Optical Force and Torque on Dipolar Dual Chiral Particles

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On the one hand, electromagnetic dual particles preserve the helicity of light upon interaction. On the other hand, chiral particles respond differently to light of opposite helicity. These two properties on their own constitute a source of fascination. Their combined action, however, is less explored. Here, we study on analytical grounds the force and torque as well as the optical cross sections of dual chiral particles in the dipolar approximation exerted by a particular wave of well-defined helicity: A circularly polarized plane wave. We put emphasis on particles that possess a maximally electromagnetic chirality and hence dual response. Besides the analytical insights, we also investigate the exerted optical force and torque on a real particle at the example of a metallic helix that is designed to approach the maximal electromagnetic chirality condition. Various applications in the context of optical sorting but also nanorobotics can be foreseen considering the particles studied in this contribution.

PACS numbers: 78.20.Bh, 78.67.Bf, 87.85.St, 81.05.Xj

Electromagnetic (EM) duality is the symmetry of nature for electric and magnetic quantities, and it can be exploited in the study of light-matter interaction. This symmetry, as implied by the source-free Maxwell’s equations, holds in free space, but it is normally broken inside a material. This is because materials respond differently to electric and magnetic fields, i.e. the permittivity is different from the permeability. However, dual particles, at least in the dipolar approximation, are realizable. Then, it is only required that their electric and magnetic dipole polarizabilities are identical and that the cross polarizabilities are equal in magnitude but opposite in sign. This can be achieved even using basic objects such as a sphere made from a material with a sufficiently large permittivity. For a certain combination of diameter, permittivity, and wavelength, the lowest order electric and magnetic Mie coefficient will be the same, satisfying the condition of duality.

Mathematically, EM duality is the invariance of Maxwell’s equations under the non-geometric duality transformation:

\[ \mathbf{E} \rightarrow \mathbf{E}\cos \theta - Z\mathbf{H}\sin \theta, \]
\[ Z\mathbf{H} \rightarrow \mathbf{E}\sin \theta + Z\mathbf{H}\cos \theta, \]

where \( \theta \) is an arbitrary angle, \( Z \) is the impedance of the medium; and \( \mathbf{E} \) and \( \mathbf{H} \) are the electric and magnetic field vectors, respectively. The importance of dual particles is that they preserve the helicity of the incident light. Helicity \( \Lambda \) is the light’s total angular momentum \( \mathbf{J} \) in the direction of the light’s linear momentum \( \mathbf{P} \), i.e. \( \Lambda = \mathbf{J} \cdot \mathbf{P} / |\mathbf{P}| \).

While EM duality necessitates the preservation of the incident light’s helicity, chirality allows for a different strength in the response of the particle to light possessing an opposite helicity. Chirality, as an intrinsic asymmetry in nature, is an important footprint of biological systems. An object is said to be chiral, as it was coined by Lord Kelvin, if it is not superimposable onto its mirror image by any rotation or translation. The necessary asymmetry is the reason for the different response of the particle when illuminated by waves of opposite helicity.

Chirality on its own, however, is only a binary condition. It neither allows ranking particles according to their chirality nor it allows to conclude how chiral a given object is with respect to a maximal chirality it might attain. These issues have been recently solved by introducing a measure of chirality, defined as the EM chirality. EM chirality has a well-defined upper bound. It has been also shown that a maximally EM chiral particle is necessarily dual, and transparent to one of the polarization handedness of the field. The analysis of such particles will be a scientifically rich exploration. In this contribution,
we concentrate on all aspects related to the optical force and torque exerted on such particles.

The sorting of chiral particles that are deposited on a substrate or while being in solution has been the main objective in many analytical studies on the optical force. In Ref. [33], the optical force and torque on dual spheres has been calculated and it was shown that duality leads to a maximal exerted torque. However, the analysis of the optical force and torque exerted on particles that are simultaneously chiral and dual has not yet been reported. Such analysis is timely, since meeting simultaneously the condition of chirality and duality can be realized with tailored particles.

To close this gap, we study in this contribution analytically the optical cross sections and the exerted optical force and torque on a dual chiral particle and also a maximally EM chiral particle in the dipolar approximation. A metallic helix is designed to approximate the conditions of maximal EM chirality at THz frequencies. To compare our analytical prediction to numerical simulations, the induced electric and magnetic dipole moments (electric and magnetic multipole moments). Neglecting higher orders, the induced electric and magnetic dipole moments can be approximated by dipole moments in a certain spectrum, and some restrictions on the polarizability tensor. For a reciprocal dipolar particle, the following Onsager relations hold for both static and dynamic polarizability tensors:

\[ \tilde{\alpha}^{ee} = (\tilde{\alpha}^{ee})^T, \quad \tilde{\alpha}^{mm} = (\tilde{\alpha}^{mm})^T, \quad \tilde{\alpha}^{em} = - (\tilde{\alpha}^{me})^T, \]

where superscript T denotes the matrix transpose.

If \( \tilde{\alpha}^{em} = - (\tilde{\alpha}^{me})^T \neq 0 \), the particle is bianisotropic. A bianisotropic particle is both anisotropic and magnetoelectric. Magnetoelectricity is the cross-coupling between the incident electric/magnetic fields and the induced magnetic/electric multipole moments.

The two general categories of bianisotropic materials/particles are reciprocal and nonreciprocal. Without external bias fields or some specific cases (i.e., moving particles), all materials/particles are reciprocal. Chiral particles are an important category of bianisotropic particles. We define a dipolar chiral particle in the following way: A dipolar particle is electromagnetically chiral if its mirror dipolar polarizability tensor \( \tilde{\alpha}(\omega) \) cannot be brought back to its initial form by any 3D rotation of the tensor.

In other words, \( \tilde{M} \tilde{\alpha} \tilde{M}^{-1} \) should not be superposable on itself by any rotation, where \( \tilde{M} \) is the mirror operator. A mirror operation is a space inversion and a \( \pi \) rotation with respect to the mirror plane, i.e., \( \tilde{M}_j = \tilde{\Pi} \cdot \tilde{R}(j, \theta = \pi) \), \( j = x, y, z \), where \( \tilde{M}_j \) is the mirror operator with respect to the \( j = 0 \) plane, \( \tilde{\Pi} \) is the parity operator doing the space inversion (\( r \to -r \)) and \( \tilde{R}(j, \theta = \pi) \) is a \( \pi \) rotation with respect to the \( j = 0 \) plane. Rotation and parity operators commute, i.e., \( \tilde{\Pi} \cdot \tilde{R} = \tilde{R} \cdot \tilde{\Pi} \).

Therefore, in order to prove that a particle is not chiral, it would be enough to find only one possible rotation \( \tilde{R} \) in the three-dimensional space to satisfy the expression:

\[ \tilde{R} \tilde{\alpha}(\omega) \tilde{R}^{-1} = \tilde{\Pi} \tilde{\alpha}(\omega) \tilde{\Pi}^{-1}. \]

It can be proven that a particle with broken symmetries in three orthogonal planes is necessarily chiral. However, not all bianisotropic particles are chiral. A particle which is bianisotropic \( \tilde{\alpha}^{em} \neq 0 \) but not chiral is called an omega particle. It is called omega because a structural implementation that possesses such a polarizability tensor has the shape of an omega letter (Ω).

**Optical field scattering and duality:** The scattered light into the far-field of a dipolar particle can be written as:

\[ E_{scs} = \frac{k^2}{4\pi} \left[ (n \times cp) \times n - (n \times m) \right] \frac{e^{ikr}}{r}, \]

\[ H_{scs} = \frac{k^2}{4\pi} \left[ (n \times m) \times n + (n \times cp) \right] \frac{e^{ikr}}{r}, \]

where \( n \) is the unit vector in the direction of the far-field radiation and \( k \) is the wavenumber. For simplicity, space
and frequency arguments are suppressed from here on. There is an interesting symmetry between the electric and magnetic dipole moments in the equation above. If \( \mathbf{cp} = \pm \mathbf{im} \), then we have \( \mathbf{H}_{\text{sc}} = \mp \mathbf{E}_{\text{sc}} / Z_0 \), which describes a wave with a well-defined helicity. Therefore, for the two conditions, the particle scatters only waves of a well-defined helicity.\(^{[10]} \) In other words, if the particle is illuminated by a wave of well-defined helicity, the scattered field also have a well-defined helicity. Therefore, satisfying \( \mathbf{cp} = \pm \mathbf{im} \) is enough to realize EM duality or anti-duality for a dipolar particle for all incident fields.\(^{[15]} \) Here, we will only focus on dipolar dual particles.

**Dual chiral particles:** Assume a very simplistic representation of a chiral particle that only shows a response to a z-polarized electric or magnetic field. Then, the polarizabilities are as follows:

\[
\tilde{\alpha}^{ee} = \alpha^{ee}_{zz} \mathbf{e}_z \mathbf{e}_z, \quad \tilde{\alpha}^{mm} = \alpha^{mm}_{zz} \mathbf{e}_z \mathbf{e}_z, \\
\tilde{\alpha}^{em} = -\tilde{\alpha}^{me} = \alpha^{em}_{zz} \mathbf{e}_z \mathbf{e}_z,
\]

with \( \mathbf{e}_z \) being the unit vector in the z-direction.

For simplicity we will use the following notations:

\[
\alpha^{ee}_{zz} = \alpha^{e}, \quad \alpha^{mm}_{zz} = \alpha^{m}, \quad \alpha^{em}_{zz} = -\alpha^{me}_{zz} = \chi = \chi' + i \chi''.
\]

(10)

Under a circularly polarized plane wave illumination \( \mathbf{E} = E_0 e^{i k x} (\mathbf{e}_y + i \sigma \mathbf{e}_z) / \sqrt{2} \), the dipole moments induced in the particle can be derived as (\( \sigma = \pm 1 \) is the handedness of the wave):

\[
\mathbf{p} = p_z \mathbf{e}_z = \frac{\epsilon_0 E_0}{\sqrt{2}} (\chi + i \sigma \alpha) \mathbf{e}_z, \quad (11)
\]

\[
\mathbf{m} = m_z \mathbf{e}_z = \frac{E_0}{\sqrt{2} Z_0} (\alpha^m - i \sigma \chi) \mathbf{e}_z. \quad (12)
\]

If \( \alpha^m = \alpha^e \), then, depending on the handedness of the wave \( \sigma \), we have \( \mathbf{p} = \pm \mathbf{im}/c \). In other words \( \alpha^m = \alpha^e = \alpha \) is an adequate condition for this reciprocal dipolar particle to be dual. Therefore, we identify the dual chiral particle as follows:

\[
\begin{align*}
  p_z &= \frac{\epsilon_0 E_0}{\sqrt{2}} (\chi + i \sigma \alpha), \\
  m_z &= \frac{E_0}{\sqrt{2} Z_0} (\alpha - i \sigma \chi).
\end{align*}
\]

Maximally EM chiral particles: The response of the chiral particle in Eqs. \( 11 \) and \( 12 \) is \( \sigma \) dependent and it reacts with different strength to right- and left-handed circularly polarized plane waves. Let us assume that we want to maximize the recently introduced EM chirality measure\(^{[112]} \) for the particle, or in other words to make the particle transparent to one helicity and responsive to the other without coupling the two. For the particle in Eq. \( 10 \) if we enforce:

\[
\alpha^e = \alpha^m = \varsigma i \chi,
\]

with \( \varsigma = \pm 1 \), for one polarization \( \sigma \) the dipole moments totally cancel out, while for the other polarization, the induced dipole moments are significant. \( \varsigma \) can be defined as the right (\( \varsigma = -1 \)) or left (\( \varsigma = +1 \)) handedness of the chiral particle. Please note that this handedness is a choice based on the geometrical handedness of the corresponding helix.\(^{[12]} \) For a maximally right-handed (\( \varsigma = -1 \)) EM chiral particle, we have:

\[
\begin{align*}
  p_z &= \sqrt{2} \epsilon_0 E_0 \delta_{1 \sigma}, \\
  m_z &= -\sqrt{2} \epsilon_0 E_0 \delta_{1 \sigma} = -ic p_z.
\end{align*}
\]

(16)

(17)

where \( \delta_{1 \sigma} \) is the delta Kronecker function for right-handed circularly polarized plane wave illumination and \( \delta_{1 \sigma} = 0 \) for left-handed circularly polarized plane wave illumination. It can be inferred that a maximally right-handed EM chiral particle is only sensitive to a right-handed circularly polarized plane wave illumination. In general, for reciprocal objects, to maximize their EM chirality, they should be dual and transparent to one helicity.\(^{[29]} \)

Below, we calculate the optical cross sections and the exerted force and torque on the dual chiral and maximally EM chiral particle.

**Optical cross sections:** The scattering, extinction, and absorption cross sections characterize the fraction of power a particle scatters, extincts, or absorbs from an incident illumination. For a dipolar particle they are defined as\(^{[21\text{b}]} \):

\[
\begin{align*}
  C_{\text{sca}} &= \frac{\epsilon^2 Z k^4}{12 \pi I_0} \left( |\mathbf{p}|^2 + |\mathbf{m}|^2 \right), \quad (18) \\
  C_{\text{ext}} &= -\frac{k c}{2 I_0} \Im (\mathbf{p} \cdot \mathbf{E} + \mu_0 \mathbf{m} \cdot \mathbf{H}), \quad (19) \\
  C_{\text{abs}} &= C_{\text{ext}} - C_{\text{sca}}, \quad (20)
\end{align*}
\]

where \( I_0 = |E_0|^2 / (2 Z_0) \) is the intensity of the incident light and \( \mu_0 \) is the permeability of the free space. The scattering and extinction cross sections for the dual chiral particle under the circularly polarized plane wave illumination (\( \mathbf{k} = k \mathbf{e}_z \)) are derived as:

\[
\begin{align*}
  C_{\text{sca}} &= \frac{k^4}{6 \pi} \left[ |\alpha|^2 + |\chi|^2 + 2 \Im (\sigma \chi \alpha^*) \right], \quad (21) \\
  C_{\text{ext}} &= k \Im (\alpha - i \sigma \chi). \quad (22)
\end{align*}
\]

The optical cross sections for the maximally right-handed chiral particle under the circularly polarized plane wave illumination (\( \mathbf{k} = k \mathbf{e}_z \)) are derived as:

\[
\begin{align*}
  C_{\text{sca}} &= \frac{2 k^4}{3 \pi} |\alpha|^2 |\delta_{1 \sigma}|, \quad (23) \\
  C_{\text{ext}} &= -2 k |\chi | |\delta_{1 \sigma}|, \quad (24) \\
  C_{\text{abs}} &= -2 k \left[ \frac{3}{k^3} |\chi|^2 + \chi' \right] |\delta_{1 \sigma}|. \quad (25)
\end{align*}
\]
As a conclusion for the maximally right-handed EM chiral particle:

1. The optical cross sections are zero for a left-handed polarization and maximal for a right-handed polarization of the illuminating plane wave.

2. The maximal values are related to $|\chi|^2, \chi'$ and $k^3 |\chi|^2 + \chi'$ for the scattering, extinction, and absorption cross sections, respectively.

3. For a maximum absolute value of the handedness-contrast for the absorption cross section, $-2k^3 |\chi|^2 + \chi'$ should be maximized, which can be realized for an optimum absorption of the particle.

For a non-absorbing maximally chiral particle, $C_{\text{abs}}$ is zero. Inspired by previous research, it can be argued that a non-absorptive maximally EM chiral particle can lead to a maximum scattering and extinction cross section by a plane wave incidence of the same handedness.\(^{33}\)

Optical force and torque: The optical force and torque can be expressed in terms of multipole moments of the particle induced by a specific illumination. The multipolar description of force and torque has been presented in Refs. 46 and 47. The results are exact but lengthy. A full-wave code is developed to calculate the force and torque numerically.\(^{33}\) The time averaged optical force and torque exerted on a dipolar particle by an arbitrary incident wave are simplified to (in SI units)\(^{32,35}\).

\[
\mathbf{F} = \frac{1}{2} \Re \left[ \nabla \mathbf{E}^* \cdot \mathbf{p} + \nabla \mathbf{B}^* \cdot \mathbf{m} - \frac{Z_0 k^4}{6\pi} (\mathbf{p} \times \mathbf{m}^*) \right],
\]

\[
\mathbf{N} = \frac{1}{2} \left\{ \Re (\mathbf{p} \times \mathbf{E}^* + \mathbf{m} \times \mathbf{B}^*) - \frac{k^3}{6\pi} \left[ \frac{1}{\epsilon_0} \Im (\mathbf{p}^* \times \mathbf{p}) + \mu_0 \Im (\mathbf{m}^* \times \mathbf{m}) \right] \right\}. \quad (26)
\]

Under the circularly polarized plane wave $\mathbf{E} = E_0 e^{i k x} (\mathbf{e}_y + i \sigma \mathbf{e}_z) / \sqrt{2}$ illumination, the time averaged optical force and torque exerted on the dual chiral particle for the two polarization handedness are derived as:

\[
\mathbf{F} = \frac{k^3}{6\pi} (F_p)_{\text{max}} [\sigma \Im (\alpha) - \Re (\chi)] \mathbf{e}_x, \quad (27)
\]

\[
\mathbf{N} = \frac{2k^3}{3\pi} (N_p)_{\text{max}} [\sigma \Im (\alpha) - \Re (\chi)] \mathbf{e}_x, \quad (28)
\]

where $(F_p)_{\text{max}} = 3(I_0/\omega)(\lambda^2/2\pi)$ and $(N_p)_{\text{max}} = 3(I_0/\omega)(\lambda^2/8\pi)$ are the upper bounds for the optical force and torque that a plane wave can exert on an isotropic electric dipolar particle.\(^{33}\) It can be concluded that for a dual chiral particle, although the helicity is preserved, the exerted torque can only be zero for one of the polarizations when $\sigma \Im (\alpha) = \Re (\chi)$, which is the condition for maximal EM chirality. The relations derived for the force and torque are very similar. This symmetry might be a direct consequence of the duality symmetry.

For the \textit{ideally} maximally right-handed EM chiral particle the force and torque derive as:

\[
\mathbf{F} = F_x \mathbf{e}_x = -\frac{k^3}{3\pi} (F_p)_{\text{max}} \chi' \delta_{1\sigma} \mathbf{e}_x, \quad (29)
\]

\[
\mathbf{N} = N_x \mathbf{e}_x = -\frac{4k^3}{3\pi} (N_p)_{\text{max}} \chi' \delta_{1\sigma} \mathbf{e}_x. \quad (30)
\]

The optical force and torque for the maximally right-handed EM chiral particle vanishes totally for $\sigma = -1,$
whereas for a right-handed circularly polarized plane wave illumination ($\sigma = +1$), the value depends on the real part of the chirality factor $\chi'$. For simplicity, we define the normalized optical force and torque as $F = F/(F_p)_{\text{max}}$ and $N = N/(N_p)_{\text{max}}$. As a conclusion for the maximally right-handed EM chiral particle:

1. The optical force and torque are zero for left-handed polarization and maximal for right-handed polarization of the incident plane wave.

2. The maximal values of the torque and force only depend on $\chi'$. Which directly relates it to the optical extinction cross section.

3. Contrary to isotropic particles, where absorption is a necessary condition to exert a torque by a circularly polarized plane wave, an optical torque can be exerted on a non-absorbing dual chiral or maximally EM chiral particle.

Similar to the case made for the optical cross sections, it can also be argued that for a non-absorbing maximally EM chiral particle, the exerted force and torque can achieve their maximum value.

Maximally EM chiral helix: Now that we have analyzed the theoretical aspects, we provide here results of simulations concerning an optimized silver helix in the THz regime. The silver helix has been optimized to satisfy the maximal EM chirality condition as discussed in Ref. [29]. The helix is schematically shown in Fig. 2. Here, we have retrieved the polarizabilities from the T-matrix of the particle (calculated and discussed in Ref. [44] using an existing full-wave code [45]). The polarizabilities are in the following form and are shown in Fig. 3:

$$\tilde{\alpha}_{ee}^{xx} = \alpha_{ee}^{xx} e_z e_z + \alpha_{ee}^{xy} e_y e_z + \alpha_{ee}^{yx} e_z e_y,$$

$$\tilde{\alpha}_{ee}^{mm} = \alpha_{ee}^{mm} e_z,$$

$$\tilde{\alpha}_{em}^{ym} = \alpha_{em}^{ym} e_x e_z + \alpha_{em}^{ym} e_y e_z,$$

$$\tilde{\alpha}_{me}^{ym} = \alpha_{me}^{ym} e_x e_z + \alpha_{me}^{ym} e_y e_z.$$

There are non-desirable nonzero elements as shown in the figure, i.e. those related to a response for a y-polarized field. This might cause some deviations between the exact numerical results and the analytical predictions in Eqs. [29, 30]. Nevertheless, it can be seen that the reciprocity conditions hold perfectly and the maximal dipolar EM chirality condition (Eq. 15) is also approximately met. The current distribution on the surface of the helix is also calculated for the two illuminations and is shown in Fig. 4. The excitation frequency corresponds to the resonance, i.e. 1.5 THz. The induced current is very small for the left-handed circularly polarized illumination, demonstrating the different response to light with different circular polarization.

The exact force and torque exerted on the helix by a circularly polarized plane wave were calculated numerically using the retrieved T-matrix and the multipole expansion of the optical force and torque [46, 47]. The numerical calculations are done using a full-wave code [49]. Results are shown in Fig. 5. The analytical results assuming that the helix was an ideal dipolar maximally EM chiral object are plotted using the retrieved cross term polarizability $(\tilde{\alpha}_{em}^{ym})$ and the analytical Eqs. [29, 30]. The agreement between the exact and ideal results is almost perfect. A non-zero but rather small force and torque in the exact numerical simulation can be seen upon illuminating the right-handed particle with a left-handed circularly polarized plane wave. It is attributed to the fact that the helix is not a perfect maximally EM chiral dipolar object, as can be for example appreciated in the finiteness of the already mentioned entries in the polarizability matrix.

Conclusion: In summary, we have calculated the optical force and torque on dual chiral and maximally EM chiral particles. We have simulated the optical force and torque on a designed maximally EM chiral silver helix. It is shown that a maximally right-handed EM chiral particle can be maximally rotated or accelerated by a right-handed circularly polarized plane wave and become almost transparent to a left-handed circularly polarized.
plane wave. Of course, the opposite holds for a maximally left-handed EM chiral particle. Our study will be useful in two perspectives. On the one hand, it can contribute to the current research on the optical sorting of racemic mixtures. On the other hand, it can prove useful in optically driven nanorobots. A maximally EM chiral particle can be used as a building block of a robot which is only sensitive to one polarization.

Acknowledgements: We acknowledge partial financial support by the Deutsche Forschungsgemeinschaft through CRC 1173. A.R. and M.F. also acknowledge support from the Karlsruhe School of Optics and Photonics (KSOP).

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