \\ z_{l+1}^{(j)}\boldsymbol{Y}_{lm}^{l+1} \end{pmatrix} = \begin{pmatrix} -\frac{il\sqrt{l+1}}{\sqrt{2l+1}} & 0 & -\frac{i\sqrt{l+1}}{\sqrt{2l+1}} \\ 0 & 1 & 0 \\ -\frac{i\sqrt{l(l+1)}}{\sqrt{2l+1}} & 0 & i\sqrt{\frac{l}{2l+1}} \end{pmatrix} \begin{pmatrix} \boldsymbol{L}_{lm}^{(j)} \\ \boldsymbol{M}_{lm}^{(j)} \\ \boldsymbol{N}_{lm}^{(j)} \end{pmatrix}$$

$$\begin{aligned} \boldsymbol{a}e^{i\boldsymbol{kr}} = 4\pi \sum_{lm} i^l \Big(& \left\{\boldsymbol{a}\cdot\boldsymbol{Y}_{lm}^{l-1*}(\hat{\boldsymbol{k}})\right\}\left(-\tfrac{l\sqrt{l+1}}{\sqrt{2l+1}}\boldsymbol{L}_{lm}^{(1)} - \tfrac{\sqrt{l+1}}{\sqrt{2l+1}}\boldsymbol{N}_{lm}^{(1)}\right) \\ & +\left\{\boldsymbol{a}\cdot\boldsymbol{Y}_{lm}^{l*}(\hat{\boldsymbol{k}})\right\}\boldsymbol{M}_{lm}^{(1)} \\ & +\left\{\boldsymbol{a}\cdot\boldsymbol{Y}_{lm}^{l+1*}(\hat{\boldsymbol{k}})\right\}\left(\tfrac{\sqrt{l(l+1)}}{\sqrt{2l+1}}\boldsymbol{L}_{lm}^{(1)} - \sqrt{\tfrac{l}{2l+1}}\boldsymbol{N}_{lm}^{(1)}\right)\Big) \\ = 4\pi \sum_{lm} i^l \Big(& -\sqrt{l(l+1)}\boldsymbol{a}\cdot\left(\tfrac{\sqrt{l}}{\sqrt{2l+1}}\boldsymbol{Y}_{lm}^{l-1*}(\hat{\boldsymbol{k}}) - \tfrac{\sqrt{l+1}}{\sqrt{2l+1}}\boldsymbol{Y}_{lm}^{l+1*}(\hat{\boldsymbol{k}})\right)\boldsymbol{L}_{lm}^{(1)} \\ & +\left\{\boldsymbol{a}\cdot\boldsymbol{Y}_{lm}^{l*}(\hat{\boldsymbol{k}})\right\}\boldsymbol{M}_{lm}^{(1)} - \boldsymbol{a} \\ & \cdot\left(\tfrac{\sqrt{l+1}}{\sqrt{2l+1}}\boldsymbol{Y}_{lm}^{l-1*}(\hat{\boldsymbol{k}}) + \tfrac{\sqrt{l}}{\sqrt{2l+1}}\boldsymbol{Y}_{lm}^{l+1*}(\hat{\boldsymbol{k}})\right)\boldsymbol{N}_{lm}^{(1)}\Big) \end{aligned}$$

$$\begin{aligned} \boldsymbol{Y}_{lm}^{(-1)}(\hat{\boldsymbol{k}}) &= \tfrac{\sqrt{l}}{\sqrt{2l+1}}\boldsymbol{Y}_{lm}^{l-1}(\hat{\boldsymbol{k}}) - \tfrac{\sqrt{l+1}}{\sqrt{2l+1}}\boldsymbol{Y}_{lm}^{l+1}(\hat{\boldsymbol{k}}),\ \boldsymbol{Y}_{lm}^{(+1)}(\hat{\boldsymbol{k}}) \\ &= \left(\tfrac{\sqrt{l+1}}{\sqrt{2l+1}}\boldsymbol{Y}_{lm}^{l-1}(\hat{\boldsymbol{k}}) + \tfrac{\sqrt{l}}{\sqrt{2l+1}}\boldsymbol{Y}_{lm}^{l+1}(\hat{\boldsymbol{k}})\right) \end{aligned}$$

We arrive at

$$\boldsymbol{a}e^{i\boldsymbol{kr}} = 4\pi\sum_{lm} i^l\left(-\sqrt{l(l+1)}\left\{\boldsymbol{a}\cdot\boldsymbol{Y}_{lm}^{(-1)*}(\hat{\boldsymbol{k}})\right\}\boldsymbol{L}_{lm}^{(1)} + \left\{\boldsymbol{a}\cdot\boldsymbol{Y}_{lm}^{l*}(\hat{\boldsymbol{k}})\right\}\boldsymbol{M}_{lm}^{(1)} - \left\{\boldsymbol{a}\cdot\boldsymbol{Y}_{lm}^{(+1)*}(\hat{\boldsymbol{k}})\right\}\boldsymbol{N}_{lm}^{(1)}\right)$$

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