Proposal for Graduation with Honors in Physics

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Abstract

One of the interests of the Department of Physics and Optical Science at UNC Charlotte is the application of the natural properties of light to help answer questions regarding specific materials, and aid in the development of new technologies that advance modern science. In this research, we apply Mie Theory to answer questions about the nature of materials created right here in the UNC Charlotte lab. Mie’s solution is an infinite series of partial waves describing the scattering of light off particles larger than the wavelength of incident light. One certain parameter that influences the degree of scattering is \( n \), the material’s index of refraction. We first attempt to calibrate Mie’s solution for the scattering of a diode laser incident upon a bare silicon dioxide fiber core with an index of refraction \( n \) that is known. Secondly, we attempt to determine Mie’s solution for the scattering off a Bragg fiber made of three different materials, where two index of refraction values are known, such that we may determine the third.

1 Introduction

1.1 Background

Electromagnetic waves, or light, have been the subject of much study and debate over the past four hundred years. In 1805, Isaac Newton published his theory on “corpuscles”, small discrete particles of light, in his book *Optiks*, expanding on the work done by Pierre Gassendi. But shortly beforehand, Dutch physicist Christiaan Huygens proposed his wave theory of light in 1678, the theory in which Newton had originally sought to confirm [1]. Newton’s corpuscular theory became widely favored up until 1801, when Thomas Young proved Huygens wave theory correct with his famed double-slit experiment.

However, Albert Einstein returned to Isaac Newton’s proposal of small packets of light to explain the photoelectric effect in 1905, for which waves simply
could not account for. Einstein’s theory was built upon Max Planck’s results in 1899 that indicated a quantization of energy; American physicist Robert Milliken proved both Einstein’s photoelectric equation and Planck’s constant $h$ by the year 1916 [2]. These small packets of energy, originally called “quanta” would eventually become known as “photons”, thanks to the coinage by American chemist Gilbert Lewis in 1926 [3].

But the study of the nature of light predates even the seventeenth century, extending back to the time of Classical Greece. Plato (429 – 347 BC)[4] developed *The Emission Theory of Light* in the fifth century, making it the first known study on record.

1.2 Gustav Mie

Gustav Mie was a German mathematician and physicist predominately interested in electromagnetic theory. He studied Maxwell’s equations for the majority of his research career, and in fact, when he found the solutions now known as Mie’s theory he did not think much of it, as it was written as an explanation of the behavior his graduate student had observed at the time [5].

The paper was published in 1908 and went virtually unnoticed for fifty years before the scientific community realized the magnitude of his work. His original paper, *Beiträge zur Optik trüber Medien, speziell kolloidaler Metallsungen* which translates as *Contributions to the Optics of Turbid Media, specially colloidal Metal solutions*, has been cited over 8300 times according to Google scholar.

The Mie Solution is an infinite series of partial waves, and the number of terms included in the series depends on the incident wavelength and the size of the scattering object. As there were no computers back in 1908, Mie was only able to determine a solution for a maximum of three terms [5]. This condition imposed a constraint on the size of the object, and Mie could not work with any particles larger than 200 nm [5].

2 Mie’s Solution for a Sphere

![Diagram of the Rayleigh scattering pattern versus a Mie scattering pattern.](Image: Hyperphysics, Georgia State University)

*Figure 1: Diagram of the Rayleigh scattering pattern versus a Mie scattering pattern.*

(Image: Hyperphysics, Georgia State University)
There are three regimes recognized in scattering theory which are determined by scale. For instances when the wavelength is larger than the particle, the process is classified as Rayleigh scattering. For wavelengths roughly the same size as the particle or slightly smaller, the process is Mie scattering (see Figure 1). And lastly, when the wavelengths are much smaller than the particles (or objects), then the scattering falls under the geometric regime.

Mie’s solution is the name given to the following pair of partial wave solutions in the far-field for the case of spherical scattering, as given by [6]:

\[ E_\theta(\theta, \phi) = i \cos \phi \frac{e^{-ik_2 r}}{k_2 r} \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} a_n \pi_n(\cos \theta) + b_n \tau_n(\cos \theta), \]  

\[ E_\phi(\theta, \phi) = -i \sin \phi \frac{e^{-ik_2 r}}{k_2 r} \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} a_n \pi_n(\cos \theta) + b_n \tau_n(\cos \theta), \]

where \( k_2 = 2\pi n_2 / \lambda \). The angular functions \( \pi_n \) and \( \tau_n \) are defined as:

\[ \pi_n(\cos \theta) = \frac{P_1^n \cos \theta}{\sin \theta}, \]

\[ \tau_n(\cos \theta) = \frac{d}{d\theta} P_1^n \cos \theta, \]

and the associated Legendre polynomials \( P_1^n \cos \theta \) are given by [7]:

\[ P_1^n \cos \theta = \frac{\sin \theta}{2^n} \sum_{k=0}^{n/2} (-1)^k n; k2n - 2k; n(n - 2k)\cos \theta^n - 2k - 1. \]

The integers \( u \) and \( v \) are the binomial coefficients:

\[ u; v = \frac{u!}{v!(u-v)!}. \]

### 3 Bessel Functions

The Bessel functions of the first kind \( J_n(x) \) are solutions to the differential equation known as Bessel’s equation, named after German mathematician and astronomer Friedrich Wilhelm Bessel (1784-1846):

\[ x^2 \frac{d^2 y}{dx^2} + x \frac{dy}{dx} + (x^2 - n^2) = 0, \]

where \( n \) is the order of the function. The terms are found using an infinite power series expansion, where the first six terms are shown in Figure 1.

The Neumann functions, also known as the Bessel functions of the second kind, are denoted \( N_n(x) \). The Bessel functions of the second kind are related to the first kind through the following formula:
Figure 2: Bessel functions of the 1st kind. (Graph: Wolfram mathworld)

\[ N_n(x) = \frac{J_n(x) \cos(n\pi) - J_{-n}(x)}{\sin(n\pi)}, \]  

(8)

where \( J_{-n}(x) = (-1)^n J_n(x) \). See Figure 2 for the Bessel functions of the second kind.

Figure 3: Bessel functions of the 2nd kind. (Graph: Wolfram mathworld)

The Hankel functions, denoted \( H_n(x) \) are linear combinations of the Bessel functions of the first and second kind, where:

\[ H_n^1 = J_n(x) + iY_n(x) \]  

(9)

is the Hankel function of the first kind, and

\[ H_n^2(x) = J_n(x) - iY_n(x) \]  

(10)

is the Hankel function of the second kind. The Hankel functions of the first kind appear in the Mie Solution for an infinite cylinder. In the solutions for
scattering off a sphere, the spherical Bessel functions of the first and second kind are used in conjunction with the spherical Hankel functions.

4 MatScat Code

By 1961, Milford Kerker had extended Mie’s solution to the case of an infinite cylinder, the ideal geometry for the cylindrical Bragg fiber. The pair of partial wave equations given in Equations 1 and 2 were modified by Kerker in his paper *Scattering of Electromagnetic Waves from Concentric Infinite Cylinders* and expressed in terms of the Bessel functions $J_n(x)$ and $H_n(x)$. The partial wave scattering coefficients $a_n$ and $b_n$ are determined by:

$$a_n = \begin{pmatrix}
J_n'(m_2\alpha) & N_n'(m_2\alpha) & J_n'(m_1\alpha) & 0 \\
J_n'(m_2\beta) & N_n'(m_2\beta) & J_n'(m_1\beta) & 0 \\
J_n'(m_2\alpha) & m_2N_n(m_2\alpha) & m_1J_n(m_1\alpha) & 0 \\
J_n'(m_2\beta) & m_2N_n(m_2\beta) & m_1J_n(m_1\beta) & 0 \\
\end{pmatrix}$$

$$b_n = \begin{pmatrix}
J_n'(m_2\alpha) & m_2J_n'(m_2\alpha) & m_1J_n'(m_1\alpha) & 0 \\
J_n'(m_2\beta) & m_2J_n'(m_2\beta) & m_1J_n'(m_1\beta) & 0 \\
J_n(m_2\alpha) & N_n(m_2\alpha) & N_n(m_1\alpha) & 0 \\
J_n(m_2\beta) & N_n(m_2\beta) & N_n(m_1\beta) & 0 \\
\end{pmatrix}$$

where $m_1 = k_1/k_3$ and $m_2 = k_2/k_3$ [6]. The propagation constants $k_1$, $k_2$ and $k_3$ correspond to the material of the core, shell and medium [6].

Because the fiber is so much larger than the incident wavelength, we need to include a large number of terms in the series. This is a direct consequence of the Mie Solution, and the reason Gustav Mie could only solve the equation for a sphere much smaller than the incident wavelength [5].

The Matlab code we selected for this experiment includes over one thousand terms. This means that in total there are over two thousand $a_n$ and $b_n$ coefficients to determine. Calculations of this nature are perhaps best suited for computers, and in this experiment we will be using Jan Schäfer’s MatScat code.

5 Experimental Goals

The goal of this research project is to determine the index of refraction of the Bragg fiber layers being fabricated right here at UNC Charlotte. The index of
refraction of one of the two Bragg layers, which are on the scale of nanometers, has changed recently. The reason for this change is due to a new fabrication method implemented as the result of a research project I participated in as a Charlotte Research Scholar during the summer of 2012.

My previous research project, entitled *Iridescence of Bragg Fibers and its Application in Non-Invasive Characterization of Conformal Thin Film Uniformity* discovered that the Bragg fibers fabricated at UNC Charlotte were not uniform, and proposed a new method of fabrication to produce uniform fibers. This new method was implemented, and the Bragg fibers are now uniform. However, the index of refraction of one of the Bragg fiber layers has changed.

The goal of this research project will be to determine the new index of refraction using Mie scattering theory. I will contribute to the scope of this research project, currently being carried out by graduate student Zeba Naqvi, as described in section 7.

6 Challenges

In this experiment, a 632.8 nm diode laser is used as the incident light source. The object we are scattering the laser off is a bare silicon dioxide fiber core of diameter 50 microns. According to the scale of Mie Theory, we should not achieve accurate results for the scattering process because the object is so much larger than the wavelength. However, Mie scattering could theoretically be applied to any object larger than the wavelength, regardless of size. But what limits this in practice is the mathematics and the nature of an infinite series. The larger the object is, the more terms are needed in the series.

The greatest difference in size that can accurately be modeled using Mie theory is $80\lambda$ [7], as described in section xx. In our experiment, the factor is $320\lambda$. To resolve this, we installed a multi precision toolbox to work in conjunction with the Matlab code in order to track the significant figures. Doing so may allow us to include even more terms in the series, making the code more accurate. Computation time was rather slow on the laboratory computers, therefore we decided to switch to the University cluster computing system. However, after running the code on the cluster, we discovered the graphs were not displaying.

Calibrating this code to our fiber core scattering pattern has proved difficult, and we are testing various methods to improve our result. Firstly, the experiment will be performed again using a modified set up. Secondly, we will test if including more terms in the series will lead to more accurate results. We initially included three thousand terms, but after I performed the very simple calculation here:

$$\frac{3}{180nm} = \frac{N}{200\mu m}$$  \hspace{1cm} (13)

$$\frac{3}{180 \times 10^{-9}} = \frac{N}{200 \times 10^{-6}}$$  \hspace{1cm} (14)

$$N = \frac{600 \times 10^{-6}}{180 \times 10^{-9}} = 3,333.33$$  \hspace{1cm} (15)
it is possible we still need about three hundred more terms in order to accurately
describe the scattering pattern using Mie Theory. These ratios are the number
of terms needed in the series over the diameter of the particle.

Additionally, there still remains a portion of the code that must be written
that analyzes the results the MatScat code returns. We are determining the
index of refraction indirectly, by comparing the graphs of our experimental
scattering pattern to the scattering pattern generated by the code. We will
guess the index of refraction and input it into the code, and then compare that
output with our actual data. A code would be ideal for this process.

7 Responsibilities

i). The study and understanding of the Mie solution
ii). The study and understanding of the Bessel functions of the first, second and
third kinds involved in Mie Theory
iii). The study and understanding of the conditions under which Mie Theory applies
iv). The study and understanding of Jan Schäfer’s MatScat codes
v). Learning and using the University Research Computing ”VIPER” cluster
vi). Researching different methods that would allow us to plot the results of the
MatScat code within the ”VIPER” cluster
vii). Researching different methods that would allow us to calibrate Jan Schäfer’s
MatScat code with the results obtained from our experiment
viii). Contributing to the set up of the experiment that will gather the scattering
patterns
ix). Contributing to any other unforeseen problems that might arise during the
project
x). Contributing to the modification of Jan Schäfer’s MatScat code to include
root searching (time permitting)
xi). Writing a thesis proposal and final report

8 Conclusion

This project will aim to characterize the index of refraction of one of the two
Bragg layers currently fabricated in the UNC Charlotte clean room using Mie
scattering. The Mie Theory solution for a layered cylinder was discovered over
forty years ago, and has since been implemented into various computer lan-
guages. We have researched and selected what we believe is the best computa-
tional program available today. Calibrating this code to our fiber core scattering
pattern has proved difficult, and we are testing various methods to improve our
result. Once the calibration has been achieved for the bare fiber core, we can
move forward and characterization the index of refraction of the Bragg layer
that has changed.
References


