

Light scattering by horizontally oriented square pyramid in the Wentzel–Kramers–Brillouin approximation

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In this research, we studied the sensitivity of the form factor of a pyramidal ice crystal in the Wentzel–Kramers–Brillouin (WKB) approximation to its geometrical characteristics: the shape, spatial orientation, aspect ratio and size parameter. Using the WKB method, we derive an analytical formula of the form factor of horizontally oriented square pyramid. We will begin this work by applying the WKB approximation to the case of a particle which rotates about its main axis. Then, we will move to deal with the case of a particle which rotates about an axis perpendicular to its main axis in a future work. In addition, the coefficient of extinction is also given. To illustrate our analytical results, some numerical examples are analyzed.

Keywords: form factor, light scattering, pyramidal ice crystal, Wentzel–Kramers–Brillouin approximation.

1. Introduction

For many years, the importance of studying the phenomenon of scattering and absorption of electromagnetic light in an isotropic medium has grown steadily and is widely used in several applications of science and technology for the study of the structure and properties of inhomogeneous media. In recent years, due to their great importance, particularly in the fields of atmospheric and oceanic optics, geophysics, metrology, computed tomography, solar energy technologies, radio wave propagation, biophysics, laser biomedicine, light scattering theory and practice, the techniques have been sufficiently developed [1–9]. Several studies have been carried out to treat the interaction between a plane electromagnetic wave and a non-absorbent homogeneous spherical particle [10]. It has been shown that the scattering of an electromagnetic wave depends only on two complementary parameters (the parameter of size ka , where a is the radius

of the spherical particle, k wave number, and the second parameter is the relative refractive index m). Depending on the particle size to wavelength ratio, several methods can be cited to study the scattering of light by a spherical particle, among these methods, the Lorenz–Mie theory, the Rayleigh theory, the anomalous diffraction theory. In general, the interaction of the particle with the radiation electromagnetic incident can be determined by solving the Maxwell equations with the boundary conditions corresponding to the shape of the particle. However, there are solutions for certain forms such as spheres, ellipsoids and infinite cylinders (VAN DE HULST, 1957 [2], BARBER and HILL, 1990 [11]), Recently, a number of techniques and approaches have been applied to find a solution to this problem. Konstantin A. Shapovalov, obtained the analytical expressions of the amplitude of light scattering by a prism and an arbitrary polygonal base pyramid in the RGD approximation [12]. Gustav Mie (1908) provided the first solution of Maxwell's equations for dielectrics and spheres and obtained a rigorous general solution based on the electromagnetic theory for the scattering of light by a homogeneous sphere of arbitrary size in a homogeneous medium [11]. Extension to other less ideal particle shapes is proving to be a difficult problem. These systems are of great interest to many scientific disciplines, such as astronomy, geophysics and chemistry. We can cite two general approaches:

1) Numerical methods like: T-matrix or extended boundary condition method (ECBM), discrete dipole approximation (DDA), finite difference time domain method (FDTD), *etc.*

2) The use of approximate analytical methods; Mie theory and its extensions have been used to obtain exact analytic solutions for scattering of light by: homogeneous and concentric spheres [13] and chiral spheres [14], homogeneous and concentric infinitely long cylinders, homogeneous and concentric spheroids and ellipsoids, *etc.* But for particles of irregular shapes, it is often advantageous to use approximate methods, such as: Rayleigh–Gans–Debye (RGD) approximation, anomalous diffraction (AD), Wentzel–Kramers–Brillouin (WKB) approximation, *etc.*

Among the analytical methods used to treat non spherical particles we find the WKB approximation. In this approximation, the internal field is equal to the incident field modulated by a phase delay factor, which corresponds to an additional phase shift of the wave that propagates inside the particle. Therefore, the WKB approximation is a refinement of the RGD approximation [15]. The WKB method, introduced by Rayleigh in 1912 to solve the problems of wave propagation [16], was applied for the first time to quantum mechanics by JEFFREYS in 1923 [17]. SAXON applied the method of the WKB approximation to the scattering of electromagnetic waves by a dielectric sphere [18]. In 1959, DIERMENDJIAN introduced this analytical method to calculate the scattering of light by spheres and proved his interest [19]. Due to the complexity of the general scattering theory for non-spherical particles, the possibility of applying the WKB approximation to the modeling of light scattering by pyramidal objects deserves to be studied. This approach has been applied earlier to spheres, cylinders and spheroids [20–22], and also applied to the cube and hexagon as non-spherical particles [23, 24]. In this study, we apply the WKB method to non-spherical particles to obtain an ana-

lytical expression of the form factor for horizontally oriented pyramidal particle. This work concerns the study of a particle which rotates around its main axis. Then, we calculate the extinction coefficient to illustrate the results.

2. Analytical formulation of the WKB approximation for horizontally oriented square pyramid

2.1. Theory

Let us consider a particle of volume v and the relative complex refractive index m ($m = m_r + im_i$), illuminated by a plane wave of wave number k ($k = 2\pi/\lambda$), polarized in the direction \mathbf{e}_x and propagating along the z -axis (Fig. 1). It is known that the scattering amplitude is derived from Maxwell's equation. In WKB approximation, the unknown field inside the particle is replaced by a plane wave that propagates without reflection and with no change in direction. This amplitude is related to the form factor $F(\theta, \varphi)$ by [21]

$$|f(\mathbf{s}, \mathbf{i})| = \sin(\zeta) \frac{k^2}{2\pi} |(m - 1)F(\theta, \varphi)| \tag{1}$$

We denoted \mathbf{s} and \mathbf{i} are the unit vectors of the scattered light and the propagation of incident light, respectively, θ is the scattering angle between \mathbf{i} and \mathbf{s} , and φ is the azimuth angle, \mathbf{r} is a vector position of any point in side the scattered, ζ is the angle between the polarization vector \mathbf{e}_x and the unit vector \mathbf{s} . Thus the form factor is given by the following expression

$$F(\theta, \varphi) = \iiint_v \exp[ik\mathbf{r}(\mathbf{i} - \mathbf{s})] \exp(ikw) dv \tag{2}$$

where w is the optical path which is introduced by the scatterer defined as follows

$$w = \int_{z_e}^z [m(z') - 1] dz' = (m - 1) \times (z - z_e) \tag{3}$$

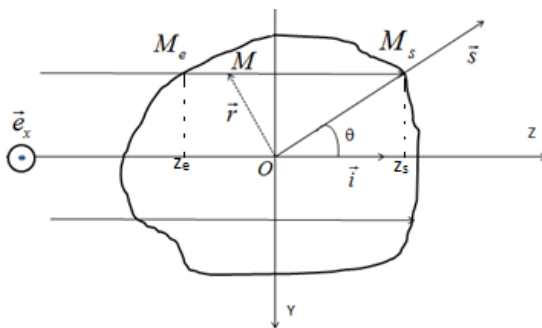


Fig. 1. Description of the scattering problem.

For non-spherical particles, it is convenient to use a Cartesian coordinate system, orthonormal $R(o, x, y, z)$ whose origin coincides with the center of the particle. Thus, the form factor for homogeneous particle is expressed in the simple form

$$F(\theta, \varphi) = \iiint_v \exp\left[ikx \sin\theta \cos\varphi\right] \exp\left[-iky \sin\theta \sin\varphi\right] \times \exp\left[ikz(m - \cos\theta)\right] \exp\left[-ikz_e(m - 1)\right] dv \quad (4)$$

where $x, y,$ and z are the components of the position of the scattering element inside the object, and z_e is the z coordinate of the intersection between the incident light and the body surface.

2.2. Application to the square pyramid

Consider a pyramidal particle to be a square base of height h and side length a , with relative complex refractive index m , illuminated by a plane wave of wave number k , polarized in the direction e_x and propagating along the z -axis. The origin of the Cartesian coordinate system $R(o, x, y, z)$ coincides with the center of the particle and the principal axis of the particle is oriented along the x -axis. In this section we apply the WKB method to horizontally oriented pyramid (Fig. 2).

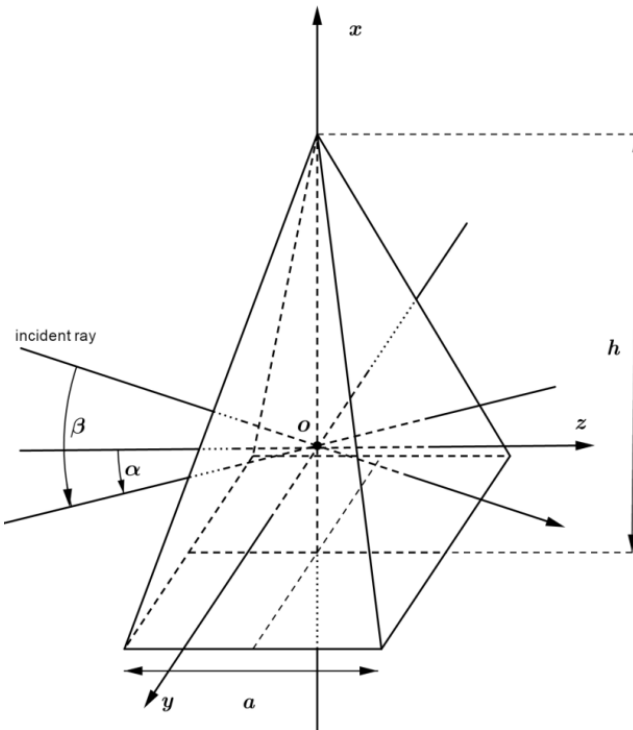


Fig. 2. Geometry of a pyramidal particle with obliquely incident ray.

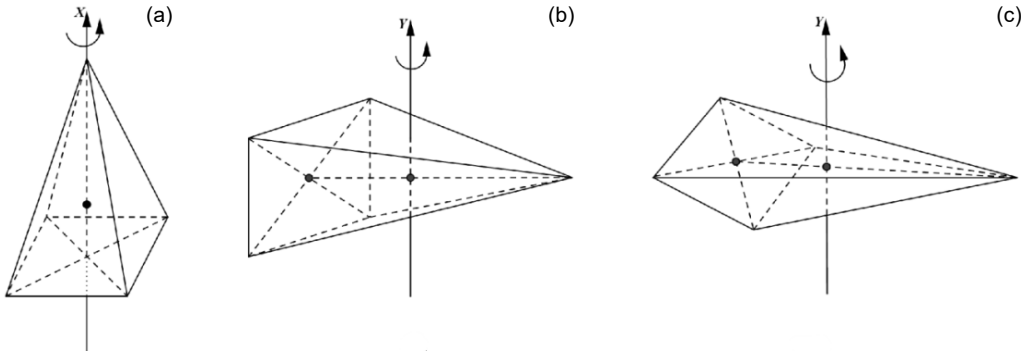


Fig. 3. Schemes for each orientation.

The obliquely incident ray is characterized by azimuth angle α and elevation angle β . From the symmetry of the pyramid, α is from 0 to $\pi/4$, and β is from 0 to $\pi/2$, α is zero when the incident ray is perpendicular to one of the ribs of the base of the pyramid. In the following, Fig. 3 shows in details the different “schemes” for horizontally oriented incidence.

The use of the WKB approximation for oblique incidence presents some difficulties. So, we will focus in this work on studying the rotation of the particle around the principal axis (x -axis) (*i.e.*, $\beta = 0$, $0 \leq \alpha \leq \pi/4$). Special cases of normal incidence (*i.e.*, flat incident light $\alpha = 0$ and edge-on incidence $\alpha = \pi/4$) are studied in another work submitted for publication, so we will focus in this article on the horizontal incidence such as ($0 < \alpha < \pi/4$). To facilitate this study, we will cut the pyramid into small slices (squares) horizontally, so that the planes of these squares (slices) are perpendicular to the x -axis, with thickness dx and side length $a(x)$ (Fig. 4a).

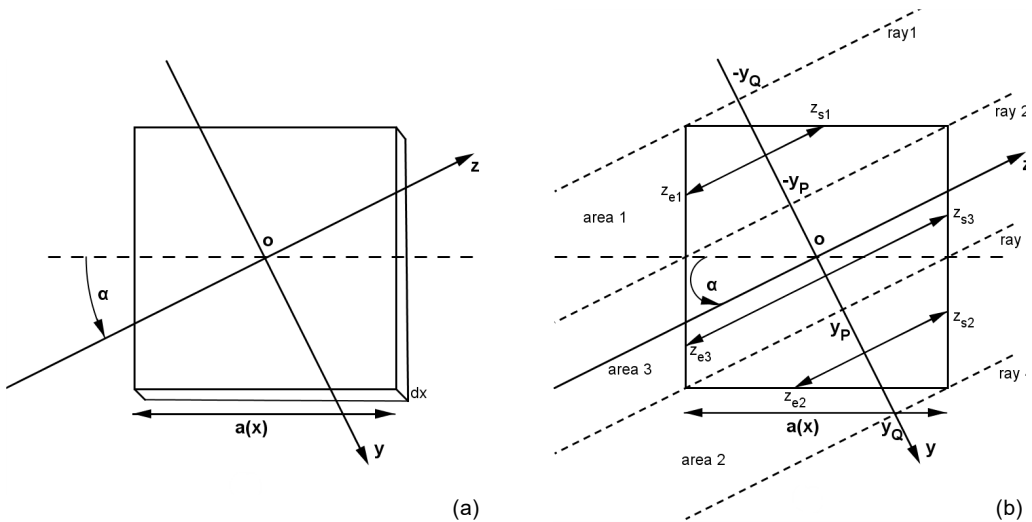


Fig. 4. Decomposition of the pyramidal particle.

For obliquely incident ray with angle α , the square of each thickness can be divided into three areas by rays: 1, 2, 3, and 4 (Fig. 4b). Furthermore, Fig. 4b shows how to measure the ray paths in each area. The ray paths in each area denoted $\Delta z_j = z_{sj} - z_{ej}$, $j = 1, 2$, and 3, are functions of the variable x and y with z_{sj} and z_{ej} are the z -coordinates of the intersection of the incident light and the slice lateral surfaces.

From Fig. 4b, we have

$$\begin{cases} z_{e1} = -\frac{a(x)}{2 \cos \alpha} - y \tan \alpha \\ z_{s1} = \frac{a(x)}{2 \sin \alpha} + y \cot \alpha \end{cases}, \quad -y_Q \leq y \leq -y_P \quad (5a)$$

$$\begin{cases} z_{e2} = -\frac{a(x)}{2 \sin \alpha} + y \cot \alpha \\ z_{s2} = \frac{a(x)}{2 \cos \alpha} - y \tan \alpha \end{cases}, \quad y_P \leq y \leq y_Q \quad (5b)$$

$$\begin{cases} z_{e3} = -\frac{a(x)}{2 \cos \alpha} - y \tan \alpha \\ z_{s3} = \frac{a(x)}{2 \cos \alpha} - y \tan \alpha \end{cases}, \quad -y_P \leq y \leq y_P \quad (5c)$$

where

$$a(x) = \frac{3a}{4} - \frac{ax}{h} \quad (5d)$$

$$\begin{cases} y_P = \frac{a(x)}{2} (\cos \alpha - \sin \alpha) \\ y_Q = \frac{a(x)}{2} (\cos \alpha + \sin \alpha) \end{cases} \quad (5e)$$

After integrating the Eq. (4) over the variable z , the expression of the form factor is given by the following expression

$$F(\theta, \varphi, \alpha) = \frac{1}{ik(m - \cos \theta)} \iint \exp(-ikx \sin \theta \cos \varphi) \times \exp(-iky \sin \theta \sin \varphi) G(z_e, z_s) dx dy \quad (6)$$

with

$$G(z_e, z_s) = \exp[ik(m - \cos \theta)z_e] \exp[-ik(m - 1)z_e] - \exp[ik(1 - \cos \theta)z_e] \quad (7)$$

We must therefore consider the particular case for which the analytical expression of the integral defined by Eq. (6) is not defined for the value of θ , and a general case.

2.2.1. Case of $\theta = 0$

After some algebraic manipulations, we obtain

$$F(0, \varphi, \alpha) = F_1(0, \varphi, \alpha) + F_2(0, \varphi, \alpha) + F_3(0, \varphi, \alpha) \tag{8}$$

where

$$F_1(0, \varphi, \alpha) = F_2(0, \varphi, \alpha) = \frac{ah \sin \alpha}{ik(m-1)} \left\{ \frac{1}{i\rho} \left[\frac{\exp(i\rho) - 1}{i\rho} - 1 \right] - \frac{1}{2} \right\} \tag{9a}$$

$$F_3(0, \varphi, \alpha) = ah \frac{\sin \alpha - \cos \alpha}{ik(m-1)} \left\{ \left(\frac{1}{i\rho} - 1 \right) \left[\frac{\exp(i\rho) - 1}{i\rho} - 1 \right] - \frac{1}{2} \right\} \tag{9b}$$

and

$$\rho = ka \frac{m-1}{\cos \alpha} \tag{9c}$$

2.2.2. Case of $\theta \neq 0$

By calculating the integral in Eq. (6) over the variable y we can find the contribution from the slice to the form factor $F(\theta, \varphi, \alpha)$ denoted as

$$f^0(\theta, \varphi, \alpha, x) = f_1^0(\theta, \varphi, \alpha, x) + f_2^0(\theta, \varphi, \alpha, x) + f_3^0(\theta, \varphi, \alpha, x) \tag{10}$$

where $f_1^0(\theta, \varphi, \alpha, x)$, $f_2^0(\theta, \varphi, \alpha, x)$ and $f_3^0(\theta, \varphi, \alpha, x)$ are the contribution from area 1, area 2 and area 3 of each slices to the form factor respectively, with

$$f_1^0(\theta, \varphi, \alpha, x) = \frac{\exp(-ikx \sin \theta \cos \varphi)}{ik(m - \cos \theta)} \int_{-y_Q}^{-y_P} \exp(-iky \sin \theta \sin \varphi) G(z_{e1}, z_{s1}) dy \tag{11a}$$

$$f_2^0(\theta, \varphi, \alpha, x) = \frac{\exp(-ikx \sin \theta \cos \varphi)}{ik(m - \cos \theta)} \int_{y_P}^{y_Q} \exp(-iky \sin \theta \sin \varphi) G(z_{e2}, z_{s2}) dy \tag{11b}$$

$$f_3^0(\theta, \varphi, \alpha, x) = \frac{\exp(-ikx \sin \theta \cos \varphi)}{ik(m - \cos \theta)} \int_{-y_P}^{y_P} \exp(-iky \sin \theta \sin \varphi) G(z_{e3}, z_{s3}) dy \tag{11c}$$

Then the form factor can be expressed in a simple form

$$F(\theta, \varphi, \alpha) = \int_{-h/4}^{3h/4} f^0(\theta, \varphi, \alpha, x) dx \tag{12}$$

Due to the additivity of the integral, the form factor Eq. (12) can be written as a sum of the contributions of each area.

$$F(\theta, \varphi, \alpha) = F_1(\theta, \varphi, \alpha) + F_2(\theta, \varphi, \alpha) + F_3(\theta, \varphi, \alpha) \quad (13)$$

where

$$F_1(\theta, \varphi, \alpha) = \int_{-h/4}^{3h/4} f_1^0(\theta, \varphi, \alpha, x) dx \quad (14a)$$

$$F_2(\theta, \varphi, \alpha) = \int_{-h/4}^{3h/4} f_2^0(\theta, \varphi, \alpha, x) dx \quad (14b)$$

$$F_3(\theta, \varphi, \alpha) = \int_{-h/4}^{3h/4} f_3^0(\theta, \varphi, \alpha, x) dx \quad (14c)$$

Substituting the values of z_{ej} and z_{sj} in Eqs. (14a), (14b) and (14c), and integrating over the variable x , after some algebraic manipulations, the contributions of each area can be expressed in a simple form

$$F_1(\theta, \varphi, \alpha) = \frac{ah \exp\left(-i \frac{3}{4} d\right)}{ik(m - \cos\theta)} \left\{ \frac{1}{iA} \left[\frac{\exp(iB) - 1}{iB} - \frac{\exp(iB') - 1}{iB'} \right] - \frac{1}{iA'} \left[\frac{\exp(iC) - 1}{iC} - \frac{\exp(iC') - 1}{iC'} \right] \right\} \quad (15a)$$

$$F_2(\theta, \varphi, \alpha) = \frac{ah \exp\left(-i \frac{3}{4} d\right)}{ik(m - \cos\theta)} \left\{ \frac{1}{iD} \left[\frac{\exp(iE) - 1}{iE} - \frac{\exp(iE') - 1}{iE'} \right] - \frac{1}{iD'} \left[\frac{\exp(iF) - 1}{iF} - \frac{\exp(iF') - 1}{iF'} \right] \right\} \quad (15b)$$

$$F_3(\theta, \varphi, \alpha) = \frac{ah \exp\left(-i \frac{3}{4} d\right)}{ik(m - \cos\theta)} \left\{ \frac{1}{iA'} \left[\frac{\exp(iG) - 1}{iG} - \frac{\exp(iG') - 1}{iG'} \right] - \frac{1}{iA''} \left[\frac{\exp(iH) - 1}{iH} - \frac{\exp(iH') - 1}{iH'} \right] \right\} \quad (15c)$$

where

$$A = t - 2q \sin \alpha - \frac{2\mu}{\sin \alpha} \quad (16a)$$

$$A' = t - 2q \sin \alpha \quad (16b)$$

$$B = d + \frac{t}{2}(\cos \alpha + \sin \alpha) + \cos \alpha(\cos \alpha - \sin \alpha)q \quad (16c)$$

$$B' = d + \frac{t}{2}(\cos \alpha - \sin \alpha) + g - \sin \alpha(\cos \alpha - \sin \alpha)q \quad (16d)$$

$$C = d + \frac{t}{2}(\cos \alpha + \sin \alpha) + \cos \alpha(\cos \alpha - \sin \alpha)q \quad (16e)$$

$$C' = d + \frac{t}{2}(\cos \alpha - \sin \alpha) + (1 + \sin^2 \alpha - \sin \alpha \cos \alpha)q \quad (16f)$$

$$D = t - 2q \sin \alpha + \frac{\rho}{\sin \alpha} \quad (16g)$$

$$D' = t - 2q \sin \alpha + \frac{2q}{\sin \alpha} \quad (16h)$$

$$E = d - \frac{t}{2}(\cos \alpha - \sin \alpha) + g + \sin \alpha(\cos \alpha - \sin \alpha)q \quad (16i)$$

$$E' = d - \frac{t}{2}(\cos \alpha + \sin \alpha) - \cos \alpha(\cos \alpha - \sin \alpha)q \quad (16j)$$

$$F = d - \frac{t}{2}(\cos \alpha - \sin \alpha) + \cos \alpha(\cos \alpha + \sin \alpha)q \quad (16k)$$

$$F' = d - \frac{t}{2}(\cos \alpha + \sin \alpha) - \cos \alpha(\cos \alpha - \sin \alpha)q \quad (16l)$$

$$G = d + \frac{t}{2}(\cos \alpha - \sin \alpha) + g - \sin \alpha(\cos \alpha - \sin \alpha)q \quad (16m)$$

$$G' = d - \frac{t}{2}(\cos \alpha - \sin \alpha) + g + \sin \alpha(\cos \alpha - \sin \alpha)q \quad (16n)$$

$$H = d + \frac{t}{2}(\cos \alpha - \sin \alpha) + (1 + \sin^2 \alpha - \sin \alpha \cos \alpha)q \quad (16o)$$

$$H' = d - \frac{t}{2}(\cos \alpha - \sin \alpha) + \cos \alpha(\cos \alpha + \sin \alpha)q \quad (16p)$$

The used parameters are

$$d = kh \sin \theta \cos \varphi \quad (17a)$$

$$t = ka \sin \theta \sin \varphi \quad (17b)$$

$$\rho = ka \frac{m-1}{\cos \alpha} \quad (17c)$$

$$\mu = ka \frac{m - \cos \theta}{2 \cos \alpha} \quad (17d)$$

$$g = \frac{\rho}{2} + \mu \quad (17e)$$

$$q = \frac{\rho}{2} - \mu \quad (17f)$$

Note that to find the amplitude of light scattering, it is sufficient to replace the form factor with its expression in Eq. (1).

3. Results

We have previously established the analytical expressions for the form factor of a horizontally oriented pyramidal particle in the framework of the WKB approximation. First, we have checked the correctness of the analytical expressions of the form factor. For this, we have calculated numerically the different double integrals which intervene

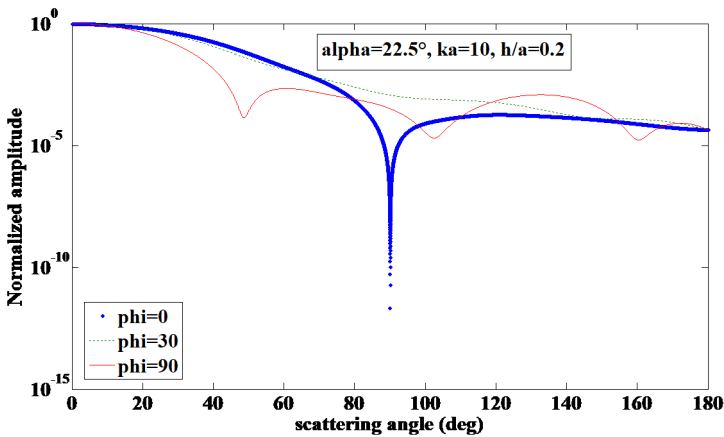


Fig. 5. Normalized amplitude *versus* the scattering angle θ for absorbing pyramidal ice crystal with aspect ratio $h/a = 2$, and $h/a = 0.2$, at the wavelength $\lambda = 0.55 \mu\text{m}$, the complex index of refraction $m = 1.311 + 0.31 \times 10^{-8}i$, for three values of $\varphi = 0^\circ, 30^\circ$ and 90° .

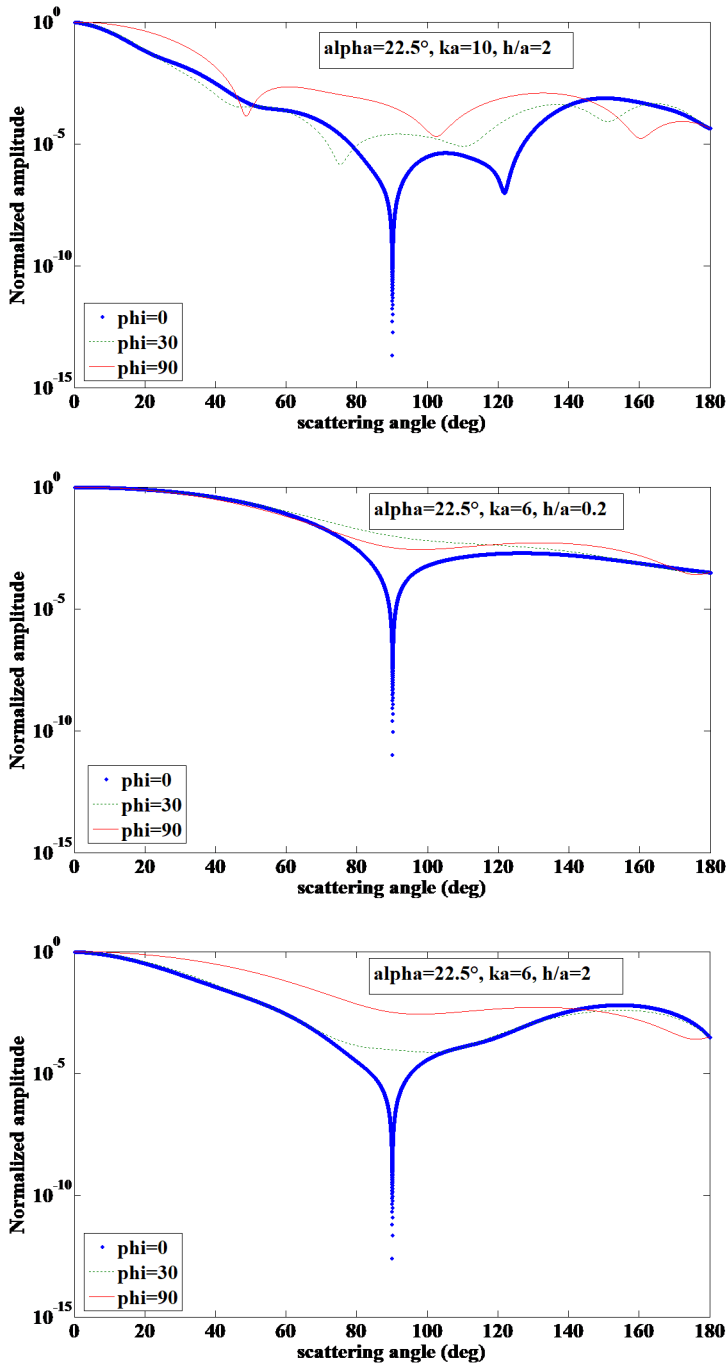


Fig. 5. Continued.

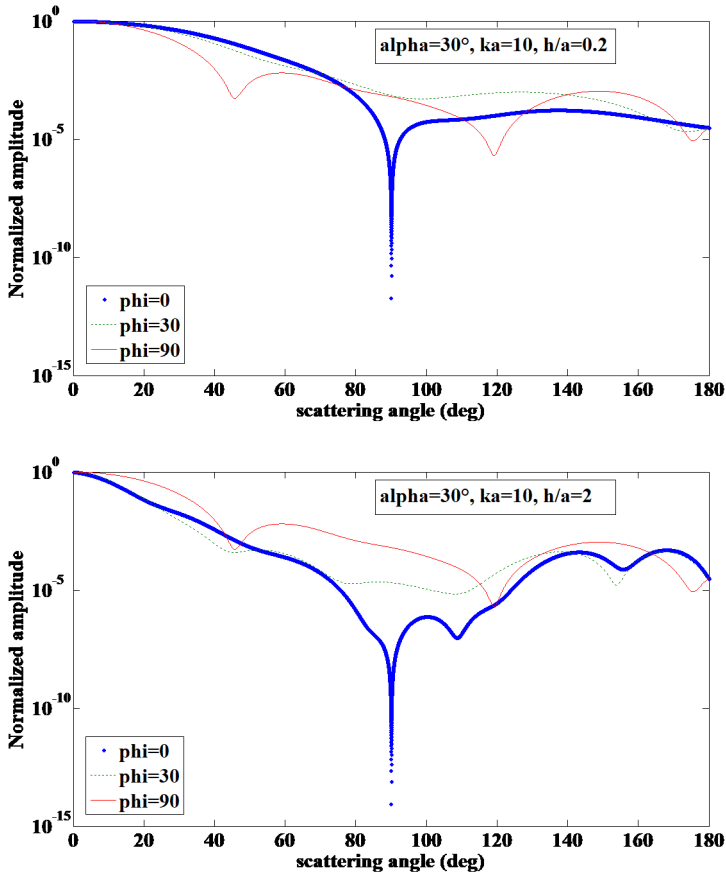


Fig. 5. Continued.

here using the Gauss-Legendre quadrature method. By taking 16×16 integration points for this quadrature, we have reproduced numerically the results obtained with the analytical expression of the form factor.

For illustration, we show in Fig. 5, the behavior of the normalized amplitude of light scattering as a function of the scattering angle θ in the case of absorbing pyramidal crystals for three values of the azimuth angle $\varphi = 0^\circ, 30^\circ$ and 90° , the wavelength $\lambda = 0.55 \mu\text{m}$, the complex index of refraction $m = 1.311 + 0.31 \times 10^{-8}i$.

The graphs representing the normalized amplitude of light scattering show that this amplitude exhibits some lobes with intensity decreasing with increasing the scattering angle. We note that the number of the extreme of the light increases with increasing the aspect ratio h/a for the same value of the azimuth angle φ , except when the value of this angle is equal to 90° . The normalized amplitude varies greatly with this angle and with the orientation angle of the particle (angle α). This is manifested by the appearance of a number of lobes and extremes. Consequently, the azimuth angle φ plays

an important role in the study of the scattering of light by a nonspherical particle, unlike the case of spherical particle. In addition to the non-spherical effect of ice crystals, the orientations of these particles are also important to their optical properties. We can also conclude that the amplitude is sensitive to the size parameter and aspect ratio. Finally, we note that the backscatter is almost unnoticeable compared to the front scattering.

4. Extinction efficiency

From the definition of the extinction efficiency and the cross section of extinction introduced in the reference [2, 25], we can show that the extinction efficiency is expressed by the following formula

$$Q_{\text{ext}} = \frac{2k}{P} \text{Im}((m-1)F(0, 0)) \quad (18)$$

where P is the projected area of the particle on the plane perpendicular to the direction of the incident wave, and the Im indicates the imaginary part.

The project area of the pyramid in this case is given by $P = \frac{ah}{2}(\sin\alpha + \cos\alpha)$. For real refractive index, the extinction efficiency becomes

$$Q_{\text{ext}} = 2 \left\{ 1 + 2 \frac{\sin\alpha - \cos\alpha}{\sin\alpha + \cos\alpha} \frac{\sin\rho}{\rho} - \frac{3\sin\alpha - \cos\alpha}{\sin\alpha + \cos\alpha} \left[\frac{\sin(\rho/2)}{\rho/2} \right]^2 \right\} \quad (19)$$

In Fig. 6, we present the behavior of the extinction efficiency factors for horizontally oriented pyramidal ice crystals in the WKB approximation, as functions of parameter $X = a/\lambda$. This parameter allows us to compare the wavelength with the largest possible ray path within the considered particle. Figure 6a shows that, the main influence of an increase in the orientation angle of the particle from 0 to $\pi/4$ on the extinction efficiency is to damp the oscillations, in particular the amplitude of the peak efficiency. One should also note that when the largest path is of the order of the wavelength, the extinction increases rapidly to a peak of maximum efficiency. Then, the extinction efficiency decreases and after some oscillations, it tends to the limiting value 2 for large quantities of X . This would suggest that the particle will block off twice the light falling upon it, an effect calling the “extinction paradox” (VAN DE HULST (1957) [2], BOHREN and HUFFMAN (1983) [14]). So it is clearly seen that the extinction efficiency is sensitive to the size parameter, and to the rotation about the principal axe of the particle (angle α). The same result was found by SUN and FU, for the hexagonal particles in the anomalous diffraction theory ADT [26].

Figure 6b shows the influence of the real part of refractive index for fixed imaginary part. As the real part increases, the amplitude of the maximum peak efficiency also increases and moves towards the small particle. In addition, there is an increase in the number of oscillations.

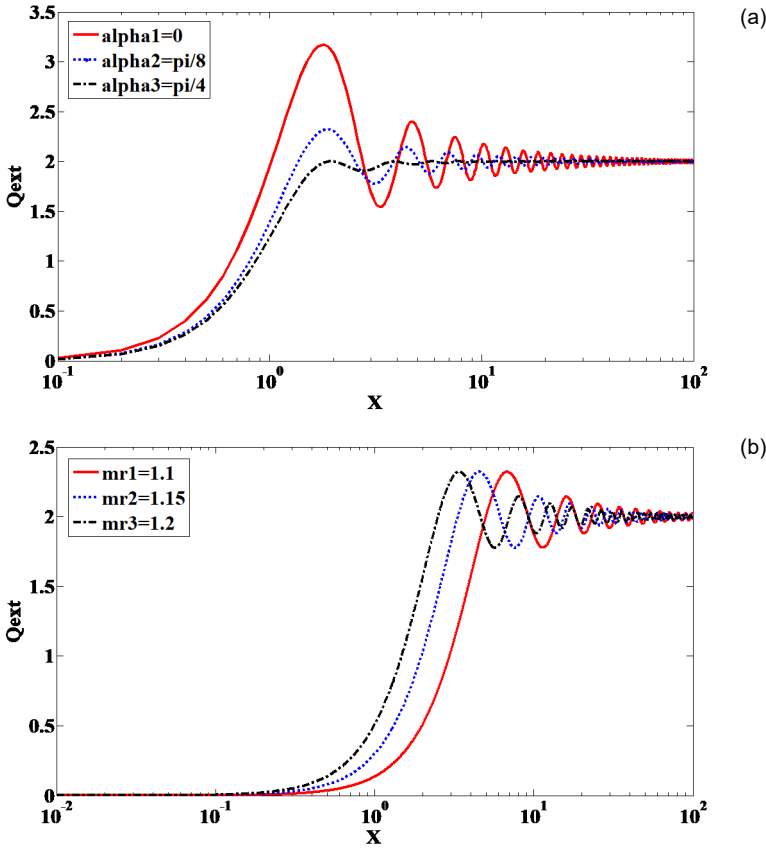


Fig. 6. Extinction efficiency factor as a function of parameter $X = a/\lambda$, for $m = 1.3645 + 0.31 \times 10^{-8}i$, (a), and $m = m_r + 0.31 \times 10^{-8}i$ (b).

5. Conclusion

This work concerns itself with the study of the scattering of a plane electromagnetic wave by a horizontally oriented non-spherical particle (in particular their rotation around its main axis) in the approximation of WKB. The particle considered is the pyramid. We observed that this form factor of the light scattering by horizontally oriented particles of the pyramid depended on the geometric shape of the particle, the size and the relative refractive index, as well as the orientation angle α of the particle with regard to the incident wave, and the azimuthally angle φ . Unlike the spherical particle, the shape factor is the same because of spherical symmetry, regardless of the orientation of the particle. Furthermore, the extinction efficiency Q_{ext} is also deduced analytically for the horizontal incidence. We can see that this coefficient depends on the orientation of particles, and also, when the value of the angle $\alpha = 45^\circ$, and for a large value of the parameter X , this coefficient converges toward the value of 2. Whereas for a value $\alpha = 0^\circ$, Q_{ext} continues to oscillate around the value of 2.

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