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Characterization and remote sensing of biological particles using circular polarization

Lev Nagdimunov [a,1], Ludmilla Kolokolova [a,*], Daniel Mackowski [b]

[a] *University of Maryland, Department of Astronomy, MD 20742, USA*
[b] *Auburn University, Mechanical Engineering Department, AL 36849, USA*

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ABSTRACT

Biological molecules are characterized by an intrinsic asymmetry known as homochirality. The result is optical activity of biological materials and circular polarization in the light scattered by microorganisms, cells of living organisms, as well as molecules (e.g. amino acids) of biological origin. Lab measurements (Sparks et al. (2009) [6,7]) have found that light scattered by certain biological systems, in particular photosynthetic organisms, is not only circular polarized but contains a characteristic spectral trend, showing a fast change and reversal of sign for circular polarization within absorption bands. Similar behavior can be expected for other biological and prebiological organics, especially amino acids. We begin our study by reproducing the laboratory measurements for photosynthetic organisms through modeling the biological material as aggregated structures and using the Multiple Sphere T-matrix (MSTM) code for light scattering calculations. We further study how the spectral effect described above depends on the porosity of the aggregates and the size and number of the constituent particles (monomers). We show that larger aggregates are characterized by larger values of circular polarization and discuss how light-scattering characteristics of individual monomers and electromagnetic interaction between them affect this result. We find that circular polarization typically peaks at medium (40–140°) scattering angles, and discuss recommendations for efficient remote observation of circular polarization from (pre)biological systems.

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1. Introduction

An emerging interest in using circular polarization to detect the presence of biological materials remotely has developed over the last 15 years. Stimulated in part by measurements of circular polarization in astronomical contexts and the astrobiological applications of such measurements, a possibility arises to employ circular polarization for remote sensing of objects that contain biological or pre-biological organics, including astronomical objects, terrestrial hydrosols, and aerosols as well as objects of bio-medical studies. In this paper we focus on particulate media, including microorganisms, dusts, and aerosols that contain either biological or pre-biological (e.g. amino acids and sugars) organics. For brevity, we call them "biological particles," "biological materials" or "biological objects."

Traditionally, astronomical circular polarization has been thought to be rarely present in the absence of high energetic phenomena. Small levels of circular polarization stemming from low energy processes have been technically difficult to measure. Nevertheless, it has now been reliably measured for planets, interstellar and interplanetary dust, and comets [1–4]. These papers also discuss the mechanisms that can be responsible for circular polarization: multiple scattering in asymmetric media, scattering

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[*] Corresponding author. Tel.: +1 301 405 1539.
E-mail addresses: lnagdi1@astro.umd.edu (L. Nagdimunov), ludmilla@astro.umd.edu (L. Kolokolova).
[1] Tel.:+1 301 405 3069.

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by aligned particles, and scattering by intrinsically asymmetric particles. We explore properties of the latter effect in this study.

Scattering by intrinsically asymmetric particles is of particular interest in remote sensing of biological particles because their material is characterized by so called homochirality. By definition [5] a molecule is said to be homochiral if it is composed entirely of one type of chiral “building blocks”, which exist in two non-superimposable mirror-symmetric forms. The vast majority of amino acids present in living tissue are “left-handed”, and most sugars present in living materials use their “right-handed” mirror-symmetric version. This preference for a single handedness is unique to biological material, no non-biological objects have ever been found to possess it. Intrinsic asymmetry of biological molecules makes biological material optically active, i.e. able to produce circular polarization.

Homochirality would be an especially useful tool in a search for biological particles if it could be remotely detectable. While it has been suggested for as long as several decades that circular polarization resulting from light scattering by homochiral materials could be remotely detectable, any detection need to be separated from the other causes of circular polarization mentioned above. To assist with this problem, we studied how homochirality of biological particles affects the circular polarization in light scattered by them. This information would facilitate the identification of circular polarization measured from a remote object, and also potentially allow us to narrow down and describe the characteristics of the observed material.

Our work was primarily motivated by recent measurements of circular polarization for light scattered by organisms that contain photosynthetic pigments by Sparks et al. [6,7]. Circular polarization produced by such pigments was found to be not only non-zero but also to vary distinctly with wavelength inside absorption bands, showing a rapid change in value and in some cases even a change in sign. An example of circular polarization measurements is shown in Fig. 1 for cyanobacteria WH8101 (adapted from [6]). Circular polarization shown in all figures of this paper is defined as the ratio of the forth Stokes parameter to the first one, i.e. V/I. Similar results were found for a variety of macroscopic vegetation as well as bacteria relying on photosynthesis for energy production. Control measurements of nonbiological chemical compounds and minerals showed either negligible circular polarization or noise-like variations of circular polarization not affected by a change in absorption [6,7].

In this paper, we present the results of computer modeling for circular polarization produced by light scattering of chlorophyll *a*, and compare them to the lab measurements of polarization by cyanobacteria and macroscopic vegetation, in which chlorophyll *a* is both abundant and essential. We study chlorophyll due to the measurements discussed above and because its optical constants are better studied and can be easier found in the literature than those of other complex organics. However, we expect that certain amino acids should also show this effect as they demonstrate similar optical constant trends in their absorption bands [8–10].

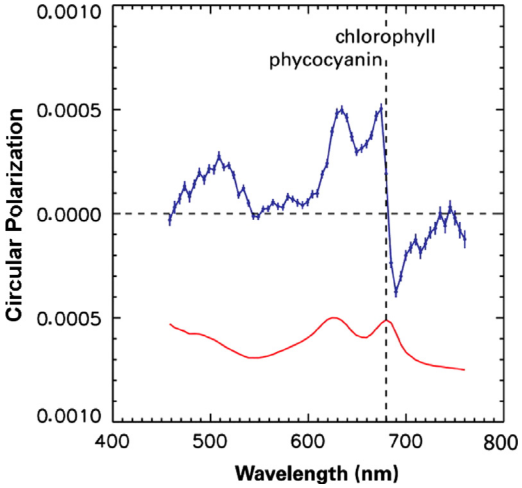

Fig. 1. Laboratory measurement of circular polarization spectra for cyanobacteria WH8101 shown at transmission (upper curve). Absorption shown in arbitrary units (lower curve). Adapted from [6].

We model biological material as aggregates of spherical particles, which provides the most realistic model (refer to Section 3) of such particles that can be treated with available computational tools. To advance both the study of circular polarization in photosynthetic pigments as well as circular polarization of homochiral molecules in general, we performed a computational survey of the effect that properties of biological particles, and the aggregates we used to model them, have on circular polarization.

2. Circular polarization induced by optically active particles

Circular polarization of light scattered by chiral molecules is caused by two material effects: optical rotation, sometimes also termed circular birefringence, and circular dichroism. Circular birefringence indicates that the material's real index of refraction is different for left and right circularly polarized light. Similarly, circular dichroism refers to different absorption for light of different handedness. Both effects, in the absence of a magnetic field, arise only in particles characterized by an intrinsic asymmetry.

There are four optical constants necessary to model circular polarization of light that is scattered by a chiral material. The first two are the real and imaginary parts of the complex index of refraction, describing refraction and absorption respectively. The other two parameters describe circular birefringence and circular dichroism. Mathematically, the complex index of refraction is $m=n+ik$, where n is different for left and right-handed polarized light in the presence of circular birefringence and k is different in the presence of circular dichroism; i is the imaginary unit. We can create a parameter β, which describes the difference in the complex index of refraction between left and right-handed circularly polarized light: $\beta=m_L-m_R=\beta_R+i\beta_I$, where β_R represents circular birefringence, β_I represents circular dichroism. If we suppose that $m_L=(n+\beta_R/2)+i(k+\beta_I/2)$ describes the optical characteristics of left-handed light, then $m_R=(n-\beta_R/2)+i(k-\beta_I/2)$

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