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Manipulating the Lorentz force via the chirality of nanoparticles

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ABSTRACT

We demonstrate that a single plane wave pulls a chiral nanoparticle toward the light source. The nanoparticle exhibits optical gain in a particular wavelength region. The equivalence of the generalized and alternative expressions of the Lorentz force density relating to bound charges for chiral media is numerically validated. By considering the two-dimensional electromagnetic problem of incident plane waves normally impinged on active chiral cylinders, it is shown that the gradient force is mainly contributed by the bound electric and magnetic current densities of the cross-polarized waves. We also investigate how the medium parameters and impedance mismatch can be used to manipulate the pulling or pushing Lorentz forces between two chiral cylinders. This finding may provide a recipe to understand the light interaction with multiple chiral nanoparticles of arbitrary shapes (in general) with the aid of the numerical approach. It could be a promising avenue in controlling the optical micromanipulation for chiral nanoparticles with mirroring asymmetry.

1. Introduction

Since the first experimental observation of the trapping of dielectric particles by a single beam [1] was demonstrated, new opportunities have been provided to study light harvesting objects [2–4] in biology, medicine, and engineering. The research on optical manipulation of particles mostly focuses on the configuration of optical fields [5–7], and medium structures [8–11], for instance, nonmagnetic anisotropic beads [8], graded-index media [9], and gain medium structures [10,11]. The light amplification of general active materials [10,11] or chiral materials with an active imaginary part of the permittivity or permeability may cause a nanoscale body to be pulled toward a light source.

The common active media include liquids, gases, solids, and semiconductors [10–17] etc. Some of the active media are non-chiral [10,11], others are chiral [12–17]. Large chiral multi-functionalized molecules [12,13], chiral metamaterials [14,15] with giant optical rotation, chiral boron nitride nanotubes [16], and green fluorescent proteins in cells [17] may be potential active chiral materials. The optical forces generated by chiral materials are mostly concentrated on passive chiral spheres using the Mie theory [18] or designing structured beams [5,6], such as nondiffractive Bessel beams [6]. Two counterpropagating incoherent plane wave sources are needed to induce a pulling force on a chiral structure made up of 25 metallic spheres [5]. The analytical Mie series method is not appropriate for the computation of non-spherical particles. Furthermore, the Mie series solution is based on the Bohren's decomposition without considering the real-time magneto-electric coupling properties of chiral media, that is, electromagnetic fields in an uncoupled effective chiral medium [18] are decomposed into a set of uncoupled waves in two equivalent isotropic media. Electromagnetic waves and energy in chiral media with chiral nihility (*i.e.*, $\varepsilon = \mu = 0$, and $\kappa \neq 0$) are analyzed [19]. In fact, the dispersive nature of the electric permittivity, magnetic permeability, and chilarity [20] must be considered for modeling the interplay of waves and chiral media.

Compared with analytical approaches [18,21], the Finite-Difference Time-Domain (FDTD) method [22–30] can record fields for various shapes of chiral materials at any specified location in space as a function of time. Compared with other numerical approaches, the FDTD method can simulate three types of chiral media [12–19,30–33], namely natural chiral materials like organic molecules [30], man-made chiral materials composed

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of rosettes or helices [14–16], and pure chiral media equivalent to dispersive media [18]. The BI-FDTD method [25] is based on a wavefield decomposition like the Mie series solution. Nevertheless, the constitutive relations for the effective chiral media can be directly implemented into some dispersive FDTD methods [20]. The Lorentz force on dielectric or magnetic dispersive achiral media has been given [26,27]. The radiation pressure of chiral slabs [29] without considering induced bound charges under a plane wave normal incidence is discussed. Compared with the one dimensional (1D) case, the distribution of spatially electromagnetic waves at oblique incidence and the Lorentz force density of chiral media with complicated shapes can be simulated with two dimensional (2D) computational methods. Moreover, the disputable equivalence of $(\mathbf{P}\cdot\nabla)\mathbf{E}$ and $(-\nabla\cdot\mathbf{P})\mathbf{E}$ [34] for chiral media needs to be further confirmed.

In this paper, the issue of manipulating the optically force via the chirality of active chiral media is considered by studying the two-dimensional electromagnetic problem of plane waves propagation in chiral cylinders. First, the auxiliary differential equation (ADE) FDTD method, as well as the generalized and alternative time-averaged Lorentz force density for chiral media are expanded and discretized in 2D Yee cells. Then, the validation of algorithms is performed by comparing computed data [27] with the numerical results of the ADE-FDTD method in the case of a dielectric cylinder under a plane wave incidence. The co- and cross-polarized field distributions in and around chiral media are obtained by using the FDTD method, which allows us to access the electromagnetic force acting on chiral objects. Finally, the possible factors affecting the positive or negative Lorentz force densities exerted on single or two chiral cylindrical rods are analyzed.

2. Theory

2.1. Constitutive relations

The magneto-electric coupling constitutive relations for bi-isotropic media in the frequency domain can be described as [31].

$$\begin{aligned}\mathbf{D}(\omega) &= \varepsilon(\omega)\mathbf{E} + [\chi(\omega) - \mathrm{j}\kappa(\omega)]\sqrt{\mu_0\varepsilon_0}\mathbf{H},\\ \mathbf{B}(\omega) &= \mu(\omega)\mathbf{H} + [\chi(\omega) + \mathrm{j}\kappa(\omega)]\sqrt{\mu_0\varepsilon_0}\mathbf{E},\end{aligned} \tag{1}$$

where $\varepsilon(\omega)$, $\mu(\omega)$, $\kappa(\omega)$, and $\chi(\omega)$ are frequency-dependent permittivity, permeability, chirality, and Tellegen parameters, respectively. A pure chiral medium, *i.e.* $\chi(\omega) = 0$ is discussed in this paper.

The effective and macroscopic medium parameters [12–16] of natural and artificial chiral media are determined by the material, physical geometric construction, and incident angle etc. The Lorentzian models are generally used to characterize the permittivity and permeability, and a Condon model is used to represent the chirality of chiral media, that is,

$$\begin{aligned}\varepsilon(\omega) &= \varepsilon_\infty\varepsilon_0 + (\varepsilon_s - \varepsilon_\infty)\varepsilon_0\omega_e^2\Big/\left(\omega_e^2 - \omega^2 + \mathrm{j}2\xi_e\omega\right),\\ \mu(\omega) &= \mu_\infty\mu_0 + (\mu_s - \mu_\infty)\mu_0\omega_h^2\Big/\left(\omega_h^2 - \omega^2 + \mathrm{j}2\xi_h\omega\right),\\ \kappa(\omega) &= \tau_\kappa\omega_\kappa^2\omega\Big/\left(\omega_\kappa^2 - \omega^2 + \mathrm{j}2\omega_\kappa\xi_\kappa\omega\right).\end{aligned} \tag{2}$$

In Eq. (2), ε_s, μ_s, ε_∞, and μ_∞ are the permittivity and permeability at zero and infinite frequencies, respectively. ω_e, ω_h, and ω_κ are resonance angular frequencies. ξ_e, ξ_h, and ξ_κ represent damping factors, and τ_κ represents a characteristic time constant measuring the magnitude of the optical rotation. The chirality of the chiral nanoparticles could be affected by the geometric dimensions, such as helix radius, width, thickness, contour length, and pitch angle. The chirality can be obtained with the circular dichroism spectroscopy of biological substances [2]. The medium parameters studied in this paper are not representative of a specific system of molecules or cells. The Lorentz force density and the ADE-FDTD method proposed in this paper can be implemented to any system that is equivalent to a dispersive chiral medium.

The wave vectors of two eigenwaves in chiral media are

$$k_\pm = k_0\sqrt{\mu_r\varepsilon_r}\pm\kappa_r, \tag{3}$$

where k_0 is the free-space wavenumber. ε_r, μ_r, and κ_r are the relative permittivity, permeability, and chirality, respectively. For an active chiral medium, at least one wave vector of the eigenwaves has a positive imaginary part; thus, one of the propagating modes will grow exponentially.

If the loss (gain) is included, conditions of the imaginary parts of permittivity, permeability, and chirality for a passive chiral medium are [22].

$$\mathrm{Im}[\varepsilon] < 0, \quad \mathrm{Im}[\mu] < 0, \quad \mathrm{Im}^2(\kappa) < [\mathrm{Im}(\varepsilon)\mathrm{Im}(\mu)/(\varepsilon_0\mu_0)]. \tag{4}$$

Otherwise, the chiral medium becomes an active one [11,22,31]. If the medium parameters do not satisfy any of the conditions in Eq. (4), the chiral medium is active.

2.2. 2D ADE-FDTD method

By introducing the transform relation between frequency domain and time domain ($\mathrm{j}\omega\to\partial/\partial t$), the electromagnetic field and current equations used to model waves propagation in chiral media can be got

$$\begin{aligned}&\nabla\times\mathbf{H} = \varepsilon_\infty\varepsilon_0\partial\mathbf{E}/\partial t + \mathbf{J} + \mathbf{K}_c,\\ &\partial^2\mathbf{J}/\partial^2 t + 2\xi_e\partial\mathbf{J}/\partial t + \omega_e^2\mathbf{J} = (\varepsilon_s - \varepsilon_\infty)\varepsilon_0\omega_e^2\partial\mathbf{E}/\partial t,\\ &\partial^2\mathbf{K}/\partial^2 t + 2\xi_h\partial\mathbf{K}/\partial t + \omega_h^2\mathbf{K} = (\mu_s - \mu_\infty)\mu_0\omega_h^2\partial\mathbf{H}/\partial t,\\ &\nabla\times\mathbf{E} = -\mu_\infty\mu_0\partial\mathbf{H}/\partial t - \mathbf{K} - \mathbf{J}_c,\\ &\partial^2\mathbf{J}_c/\partial^2 t + 2\omega_\kappa\xi_\kappa\partial\mathbf{J}_c/\partial t + \omega_\kappa^2\mathbf{J}_c = \tau_\kappa\omega_\kappa^2\sqrt{\mu_0\varepsilon_0}\partial^2\mathbf{E}/\partial^2 t,\\ &\partial^2\mathbf{K}_c/\partial^2 t + 2\omega_\kappa\xi_\kappa\partial\mathbf{K}_c/\partial t + \omega_\kappa^2\mathbf{K}_c = -\tau_\kappa\omega_\kappa^2\sqrt{\mu_0\varepsilon_0}\partial^2\mathbf{H}/\partial^2 t.\end{aligned} \tag{5}$$

Then, the field and current equations containing constitutive relations for chiral media can be deduced and numerically solved by means of the ADE-FDTD method. For the two dimensional case, the physical quantities are independent of z axis i.e. $\partial/\partial z = 0$. For simplicity, only the field components of the Transverse Magnetic (TM) waves are given in this paper. Thus, the spatial and time iterative equations for the source-free chiral media are in the following form,

$$\begin{aligned}E_z^{n+1}(i,j) = E_z^n(i,j) &- \frac{\Delta t}{\varepsilon_\infty\varepsilon_0}\left[J_z^{n+\frac12}(i,j) + K_{cz}^n\left(i+\frac12,j+\frac12\right)\right]\\ &+\frac{\Delta t}{\varepsilon_\infty\varepsilon_0}\times\left[\begin{array}{c}\dfrac{H_y^{n+\frac12}\left(i+\frac12,j\right) - H_y^{n+\frac12}\left(i-\frac12,j\right)}{\Delta x}\\ -\dfrac{H_x^{n+\frac12}\left(i,j+\frac12\right) - H_x^{n+\frac12}\left(i,j-\frac12\right)}{\Delta y}\end{array}\right],\end{aligned}$$

$$\begin{aligned}J_z^{n+\frac32}(i,j) &= \alpha_x J_z^{n+\frac12}(i,j) + \beta_x J_z^{n-\frac12}(i,j)\\ &+ \gamma_x\left[E_z^{n+1}(i,j) - E_z^{n-1}(i,j)\right],\end{aligned}$$