LIGHT SCATTERING SIMULATIONS OF SPHEROIDS USING THREE BEAMS PHASE DOPPLER SYSTEM

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Abstract: Problem presented in the paper concentrates on the light scattering on spheroids, that cross the probe volume of the laser Doppler system which exploits three laser beams. Comparison of the system responses between spheres and spheroids of different shapes is demonstrated.
An influence of Euler's rotation angles of the spheroid and differences in scattered field between two and three beam systems are shown.

Keywords: light scattering, phase Doppler system, spheroids, three beams, t-matrix, extended boundary condition method

1. INTRODUCTION

One of the well-established measurement techniques is Phase-Doppler (PDA) anemometry, which allows measuring particles velocity, size, flux, concentration and physical properties of the flow. Although a great development of the laser Doppler anemometry (LDA) techniques it is noteworthy, that many improvements are still being done. Present optical systems are able to determine simultaneously not only particle diameter and velocity of the flow but also a refractive index, absorption coefficients or physical homogeneity of the particle [1, 2].

We propose an extension of three Beams Phase Doppler Anemometer (3BPDA) to measure properties of axisymmetrical, homogenous particles (according to the idea of Onofri [3]). The system uses three coherent laser beams, which are coplanar in this case.

Volume probe in standard laser anemometers can be created by diffraction a coherent, linearly polarized laser beam onto Bragg's cell or a diffraction grating. During that process three orders diffracted beams are present: +1,0,-1. Probe volume consists +1, -1 beams; 0 order beam is classically cut off. In 3BPDA zero-order beam is also transmitted, thus volume probe is a superposition of three beams.

Usually simulations of many kind of laser Doppler Systems base on Mie theory, which describes scattering phenomenon of plane, electromagnetic wave illuminating a spherical particle placed in homogenous space without additional sources. Approximation of the shape of the scatterer as a sphere is sufficient to get valuable results in many cases. However there are situations where more sophisticated model should be considered. Such situation takes place during a development of droplets of liquid, which is a dynamic process that introduces oscillations of surface for macroscopic particles [4]. Interactions between particles in a real flow also influence on their shapes. Therefore spheroidal particle seems to be more useful in next step of considered approximations. Among many techniques extended boundary condition method (EBCM) seems to be one of the powerful end efficient tools for calculating scattering properties of media. The method provides high computational effectiveness as well as algorithms derived directly form Maxwell equations.

The paper therefore describes a scattering model used in preliminary calculations of the response of 3BPDA for cases when plane wave is taken into account as incident field and when classical Gaussian laser beam is used. Our future task is to determine limitations and measurement errors in case when particles moving through probe volume are not perfect spheres but spheroids.

2. METHODOLOGY

To calculate the scattered electromagnetic field of nonspherical particle let us choose a coordinate system with its origin placed inside, in the centre of the particle (particle coordinate system P). The particle is illuminated by plane, electromagnetic wave, separated on two components:

$$\mathbf{E}_i(\mathbf{r}) = \left(E_{i\theta}\mathbf{n}_\theta + E_{i\varphi}\mathbf{n}_\varphi\right)e^{ik\mathbf{n}_i\mathbf{r}} \qquad (1)$$

where $\mathbf{r}$ is the position vector with its origin at the origin of P, k is the wavenumber of free space, $\mathbf{n}_\varphi$, $\mathbf{n}_\theta$ are unit vectors related to φ and θ directions, respectively, $\mathbf{n}_i$ is a unit vector of propagating wave.

Both of incident $\mathbf{E}_i$ and scattered $\mathbf{E}_s$ fields can be expanded in vector spherical functions:

$$\mathbf{E}_i(\mathbf{r}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\left[a_{mn}\mathrm{Rg}\mathbf{M}_{mn}(k\mathbf{r}) + b_{mn}\mathrm{Rg}\mathbf{N}_{mn}(k\mathbf{r})\right] \quad (2)$$

$$\mathbf{E}_s(\mathbf{r}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\left[p_{mn}\mathbf{M}_{mn}(k\mathbf{r}) + q_{mn}\mathbf{N}_{mn}(k\mathbf{r})\right] \qquad (3)$$

Where $\mathbf{Rg}\mathbf{M}_{mn}$, $\mathbf{Rg}\mathbf{N}_{mn}$ are regular at the origin and $\mathbf{M}_{mn}$, $\mathbf{N}_{mn}$ are spherical wave functions. The expansion coefficients of an incident, plane wave can be expressed as:

$$a_{mn} = i^n d_n k_m \mathbf{E}\mathbf{C}_{mn}^*(\theta)\exp(-im\varphi) \qquad (4)$$

$$b_{mn} = i^{n-1} d_n k_m \mathbf{E}\mathbf{B}_{mn}^*(\theta)\exp(-im\varphi) \qquad (5)$$

$$d_n = \sqrt{[(2n+1)/(4\pi n(n+1))]}, \quad k_m = 4\pi(-1)^m \quad (6)$$

where $\mathbf{E}$ is complex constant vector, $\mathbf{C}_{mn}$, $\mathbf{B}_{mn}$ are vector spherical harmonics. Respectively, coefficients of the scattered electromagnetic field [5, 6] can be denoted as

$$p_{mn} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} (T_{mnm'n'}^{11} a_{m'n'} + T_{mnm'n'}^{12} b_{m'n'}) \qquad (7)$$

$$q_{mn} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} (T_{mnm'n'}^{21} a_{m'n'} + T_{mnm'n'}^{22} b_{m'n'}) \qquad (8)$$

Due to the linearity conditions of Maxwell equations the relation between p_{mn}, q_{mn} and a_{mn}, b_{mn} coefficients can be expressed as

$$\begin{bmatrix} \mathbf{p} \\ \mathbf{q} \end{bmatrix} = \begin{bmatrix} T^{11} & T^{12} \\ T^{21} & T^{22} \end{bmatrix} \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix} \qquad (9)$$

where $\mathbf{a}$, $\mathbf{b}$, $\mathbf{p}$, $\mathbf{q}$ are vectors of expansion coefficients given above and matrix consists elements $T^{11}... T^{22}$ is called transition matrix $\mathbf{T}$ [7].

Elements of $\mathbf{T}$ are independent of incident wave as well as scattered field. Its elements consists only information about a particle size, its refractive index and a geometrical shape and besides $\mathbf{T}$ is completely independent on incident and scattered fields, polarization and propagation directions - therefore matrix can be derived only once for physically defined particle. Only simple recalculations are required for another scattering directions.

If transition matrix is known we can describe distribution of the scattered field for an arbitrary scattering system using complex, amplitude matrix $\mathbf{S}$. Its elements consist of information about a geometry of incident and scattered directions $\mathbf{S} = \mathbf{S}(\mathbf{T}, \mathbf{n}_i, \mathbf{n}_s)$ (in global coordinate frame L), where $\mathbf{n}_s$ is unit vector of scattering direction

$$\begin{bmatrix} \mathbf{E}_{s\theta} \\ \mathbf{E}_{s\varphi} \end{bmatrix} = \mathbf{S}(\mathbf{T}, \mathbf{n}_i, \mathbf{n}_s)\begin{bmatrix} E_{i\theta} \\ E_{i\varphi} \end{bmatrix} \qquad (10)$$

This makes this technique, based on EBCM, very powerful and rigorous even then, when a formal description of the particle is not straightforward. Many kinds of optical systems can be simulated if a case of one or more illuminating waves is considered.

One of such systems is Phase Doppler System (PDA) that superposes two laser beams to obtain probe volume. For Gaussian laser beams useful description can be used. The laser beam is fully described by the set of coefficients according to the idea proposed by Doicu and Wriedt [8, 9].

For such beam a new coordinate system must be introduced with its origin placed in the center of the beam waist. Expansion coefficients are derived in the reference frame with the use of generalized local approximation.

$$a_{m'n} = \frac{1}{2}(-1)^{m'-1} C_{nm'} K_{nm'} \Psi e^{ikz_0}(s_1 + s_2) \qquad (11)$$

$$b_{m'n} = \frac{1}{2}(-1)^{m'-1} C_{nm'} K_{nm'} \Psi e^{ikz_0}(s_1 - s_2) \qquad (12)$$

$$s_1 = e^{i(m'-1)\varphi_0} J_{m'-1}\left(2\frac{Q\rho_0\rho_n}{w_0^2}\right) \qquad (13)$$

$$s_2 = e^{i(m'+1)\varphi_0} J_{m'+1}\left(2\frac{Q\rho_0\rho_n}{w_0^2}\right) \qquad (14)$$

where coefficients

$$C_{nm'} = 4i^{n-1}\frac{(n+|m'|)!}{(n-|m'|)!} \qquad (15)$$

$$K_{nm'} = \begin{cases} (-1)^{|m'|}\dfrac{i}{(n+1/2)^{|m'|-1}}, & m'\neq 0 \\ \dfrac{n(n+1)}{n+1/2}, & m'=0 \end{cases} \qquad (16)$$

$$\Psi = iQe^{-iQ\left(\frac{\rho_0^2}{w_0^2}+\frac{(n+1/2)^2}{k^2w_0^2}\right)}, \quad \rho_n = \frac{(n+1/2)}{k} \qquad (17)$$

$$Q = \frac{1}{(i-2z_0/l)}, \quad \rho_0 = \sqrt{x_0^2+y_0^2} \qquad (18)$$

$$\varphi_0 = \arctan\left(\frac{x_0}{y_0}\right) \qquad (19)$$

where w_0 is a beam waist radius and vector (x_0, y_0, z_0) describes position of the particle in the L coordinate system that is also connected with direction vectors of the Gaussian beams.

For each beam of order +1, 0, -1 of diffraction grating amplitude matrix may be derived - for simplifying computations only one scattering direction for each $\mathbf{S}$ matrix is considered (e.g. only for single point detector). Considering above simplification we may write:

$$\mathbf{S}^N(\mathbf{n}_i^N, \mathbf{n}_s^N) = \begin{bmatrix} S_{11}^N & S_{12}^N \\ S_{21}^N & S_{22}^N \end{bmatrix} \quad (20)$$

where N is number of a diffraction order (+1, 0, -1) and for each beam we have the same scattering direction: $\mathbf{n}_s^{-1} \equiv \mathbf{n}_s^0 \equiv \mathbf{n}_s^{+1}$.

The scattered field for the particle placed in probe volume superposed from three beams

$$\mathbf{E}_{s\theta} = (E_{i\theta}S_{11}^{-1} + E_{i\varphi}S_{12}^{-1} + E_{i\theta}S_{11}^0 \\ + E_{i\varphi}S_{12}^0 + E_{i\theta}S_{11}^{+1} + E_{i\varphi}S_{12}^{+1})\mathbf{n}_\theta \quad (21)$$

$$\mathbf{E}_{s\varphi} = (E_{i\theta}S_{21}^{-1} + E_{i\varphi}S_{22}^{-1} + E_{i\theta}S_{21}^0 \\ + E_{i\varphi}S_{22}^0 + E_{i\theta}S_{21}^{+1} + E_{i\varphi}S_{22}^{+1})\mathbf{n}_\varphi \quad (22)$$

Planar optical setup, when detectors and incident electrical field vectors are in yz-plane and $\varphi = \pi/2$ simplifies equations and we have only part with $\mathbf{E}_{s\theta}$.

Obviously, in non-planar systems, both terms (21) and (22) must be taken into account. Scattered intensity can be calculated with the help of Poynting's vector; and for nonmagnetic and homogeneous medium (with magnetic permeability μ):

$$I_s = \frac{1}{2\omega\mu} E_s E_s^* \quad (23)$$

3. RESULTS

General angle and vector relations in 3BPDA system are presented in figure 1. Simulations were carried out for planar system for $\varphi = \pi/2$. Therefore unit vector $\mathbf{n}_s$ lies in yz-plane. The particle is placed in the center of the L coordinate system $(x_0 = y_0 = z_0 = 0)$ and for the case of a plane wave ($w_0 \to \infty$).
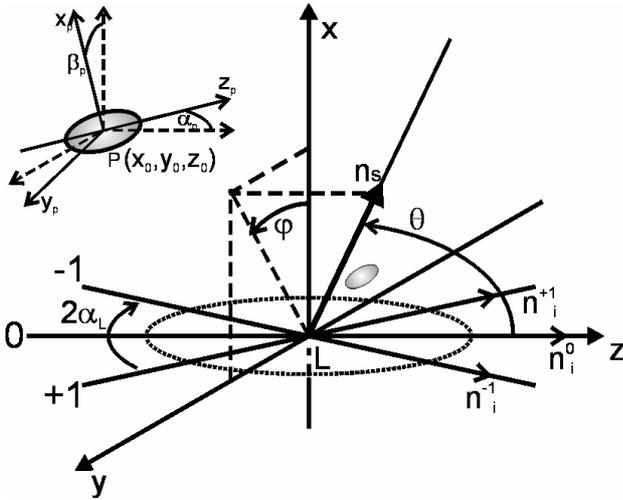

Fig. 1. Geometry of the scattering model and coordinate systems local P and global L. Ellipse shows scattering plane. Values +1, 0 ,-1 denote order of the laser beam. Vector (x₀,y₀,z₀) shows origin of the particle with respect to L reference frame. n^{-1}_i, n^0_i, n^{+1}_i are unit vectors of the propagating beams.

The system consists three beams with equal intensities for simplicity of computations. Angle between beams +1 and –1 equals $2\alpha_L$. Angles α_P, β_P are Euler's angles of rotated particle with reference to L coordinate system. The symmetry axis of the particle is aligned with P coordinate system. Computational procedures use modified routines developed by Mishchenko [10, 11]. In preliminary simulations we consider case when plane wave illuminates the particle located in the origin of L reference frame. However rotating diffraction grating introduces frequency shift between beams of +/- 1 orders (0 order beam is not frequency shifted) this property of the system for current simulations is neglected. Future analysis will take this into account. Let us also introduce an eccentricity factor $\varepsilon = a/b$ where a – is semi-axis of the particle included in $x_p y_p$ – plane and b is semi-axis aligned with z_p axis of the particle reference frame. Angle between beams $\alpha_L = 2°$. Refractive index is equal 1,33 + i0,00; particle diameter 2 μm, λ = 632,8nm. Simulations were carried out for different values of eccentricity and Euler's angles: α_P, β_P.
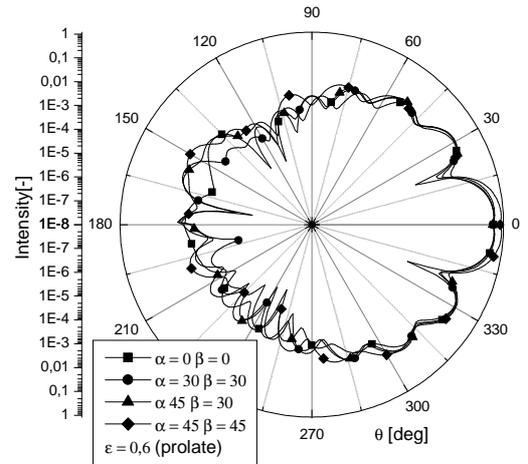
a)
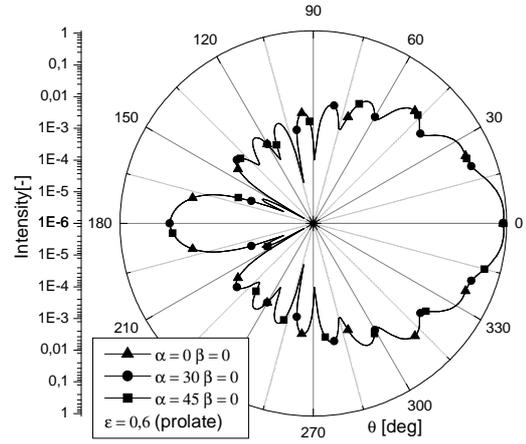
b)

Fig. 2. Normalized intensity in yz-plane vs. scattering angle θ; prolate particles with eccentricity factor $\varepsilon = 0,6$. Diagrams developed for different Euler's angles: a) – particle is changing orientation only for angle α; b) – particle is positioned in the center of L reference frame for several Euler's angles.

For preliminary results the normalized intensity in the scattering plane vs. the scattering angle was observed.
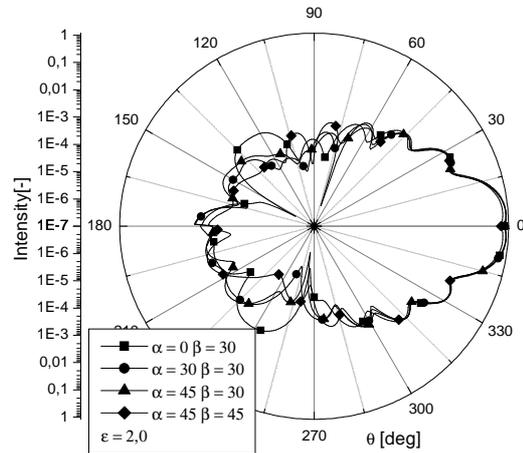
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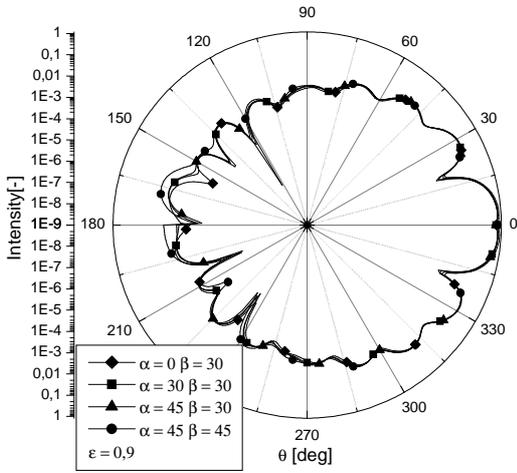
b)

Fig.3. Normalized intensity vs. scattering angle for different conditions: a) $\varepsilon = 0{,}9$ (slightly prolate particle); b) $\varepsilon = 2{,}0$ (oblate particle).

This dependence is shown in figure 2. In case of the particle only rotated by angle α ($\beta = 0$) for constant eccentricity there is no difference in scattering characteristics. The influence of rotation of the particle on intensity diagrams appears when both of the Euler's angles have non-zero values which is presented in figure 2b. Even for eccentricity ($\varepsilon = 0{,}9$ $a = 0{,}9\mu m$ and semi-axis $b = 1\mu m$) such level of shape deviation of the particle increases disturbances when position of the detector changes to greater ($\theta > 130°$) scattering angles. Relative differences in intensity level for $\varepsilon > 0{,}9$ ($\varepsilon \to 1$) shows that error due to non-sphericity may be neglected for three beam systems for carefully positioned detectors. If eccentricity factor strongly differs from 1 the range of allowable scattering angle decreases significantly to ~20° (figure 4a). On the other hand position of the detector should avoid situation of direct illumination by incident beam (angles around α_L) when a receiving unit sensitivity and sufficient dynamics must be preserved. On figure 2b, 3a, 3b rising influence of rotation

effect can be observed. For different levels of ε factor strong disturbances in characteristics can be also noticed. For greater β angles first peak of considered characteristics moves and reach maximum for $4 - 5°$. For scattering angle ranges from 0 to 40° an undesirable effect can have moderate importance on the detector placement. For greater values of scattering angle there is a strong influence of orientation of the scatterer on intensity characteristics.

Tu sum up: the effect of non-sphericity (for arbitrary and randomly positioned particles) may be significant for real systems and in many cases if geometry of the system is constrained by environmental conditions (hard accessible) or by structure of an anemometer itself (compact form in backscattering regime). For full analysis - simulations of a phase Doppler signal must be done as well. In our computations only static situation (when the particle is localized in the center of L coordinate system) is considered. Our future considerations will focus on effect of Gaussian intensity profiles of an illuminating laser beam as well as on dynamic behavior of the system.
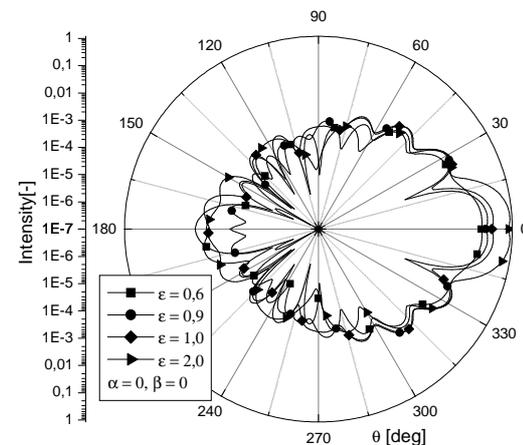
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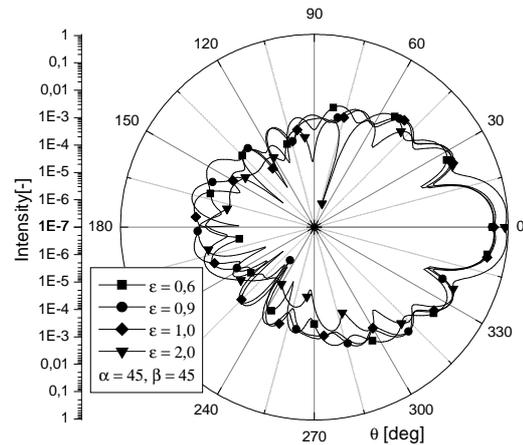
b)

Fig.4. a) – diagram for constant Euler's angles for different level of eccentricity; b) – different levels of eccentricity but for aligned with z-axis of L reference frame and centered particle.
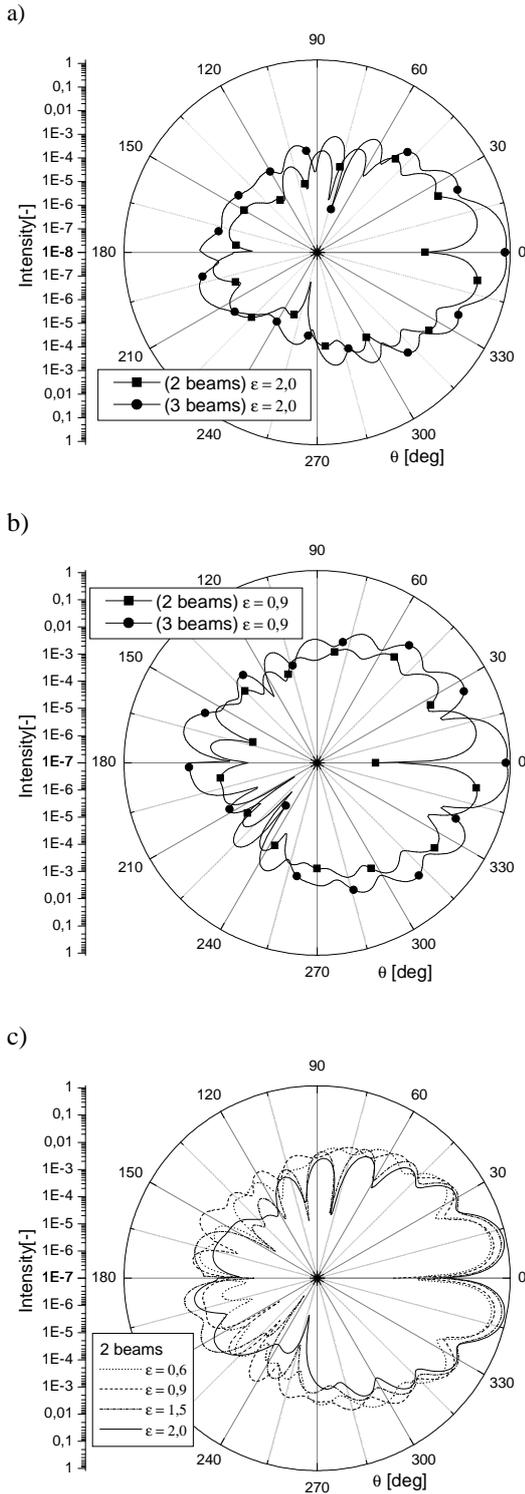
a)

b)

c)

Fig.5. Comparison of the scattering characteristics of three and two beams system for the particle located in center of L reference frame for different eccentricities; Euler's angles Euler's angles $\alpha = 45°$, $\beta = 45°$.

Figure 5 shows comparison of scattering characteristics of normalized intensity vs. scattering angle. Note that, when third beam of 0 order is present in interference pattern appears additional maximum nearby $\theta = 0°$ (figures 5a, b) – due to superposition of incident amplitudes.

4. CONCLUSION

Computational complexity brings out that simulation process is constrained to particles with medium size parameter. In our case a particle with refractive index 1,33 + i0,00 and 1μm radius was simulated. For particles with pure real refractive index oscillating characters of scattering functions can be noticed. It introduces instabilities in computational subroutines for greater size parameters and eccentricity level that ranges below 0,9 and above 1,1.

Analysis shows an influence of non-sphericity of the axially symmetric particles on scattering characteristics. The more spheroid eccentricity is induced the greater disturbances are observed. Our future work concentrates on properties of three beam system, when intensity profile of the beams is Gaussian and for the particle moving through a probe volume created from such beams. +1 and –1 order beams will be frequency shifted due to diffraction grating. If the level of eccentricity is relatively small ($\varepsilon \in \langle 0,9;1,1 \rangle$) departures from typical of spheres scattering characteristics can be neglected.

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REFERENCES

[1] Onofri F., Girasole T., Gréhan G., Gouesbet G., Brenn G., Domnick J., Tropea C., Xu T-H., Phase-Doppler Anemometry with Dual Burst Technique for Measurement of Refractive Index and Absorption Coefficient Simultaneous with Size and Velocity, *Part. and Part. Syst. Charact.*, V. 13, 212-224, 1996.

[2] Onofri F., Bergounoux L., Firpo J-L., Mesguish-Ripault J., Velocity, size and concentration measurements of optically inhomogeneous cylindrical and spherical particles*, Applied Optics,* V. 38, N. 21, 4681-4690*,* 1999.

[3] F. Onofri, S. Radev "3-Coherent Beams Phase Doppler and Laser Doppler Velocimetry Measurements Techniques", Application of Laser Techniques to Fluid Mechanics, 12th Int. Symposium 2004, Lisbon.

[4] D. S. Dandy, Theoretical studies of droplets deformation in finite Reynolds numbers flows, SPIE 1862, 1993, 237-248.

[5] L. Tsang, J. Kong, R. T. Shin, Theory of Microwave Remote Sensing, John Wiley and Sons, New York, 1985.

[6] P. C. Waterman, "Symmetry, unitarity, and geometry in electromagnetic scattering", Phys. Rev. D, 3, 825-839, 1971.

[7] Mishchenko M. I., Travis L. D., Lacis A. A., Scattering, Absorption, and Emission of Light by Small Particles, Cambridge University Press, 2002.

[8] Doicu A, Wriedt T., Bauckhage K.,"Light Scattering by Homogenous Axisymmetric Particles for PDA

Calculations to Measure Both Axes of Spheroidal Particles", Part Part. Syst. Charact. 14, 3 – 11, 1997.

[9] Doicu A., Koser J., Wriedt T., Bauckhage K., "Light Scattering Simulation and Measurement of Monodisperse Spheroids using a Phase Doppler Anemometer", Part Part. Syst. Charact. 15, 257 – 262, 1998.

[10] M. I. Mishchenko "Calculation of the amplitude matrix for a nonspherical particle in a fixed orientation", Applied Optics Vol. 39, No. 6, February 2000.

[11] M. I. Mishchenko, L.D. Travis "Capabilities and Limitations of a Current Fortran Implementation of the T-Matrix Method for Randomly oriented, Rotationally Symmetric Scaterrers", J. Quant. Spectrosc. Radiat. Transfer, Vol. 60, No. 3, pp. 309-324, 1998.