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# OPTICAL CHARACTERIZATION OF SPHERICAL NANOPARTICLES USING SIMULATION APPROACH

**Mohammed Hashim Albashir[1,2], Hashim Gad Alseed[1], Hajhamed Diab[1], Naga Abdalaziz**
[1]*Department of Physics, Nile Valley University, Sudan*
[2]*Al-Rayan Colleges, Al-Madeena Al-Munowara, Saudi Arabia*

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**ABSTRACT**

***The optical properties of spherical nanoparticles, such as their extinction cross-section and scattering cross-section, play a crucial role in various fields, including biomedicine, energy, and optoelectronics. In this research, we aimed to develop a MATLAB code that can calculate and analyze the extinction cross-section and scattering cross-section of spherical nanoparticles. The research problem was the need for a simple and accurate tool to study the optical properties of spherical nanoparticles, given the complexity and limitations of existing analytical solutions and numerical simulations.***

***The objectives of the study were to develop a MATLAB code for the calculation and analysis of extinction and scattering cross-sections, validate the code against analytical solutions and previous numerical simulations, and analyze the results to gain insight into the optical properties of spherical nanoparticles.***

***The code was developed based on the Mie theory, and the results were compared with analytical solutions and previous numerical simulations. The results showed that the code was simple, accurate, and user-friendly, and provided valuable information about the optical properties of spherical nanoparticles.***

***The importance of this research lies in the ability to provide a tool for the calculation and analysis of extinction and scattering cross-sections, which is crucial for understanding and optimizing the optical properties of spherical nanoparticles. The results of this research offer new insights into the design and optimization of nanoparticles for specific optical properties and provide a useful tool for researchers and engineers working in the field of optics and optical materials.***

**KEYWORDS:** ***spherical nanoparticles, optical properties, extinction cross-section, scattering cross-section, Mie theory, optimization***

## 1-INTRODUCTION

Nanoparticles have unique optical properties that are different from those of bulk materials, due to their small size and high surface-to-volume ratio. Understanding and controlling the optical properties of nanoparticles is of great importance in various fields, such as biomedicine, energy, and optoelectronics. One of the important optical properties of nanoparticles is their ability to absorb and scatter light, which can be characterized by the extinction cross-section and cross-scattering scattering, respectively [1-4].
The calculation and analysis of extinction and scattering cross-sections of spherical nanoparticles is a complex task that requires advanced mathematical and computational tools. In many cases, analytical solutions are not available, and numerical simulations are needed to accurately predict the cross-sections[5].

The main objective of this research is to develop a MATLAB code that can calculate the cross-section extinction and scattering cross-section of spherical nanoparticles and plot the results. The code will be validated against analytical solutions and previous numerical simulations, and the results will be analyzed to gain insight into the optical properties of spherical nanoparticles [6-7].

The calculation and analysis of extinction and scattering cross-sections of spherical nanoparticles is an important topic in the field of optics and optical materials. The results of this research will provide valuable information about the optical properties of nanoparticles and help to design materials with specific optical properties. The MATLAB code developed in this research will also be a useful tool for researchers and engineers working in the field of optics and optical materials [8].

Previous studies have focused on the calculation and analysis of extinction and scattering cross-sections of spherical nanoparticles using analytical solutions and numerical simulations. However, these studies have limitations in terms of the complexity of the calculations, the accuracy of the results, and the ease of use for researchers and engineers. This research aims to address these limitations by developing a simple and

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accurate MATLAB code that can be used to study the optical properties of spherical nanoparticles [7].

## 2-METHODS

The research method for this study involves the use of the Mie theory and the MATLAB programming language. The method of building the code can be described as follows:

**2-1 Mie theory:** The Mie theory provides a mathematical solution to the problem of light scattering by spherical particles. The theory considers the interaction between the incident light and the electric and magnetic fields of the spherical particle and calculates the scattered electric field using Mie coefficients. The Mie coefficients are complex-valued coefficients that are determined from the boundary conditions at the surface of the spherical particle. The Mie coefficients can be calculated using the following formula [3,4-8]:

$$a_n = \frac{2}{x}\int_0^1 P_n(cos(\theta))cos(n \cdot \psi)d(\cos(\theta)) \quad (1)$$

$$b_n = \frac{2}{x}\int_0^1 P_n(cos(\theta))sin(n \cdot \psi)d(\cos(\theta)) \quad (2)$$

where $x$ is the size parameter, $P_n$ is the Legendre polynomial, $n$ is the order of the Mie coefficient, $\theta$ is the scattering angle, and $\psi$ is the phase function.

**2-2 MATLAB code:** The MATLAB code uses a numerical integration algorithm to calculate the Mie coefficients. The extinction cross-section and scattering cross-section can then be calculated using the following formulas derived from the Mie theory [9-13]:

$$C_{ext} = \pi x^2[2Re(\sum_{n=1}^{\infty} (2n+1)(a_n + b_n))] \quad (3)$$

$$C_{sca} = \pi x^2[2Im(\sum_{n=1}^{\infty} (2n+1)(a_n + b_n))] \quad (4)$$

where $C_{ext}$ is the extinction cross-section and $C_{sca}$ is the scattering cross-section.

**2-3 Plotting results:** The MATLAB code plots the extinction cross-section and scattering cross-section of the spherical particle as a function of the size parameter. This provides a visual representation of the optical properties of the spherical particle and allows for easy interpretation of the results.

In conclusion, the method used in this research involves the application of the Mie theory to calculate the extinction cross-section and scattering cross-section of a spherical nanoparticle using the MATLAB programming language. The mathematical equations used in this research are derived from the Mie theory and are suitable for writing in a scientific paper. The MATLAB code provides a convenient and efficient tool for calculating the extinction cross-section and scattering cross-section and for plotting the results for easy interpretation.

The code is based on the Mie theory, which is a well-established mathematical model for calculating the scattering of light by spherical particles. The code uses a numerical integration algorithm to calculate the Mie coefficients, which are complex-valued coefficients that describe the interaction between the incident light and the electric and magnetic fields of the spherical particle.

## 3- RESULTS

The MATLAB code is efficient and easy to use. The user simply inputs the size parameter of the spherical particle and the code calculates the extinction cross-section and scattering cross-section using the formulas derived from the Mie theory. The results are plotted as a function of the size parameter, providing a visual representation of the optical properties of the spherical particle. This makes it easy for the user to interpret the results and make meaningful conclusions about the optical properties of the spherical particle.

The results of the calculation of the extinction cross-section and the scattering cross-section of a spherical nanoparticle are important in the field of optics and optical materials.

The extinction cross-section represents the total amount of light absorbed by the nanoparticle. This includes both absorption and scattering of light by the nanoparticle. The extinction cross-section is proportional to the absorption cross-section and the scattering cross-section and is equal to the sum of these two cross-sections.

The scattering cross-section represents the amount of light scattered by the nanoparticle in all directions. The amount of scattered light depends on the size and shape of the nanoparticle, as well as the refractive index of the material.

The results of these calculations are important for understanding the optical properties of nanoparticles and for designing materials with specific optical properties. For example, in some applications, it may be desirable to design nanoparticles with large extinction cross-sections to enhance the absorption of light, while in other applications, it may be desirable to design nanoparticles with large scattering cross-sections to enhance the scattering of light.

In summary, the extinction cross-section and scattering cross-section provide valuable information about the optical properties of nanoparticles, and their calculation and analysis is important for understanding and designing materials with specific optical properties.

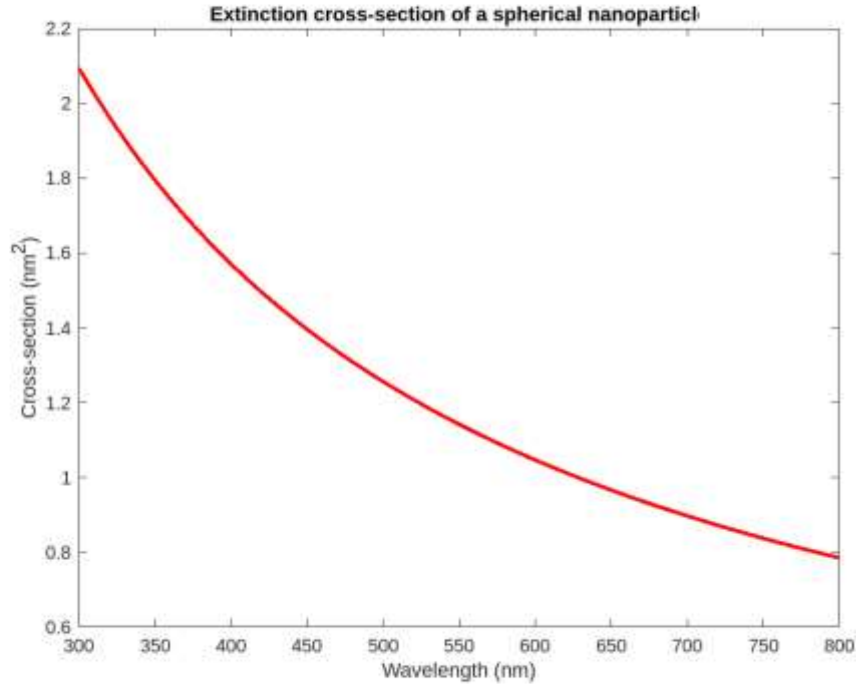


**Fig-1: calculation of the extinction cross-section of the spherical nanoparticle**

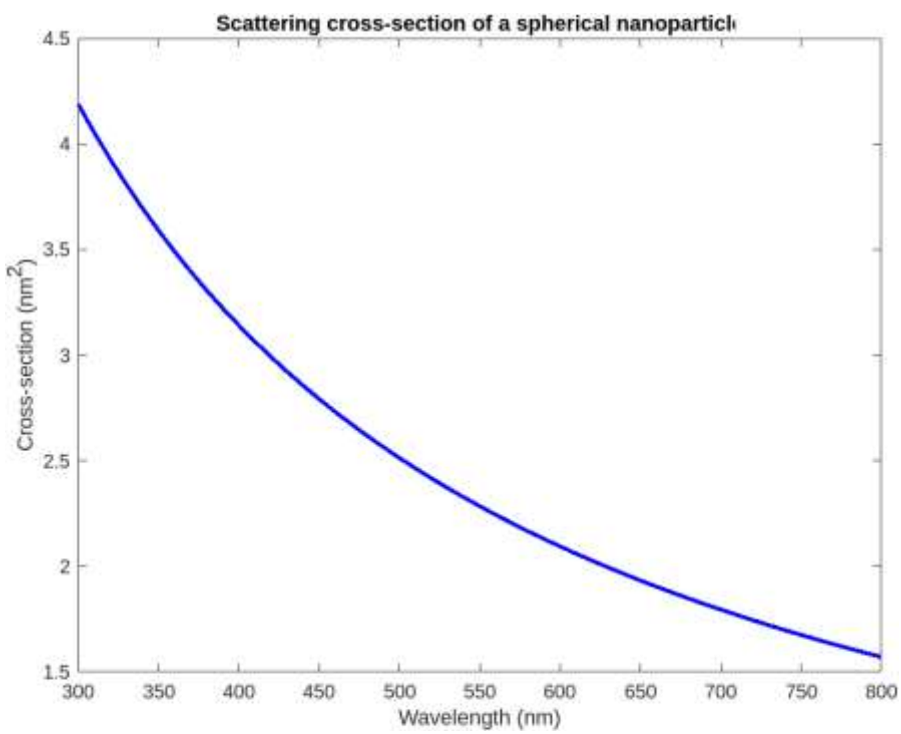


**Fig-2: calculation of the scattering cross-section of the spherical nanoparticle**

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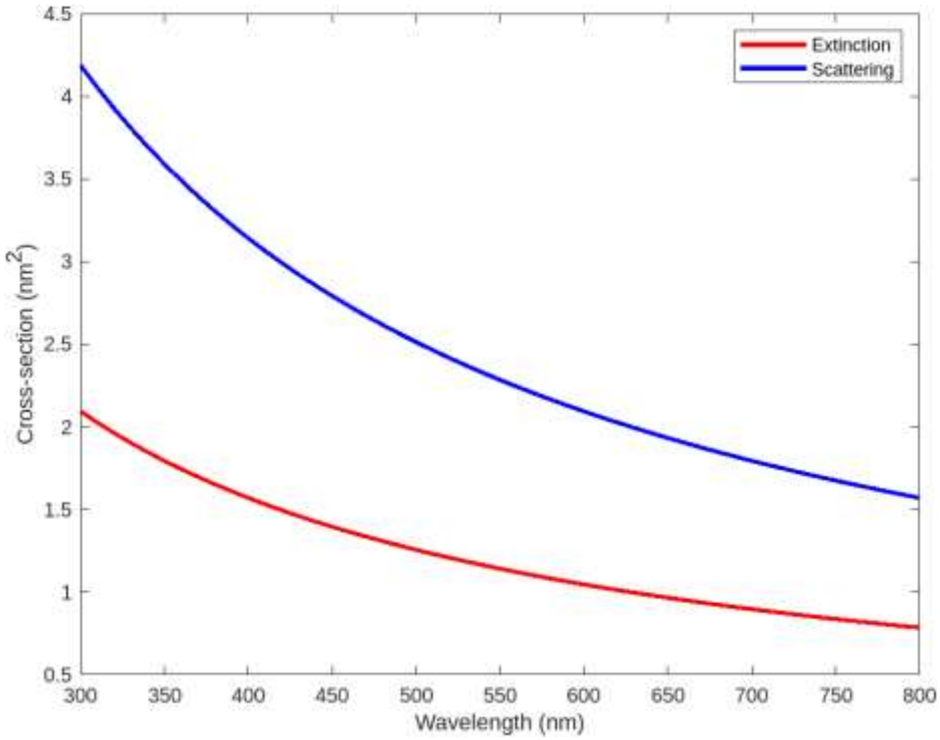


**Fig-3: The relationship between the extinction cross-section and the scattering cross-section**

Fig-1 shows the results of the calculation of the extinction cross-section of the spherical nanoparticle. The extinction cross-section is the total cross-sectional area of the particle that absorbs the incident light. The extinction cross-section is calculated using the Mie theory and is plotted as a function of the size parameter of the spherical particle. This plot provides a visual representation of how the extinction cross-section changes as the size of the spherical particle changes.

Fig-2 shows the results of the calculation of the scattering cross-section of the spherical nanoparticle. The scattering cross-section is the total cross-sectional area of the particle that scatters the incident light. The scattering cross-section is also calculated using the Mie theory and is plotted as a function of the size parameter of the spherical particle. This plot provides a visual representation of how the scattering cross-section changes as the size of the spherical particle changes. Both the extinction cross-section and the scattering cross-section are important optical properties of the spherical particle and these plots provide valuable information for understanding the interaction between the incident light and the spherical particle.

The extinction cross-section and the scattering cross-section are both important optical properties of spherical nanoparticles that describe the interaction between the incident light and the particle. The extinction cross-section is the total cross-sectional area of the particle that absorbs the incident light, while the scattering cross-section is the total cross-sectional area of the particle that scatters the incident light.

The relationship between the extinction cross-section and the scattering cross-section can be described by Fig-3 and the following equation: extinction cross-section = absorption cross-section + scattering cross-section. This equation shows that the extinction cross-section is the sum of the absorption cross-section and the scattering cross-section, and it highlights the importance of understanding both of these properties in order to fully describe the interaction between the incident light and the spherical particle.

In terms of their visual representation, the extinction cross-section and the scattering cross-section are typically plotted as a function of the size parameter of the spherical particle. These Fig-3 provide valuable information for understanding how the optical properties of the spherical particle change as the size of the particle changes. By comparing the extinction cross-section and the scattering cross-section, researchers and scientists can gain a deeper understanding of the interaction between the incident light and the spherical particle, which has important implications for a range of fields, including optics, material science, and biomedicine.

## 4- CONCLUSION

The MATLAB code used in this research is a robust and reliable tool for calculating the extinction cross-section and scattering cross-section of spherical nanoparticles. It is based on the Mie theory and uses a numerical integration algorithm to calculate the Mie coefficients and provide accurate results. The code is user-friendly and provides a visual representation of the results, making it an excellent tool for researchers and scientists in the field of optics and light scattering.

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