

Longitudinal and transverse photophoretic force on a homogeneous sphere exerted by a zero-order Bessel beam with selective polarizations

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Abstract: The prediction of photophoretic force exerted on an optical absorptive particle in a gaseous medium is a challenging problem, since the problems of electromagnetic scattering, heat transfer, and gaseous molecule dynamics are involved and coupled with each other. Based on the calculation of source function distribution inside a homogeneous sphere excited by a zero-order Bessel beam with the aid of generalized Lorenz-Mie theory (GLMT), analytical expressions of asymmetry vector, which is a crucial quantity in the calculation of photophoretic force, are given using the adjoint boundary value method. Numerical simulations are performed to analyze the influences of polarization and half-cone angle of the incident beam, particle size, and absorptivity of the particle on the asymmetry vector for both on-axis and off-axis illumination. Longitudinal and transverse photophoretic forces on a homogeneous sphere are displayed for slip-flow regime of gaseous media. The results give us insights into the working mechanism underpinning the development of novel heat-mediated optical manipulation techniques, measurement of the refractive index of particles, and others.

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1. Introduction

The rapid progress in the precise manipulation of small particles have produced significant advances in various fields, including biomedicine, physical chemistry, nanotechnology, etc. Among the various approaches used in particle trapping and manipulation, increased attention has been given to the optical methods due to their intrinsic advantages, including high resolution in space, non-intrusive and high precision in sensing [1]. The conventional optical tweezers, proposed by Ashkin in 1970, have been widely applied in various fields that he was awarded the Nobel Prize in Physics in 2018 [2]. Conventional optical tweezers based on the gradient (non-thermal) forces to trap and manipulate small particles using a tightly focused laser beam have certain limitations. For instance, the gradient force is around ~pN level, various perturbations from the ambient surroundings influence the trapping efficiency significantly that this technique is commonly used in liquid media where various perturbations can be diminished. Furthermore, the distance between the high-aperture object lens and the trapped particle is quite limited, making difficult the simultaneous implementation of other collaborative measuring techniques. Compared to the conventional optical tweezers, the new emerging heat-mediated optical manipulation technique based on photophoretic force demonstrates flexible control of lossy particles of various shapes, sizes, and compositions in gaseous media. The simple optical configurations and long manipulation range of photophoresis-based optical manipulation in experiments enable great potential applications to characterize physical and chemical properties

of aerosol particles [3, 4], in combination with other techniques, such as light scattering, Raman spectroscopy, and in realizing three-dimensional images in space known as optical trap displays [5].

Compared to the recent breakthroughs in the experimental line, theoretical analysis of photophoretic forces exerted by a structured laser beam on an absorbing particle is quite challenging and less developed, in particular because it is an interdisciplinary coupled problem involving electromagnetic scattering, thermal dynamics, and gaseous molecule dynamics, and also because most of the previous investigations were motivated by the applications in atmospheric science and astrophysics [6], where a plane wave illumination is always assumed. When an optical absorptive particle is illuminated, a temperature gradient appears on the surface of the particle originating from the non-uniform absorption of radiant energy within the particle. Then, uneven momentum transfer between the particle and the gas molecules on the particle surface results in the photophoretic force, which depends on the properties of particles (shape, size, material), the parameters of gas media (pressure, composition), and the illumination conditions. In the case of a homogeneous sphere illuminated by a plane wave, axial symmetric distributions of the internal field and the heat source function are obtained so that the photophoretic force arising from this kind of longitudinal unbalanced heat absorption in a non-volatile homogeneous lossy sphere is a longitudinal force along the propagation direction of the light. It can be attractive or repulsive, pulling the particle toward or pushing the particle away from the light source, depending on an asymmetry factor J_1 which imbeds all the information of the uneven absorption of radiation and reflects the heat source distribution in the particle [7, 8]. As far as the axial symmetry of the electromagnetic scattering is preserved, the photophoretic force has only a longitudinal component, for instance, in the case when an axisymmetric particle is illuminated by an axisymmetric beam under on-axis configuration [9-11].

However, the asymmetric factor is extended to a vectorial quantity once axial symmetry in the electromagnetic scattering is lost, which is a more practical case since the particle is in a dynamic motion and not always in the center of the beam. Then a transversal component of the photophoretic force occurs. By developing a method to predict the photophoretic force for non-spherical particles, the asymmetry factor J_1 was extended to a asymmetry vector $\mathbf{J}$ by Rohatschek and Zulehner [12], and the photophoretic force was expressed in terms of the asymmetry vector. Some attempts can be found to consider the influence of field profiles of the incident laser beam on the photophoretic force, but approximated methods or numerical methods were used, which lack efficiency, and a full analysis was not covered [13, 14]. The underlying mechanisms of photophoretic force exerted by a structured laser beam, which plays a significant role in the guide of further developments, are not fully understood.

In recent two years, the photophoresis of cylindrical particles, including a dielectric cylinder [15], a magneto-dielectric cylinder [16], a cylinder near a planar boundary and corners [17, 18], and two parallel cylinders [19], were analyzed by Mitri, where the influences of light sheets with different polarizations and incidence directions were considered. Based on the analysis performed by Mackowski [7] on the photophoretic force of a homogeneous sphere illuminated by a plane wave, Ambrosio [20] extended the investigation to the cases of axisymmetric beams of the first kind of on-axis illumination using the generalized Lorenz-Mie theory, where fundamental Gaussian beam and zero-order Bessel beam were considered as examples. A study of high-order Bessel beams in the on-axis case was then performed to analyze the characteristics of photophoretic force exerted by a hollow beam [21]. Very recently, the calculation of asymmetry vector $\mathbf{J}$ of a sphere was extended to the cases of arbitrarily shaped laser beams with arbitrary illumination [22] with the aid of the generalized Lorenz-Mie theory (GLMT), which forms a solid foundation for predicting photophoretic force on a regular-shaped particle in the case of a structured laser beam. In this paper, this method is applied to the case of Bessel

beams illumination with different polarizations. This work is motivated by the results that the trapping efficiency was confirmed to be sensitive in a photophoretic trap where a radially or azimuthally polarized laser beam was used in the experiments [23], which provides additional flexibility to the optical micromanipulation of light-absorbing particles in gaseous media. However, as far as we know, no rigorous quantitative theoretical analysis is available to interpret the influence of polarization on the photophoretic force exerted on an absorbing sphere illuminated by a structured laser field. Thus, Bessel beams of selective polarizations are implemented for both on-axis and off-axis illumination to analyze the influence of polarization and location on the photophoretic force, which casts insights into the physical mechanism of dynamic behavior of a particle trapped in a Bessel beam.

The rest of this paper is organized as follows. In Section 2, brief description of the theoretical prediction of photophoretic forces of a sphere illuminated by a Bessel beam is presented, where numerical-ready mathematical expressions are provided. Detailed simulation results are displayed in Section 3 for the behaviors of asymmetry vector and photophoretic force in different conditions. The influences of particle size, imaginary part of refractive index, half-cone angle, and particle location on the photophoretic force are explored. Section 4 is a conclusion.

2. Photophoretic force and asymmetry vector

For a homogeneous non-volatile sphere in the gaseous medium illuminated by a plane wave, analytical solutions can be obtained [7] in different conditions depending on the Knudsen number $Kn = l/a$, where l and a are the mean free path of the gas molecules and the particle size, respectively. On the one hand, in the slip-flow or continuous regime, where the size of the particle is much larger than the mean free path of the gas molecules leading to $Kn < 1$ or $Kn \ll 1$, the photophoretic force is mainly due to the thermal creep around the particle. By applying the boundary conditions, the photophoretic force for a non-volatile sphere in the slip-flow regime is given by Mackowski [7]:

$$F_p = -\frac{4\pi c_s \eta_g^2 I_\lambda a}{\rho_g k_s T_0} \frac{1}{(1 + 3c_m l/a)(1 + 2c_l l/a + 2k_g/k_s)} J_1. \quad (1)$$

where c_s , c_m and c_l are the momentum exchange coefficient, the thermal slip coefficient and the jump coefficient, respectively. T_0 is the temperature at infinity, which is assumed to be the ambient gas temperature. ρ_g and η_g are the density and viscosity of the surrounding gaseous medium, respectively. I_λ is the intensity of the incident wave. k_g and k_s are the thermal conductivity of the gas and that of the particle, respectively. For the special case $Kn \ll 1$, Eq. (1) can be approximated by:

$$F_p = -\frac{4\pi c_s \eta_g^2 I_\lambda a}{\rho_g T_0} \frac{1}{(k_s + 2k_g)} J_1. \quad (2)$$

which is the same as that given by Yalamov [9]. For a strong absorbing particle where radiation is absorbed entirely on the illuminated surface, the asymmetry factor $J_1 = -0.5$, and Eq. (1) reduced to that given by Reed [24].

On the other hand, if the size of the particle is much smaller than the mean free path of the gas molecules, we have $Kn \gg 1$. Then the kinetic theory of gases is applied to give an analytical solution to the photophoretic force for a non-volatile sphere [7]:

$$F_p = -\frac{\pi^2 \alpha \eta_g^2 I_\lambda a}{6\rho_g k_s T_0} \frac{(a/l)^2}{1 + H_m} J_1. \quad (3)$$

137 where

$$138 \quad H_m = \frac{4\alpha}{15} \frac{k_g}{k_s} \frac{a}{l}. \quad (4)$$

139 where α is the thermal accommodation coefficient defined as the ratio of the net molecular
140 kinetic energy transfer to the particle to that obtained if all reflected molecules were
141 characterized by a Maxwellian distribution evaluated at the actual local surface temperature.
142 Considering the definition [7]:

$$143 \quad l = 2\eta_g \left(\frac{\pi M}{8RT_0} \right)^{1/2} \frac{1}{\rho_g}, \quad k_s = \frac{15}{4} \eta_g \frac{R}{M} \quad (5)$$

144 where R is the gas constant, M is the mole mass of the gas. Eq. (3) can be written as:

$$145 \quad F_p = -\frac{\pi a^3 \alpha p I_\lambda}{3(ha + k_s)T_0} J_1. \quad (6)$$

146 where h is the molecular heat transfer coefficient. Eq.(6) is the same as those given by Zulehner
147 and Rohatschek [12]. For radiation absorbed entirely on the particle surface, where $J_1 = -0.5$,
148 then Eq. (6) is the same as that given by Hidy and Brock [25] with $h = \alpha p \bar{v} / (2T_0)$.

149 As shown in Eqs. (1)-(6), in both the slip-flow and the free molecule regimes, the photophoretic
150 forces have the same dependency upon the radiative absorption, which is embodied in the
151 photophoretic asymmetry factor J_1 . The J_1 incorporates the information on the heat distribution
152 which can be found from the heat source function predicted using the classical Lorenz-Mie
153 theory:

$$154 \quad J_1 = \frac{3nkx}{2\pi} \int_0^1 t^3 dt \int_0^{2\pi} d\varphi \int_{-1}^1 B(t, \mu) \mu d\mu. \quad (7)$$

155 where $x = 2\pi a / \lambda$ and $m_p = n + i\kappa$ are the size parameter and the relative refractive index of
156 the particle, respectively, with λ being the wavelength of the incident laser beam. In addition,
157 $B = (\mathbf{E} \cdot \mathbf{E}^*) / E_0^2$ is known as the normalized source function [26], $\mathbf{E}$ is the electric component
158 of the internal field inside the particle and E_0 its corresponding field strength. The $t = r / a$ is
159 a dimensionless variable, and $\mu = \cos\theta$.

160 In the case of a homogeneous sphere illuminated by a plane wave, axial symmetric
161 distributions of the internal field and the heat source function are obtained, and the asymmetry
162 factor J_1 is a scalar quantity. The photophoretic force arising from this kind of longitudinal
163 unbalanced heat absorption in a non-volatile homogeneous lossy sphere is a longitudinal force
164 along the propagation direction of the light. However, the scalar asymmetric factor J_1 is
165 extended to a vector $\mathbf{J}$ once the axial symmetry in the electromagnetic scattering is no more
166 preserved, and a transverse component of the photophoretic force occurs [16-18, 22].

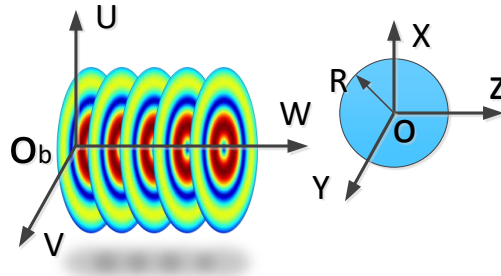


Fig. 1. Illustration of a homogeneous sphere illuminated by an off-axis Bessel beam

In the case of a homogeneous sphere illuminated by an off-axis Bessel beam, as illustrated in Fig. 1, the photophoretic force can be expressed in terms of the asymmetric vector as:

$$\mathbf{F}_{\text{ph}} = -C_{Kn} \mathbf{J}. \quad (8)$$

where C_{Kn} is a constant value depends on the ambient atmosphere condition and parameters of the particle, and $\mathbf{J}$ is the asymmetric vector:

$$\mathbf{J} = J_x \hat{x} + J_y \hat{y} + J_z \hat{z}. \quad (9)$$

where [22]

$$J_{\begin{Bmatrix} x \\ y \end{Bmatrix}} = \frac{6nk}{|M|^2 x^3} \left\{ \frac{\text{Im}}{\text{Re}} \sum_{n=1}^{\infty} [A_n^m (S_n^* + \frac{n+1}{M} R_{n+1}) + B_n^m (-S_n + \frac{n+1}{M} R_n) + iC_n^m S_n] \right\}. \quad (10)$$

$$J_z = -\frac{12nk}{|M|^2 x^3} \text{Im} \sum_{n=1}^{\infty} \sum_{m=-n}^n [D_n^m (S_n^* + \frac{n+1}{M} R_{n+1}) + E_n^m (-S_n + \frac{n+1}{M} R_n) + iF_n^m S_n]. \quad (11)$$

$$A_n^m = \frac{1}{(n+1)^2} \left\{ \sum_{m=0}^{n-1} d_n^* d_{n+1}^{m,*} g_{n+1,TE}^{m,*} g_{n,TM}^{m+1} \frac{(n+|m|+1)!}{(n-|m|-1)!} + \sum_{m=0}^n d_n^* d_{n+1}^{m,*} g_{n,TM}^{m,*} g_{n+1,TE}^{m+1} \frac{(n+|m|+2)!}{(n-|m|)!} \right. \\ \left. - \sum_{m=-n}^{-1} d_n^* d_{n+1}^{m,*} g_{n+1,TE}^{m,*} g_{n,TM}^{m+1} \frac{(n+|m|+1)!}{(n-|m|+1)!} - \sum_{m=-n}^{-1} d_n^* d_{n+1}^{m,*} g_{n,TM}^{m,*} g_{n+1,TE}^{m+1} \frac{(n+|m|)!}{(n-|m|)!} \right\} \quad (12)$$

$$B_n^m = \frac{1}{(n+1)^2} \left\{ \sum_{m=0}^{n-1} c_n^* c_{n+1}^{m,*} g_{n+1,TE}^{m,*} g_{n,TE}^{m+1} \frac{(n+|m|+1)!}{(n-|m|-1)!} + \sum_{m=0}^n c_n^* c_{n+1}^{m,*} g_{n,TE}^{m,*} g_{n+1,TE}^{m+1} \frac{(n+|m|+2)!}{(n-|m|)!} \right. \\ \left. - \sum_{m=-n}^{-1} c_n^* c_{n+1}^{m,*} g_{n+1,TE}^{m,*} g_{n,TE}^{m+1} \frac{(n+|m|+1)!}{(n-|m|+1)!} - \sum_{m=-n}^{-1} c_n^* c_{n+1}^{m,*} g_{n,TE}^{m,*} g_{n+1,TE}^{m+1} \frac{(n+|m|)!}{(n-|m|)!} \right\} \quad (13)$$

$$C_n^m = \frac{2n+1}{[n(n+1)]^2} d_n^* c_n^* \times \left\{ \sum_{m=0}^n (g_{n,TM}^{m+1} g_{n,TE}^{m,*} \pm g_{n,TM}^m g_{n,TE}^{m+1,*}) \frac{(n+|m|+1)!}{(n-|m|-1)!} \right. \\ \left. - \sum_{m=-n}^{-1} (g_{n,TM}^{m+1} g_{n,TE}^{m,*} \pm g_{n,TM}^m g_{n,TE}^{m+1,*}) \frac{(n+|m|)!}{(n-|m|)!} \right\} \quad (14)$$

$$D_n^m = \frac{1}{(n+1)^2} d_n^* d_{n+1}^{m,*} g_{n,TM}^{m,*} g_{n+1,TE}^m \frac{(n+|m|+1)!}{(n-|m|)!} \quad (15)$$

$$E_n^m = \frac{1}{(n+1)^2} c_n^* c_{n+1}^{m,*} g_{n,TE}^{m,*} g_{n+1,TE}^m \frac{(n+|m|+1)!}{(n-|m|)!} \quad (16)$$

$$F_n^m = m \frac{2n+1}{[n(n+1)]^2} c_n^* d_n^{m,*} g_{n,TE}^{m,*} g_{n,TM}^m \frac{(n+|m|)!}{(n-|m|)!} \quad (17)$$

where $g_{n,TE}^m$ and $g_{n,TM}^m$ are the beam shape coefficients (BSCs) of the GLMT which encode the structure of the illuminating laser beam. Please note that Eqs. (10)-(17) here are slightly different from those given in Ref. [22] since the conventional form of the scattering coefficients c_n, d_n in the classical Lorenz-Mie theory [27-29] for non-magnetic spheres were used here:

$$c_n = \frac{M [\psi_n(x) \xi_n'(x) - \xi_n(x) \psi_n'(x)]}{\psi_n(m_p x) \xi_n'(x) - M \xi_n(x) \psi_n'(m_p x)} \\ d_n = \frac{M [\psi_n(x) \xi_n'(x) - \xi_n(x) \psi_n'(x)]}{M \psi_n(m_p x) \xi_n'(x) - \xi_n(x) \psi_n'(m_p x)}. \quad (18)$$

While the scattering coefficients c_n, d_n in Ref. [22] are valid for arbitrary refractive index.

190 Furthermore,

$$191 \quad R_n = \frac{\text{Im}[m_p \psi_{n+1}(m_p x) \cdot \psi_n^*(m_p x)]}{\text{Im}(m_p^2)}$$

$$S_n = -\frac{i}{2\text{Im}(m_p^2)} \left[x(m_p |\psi_n(m_p x)|^2 + m_p^* |\psi_{n+1}(m_p x)|^2) - \left(m_p + 2(n+1) \frac{\text{Re}(m_p^2)}{m_p} \right) R_n + (2n+1) m_p^* R_{n+1} \right] \quad (19)$$

192

193 To simplify the numerical implementation, the followings are introduced [7]:

$$194 \quad R_n \equiv \frac{R_n}{|\psi(m_p x)|^2} = \frac{\text{Im}(m_p C_n)}{\text{Im}(m_p^2)} \quad (20)$$

$$195 \quad S_n = \frac{S_n}{|\psi(m_p x)|^2} = \frac{-i}{2\text{Im}(m_p^2)} \left\{ x(m_p + m_p^* |C_n|^2) - \left[m_p + 2(n+1) \frac{\text{Re}(m_p^2)}{m_p} \right] R_n + (2n+1) m_p^* |C_n|^2 R_{n+1} \right\} \quad (21)$$

196 where

$$197 \quad C_n = \frac{\psi_{n+1}(m_p x)}{\psi_n(m_p x)} = \frac{n+1}{m_p x} - D_n \quad (22)$$

$$198 \quad c_n = \psi_n(m_p x) c_n; d_n = \psi_n(m_p x) d_n \quad (23)$$

199 Thus, we have:

$$200 \quad J_z = -\frac{12nk}{|m_p|^2 x^3} \text{Im} \sum_{n=1}^{\infty} \sum_{m=-n}^n [D_n^m (\frac{S_n^*}{C_n} + \frac{n+1}{m_p} R_{n+1} C_n^*) + E_n^m (-\frac{S_n}{C_n} + \frac{n+1}{m_p} \frac{R_n}{C_n}) + i F_n^m S_n] \quad (24)$$

$$201 \quad J_{\{y\}} = \frac{6nk}{|m_p|^2 x^3} \left\{ \text{Im} \sum_{n=1}^{\infty} \sum_{m=-n}^n [A_{n,1}^m (\frac{S_n^*}{C_n} + \frac{n+1}{m_p} R_{n+1} C_n^*) + B_{n,1}^m (-\frac{S_n}{C_n} + \frac{n+1}{m_p} \frac{R_n}{C_n}) + A_{n,2}^m (\frac{S_n^*}{C_n} + \frac{n+1}{m_p} R_{n+1} C_n) + B_{n,2}^m (-\frac{S_n}{C_n} + \frac{n+1}{m_p} \frac{R_n}{C_n}) + i C_n^m S_n] \right\} \quad (25)$$

$$202 \quad A_{n,1}^m = \frac{1}{(n+1)^2} d_n^* d_{n+1} \left\{ \sum_{m=0}^n g_{n,TM}^{m,*} g_{n+1,TM}^{m+1} \frac{(n+|m|+2)!}{(n-|m|)!} - \sum_{m=-n}^{-1} g_{n,TM}^{m,*} g_{n+1,TM}^{m+1} \frac{(n+|m|)!}{(n-|m|)!} \right\} \quad (26)$$

$$A_{n,2}^m = \frac{1}{(n+1)^2} d_n d_{n+1}^* \left\{ \sum_{m=0}^{n-1} g_{n+1,TM}^{m,*} g_{n,TM}^{m+1} \frac{(n+|m|+1)!}{(n-|m|-1)!} - \sum_{m=-n-1}^{-1} g_{n+1,TM}^{m,*} g_{n,TM}^{m+1} \frac{(n+|m|+1)!}{(n-|m|+1)!} \right\}$$

$$203 \quad B_{n,1}^m = \frac{1}{(n+1)^2} c_n^* c_{n+1} \left\{ \sum_{m=0}^n g_{n,TE}^{m,*} g_{n+1,TE}^{m+1} \frac{(n+|m|+2)!}{(n-|m|)!} - \sum_{m=-n}^{-1} g_{n,TE}^{m,*} g_{n+1,TE}^{m+1} \frac{(n+|m|)!}{(n-|m|)!} \right\} \quad (27)$$

$$B_{n,2}^m = \frac{1}{(n+1)^2} c_n c_{n+1}^* \left\{ \sum_{m=0}^{n-1} g_{n+1,TE}^{m,*} g_{n,TE}^{m+1} \frac{(n+|m|+1)!}{(n-|m|-1)!} - \sum_{m=-n-1}^{-1} g_{n+1,TE}^{m,*} g_{n,TE}^{m+1} \frac{(n+|m|+1)!}{(n-|m|+1)!} \right\}$$

$$C_n^m = \frac{2n+1}{[n(n+1)]^2} d_n^* c_n^* \times \left\{ \sum_{m=0}^n (g_{n,TM}^{m+1} g_{n,TE}^{m,*} \pm g_{n,TM}^m g_{n,TE}^{m+1,*}) \frac{(n+|m|+1)!}{(n-|m|-1)!} \right. \\ \left. - \sum_{m=-n}^{-1} (g_{n,TM}^{m+1} g_{n,TE}^{m,*} \pm g_{n,TM}^m g_{n,TE}^{m+1,*}) \frac{(n+|m|)!}{(n-|m|)!} \right\} \quad (28)$$

$$D_n^m = \frac{1}{(n+1)^2} d_n^* d_{n+1} g_{n,TM}^{m,*} g_{n+1,TM}^m \frac{(n+|m|+1)!}{(n-|m|)!} \quad (29)$$

$$E_n^m = \frac{1}{(n+1)^2} c_n^* c_{n+1} g_{n,TE}^{m,*} g_{n+1,TE}^m \frac{(n+|m|+1)!}{(n-|m|)!} \quad (30)$$

$$F_n^m = m \frac{2n+1}{[n(n+1)]^2} c_n^* d_n g_{n,TE}^{m,*} g_{n,TM}^m \frac{(n+|m|)!}{(n-|m|)!} \quad (31)$$

Eqs. (24)-(31) can be implemented numerically, once the BSCs of the incident structured beam are known.

Detailed descriptions of vector circularly symmetric Bessel beams can be found in [30-32]. A rigorous and efficient approach was given in Ref. [33] for the calculation of BSCs of a circularly symmetric Bessel beam, which can be implemented using an angular spectrum decomposition (ASD) [34, 35] or any other more conventional methods in the framework of GLMT. Analytical expressions of BSCs for x-polarized circularly symmetric Bessel beam can be obtained from Ref. [33]:

$$g_{n,TM}^m = -g(\alpha_0)(-1)^{\frac{m-|m|}{2}} \frac{(n-m)!}{(n+|m|)!} e^{-ik_z z_0} \left\{ i^{l-m+1} e^{i(l-m+1)\phi_0} J_{l-m+1}(\sigma_0) [\tau_n^m(\cos \alpha_0) + m\pi_n^m(\cos \alpha_0)] \right. \\ \left. + i^{l-m-1} e^{i(l-m-1)\phi_0} J_{l-m-1}(\sigma_0) [\tau_n^m(\cos \alpha_0) - m\pi_n^m(\cos \alpha_0)] \right\} \quad (32)$$

$$g_{n,TE}^m = ig(\alpha_0)(-1)^{\frac{m-|m|}{2}} \frac{(n-m)!}{(n+|m|)!} e^{-ik_z z_0} \left\{ i^{l-m+1} e^{i(l-m+1)\phi_0} J_{l-m+1}(\sigma_0) [\tau_n^m(\cos \alpha_0) + m\pi_n^m(\cos \alpha_0)] \right. \\ \left. - i^{l-m-1} e^{i(l-m-1)\phi_0} J_{l-m-1}(\sigma_0) [\tau_n^m(\cos \alpha_0) - m\pi_n^m(\cos \alpha_0)] \right\}$$

where the generalized Legendre functions have been introduced:

$$\pi_n^m(\cos \alpha_0) = \frac{P_n^m(\cos \alpha_0)}{\sin \alpha_0}, \quad \tau_n^m(\cos \alpha_0) = \frac{dP_n^m(\cos \alpha_0)}{d\alpha_0}. \quad (33)$$

and $\sigma_0 = k_t \rho_0$, $\rho_0 = [x_0^2 + y_0^2]^{1/2}$, $\phi_0 = \tan^{-1}(y_0 / x_0)$. The transverse and longitudinal wavenumbers are $k_t = k_0 \sin \alpha_0$ and $k_z = k_0 \cos \alpha_0$, respectively. The $J_l(\cdot)$ represents an l -order Bessel function of the first kind. The α_0 is the half-cone angle of the Bessel beam. The $g(\alpha_0)$ is a generalization factor.

For an on-axis x-polarized Bessel beam, where $\rho_0 = 0$ and $\phi_0 = 0$, all the BSCs are zero except $m = l \pm 1$, and the BSCs $g_{n,TM}^m$ and $g_{n,TE}^m$ satisfy the relationship [33]:

$$g_{n,TM}^{l-1} = -ig_{n,TE}^{l-1}, \quad g_{n,TM}^{l+1} = ig_{n,TE}^{l+1}. \quad (34)$$

Then we have $A_n^m = B_n^m = C_n^m = 0$, which results in $J_x = J_y = 0$. Inserting Eq. (34) into Eq. (11), we have

228

$$J_z = \frac{-12nk}{|M|^2 x^3} \text{Im} \sum_{n=1}^{\infty} \left\{ -\frac{1}{(n+1)^2} \left(c_n^* c_{n+1} S_n - d_n^* d_{n+1} S_n^* \right) \left(\frac{g_{n, TM}^{l+1,*} g_{n+1, TM}^{l+1}}{(n-|l+1|)!} + \frac{g_{n, TM}^{l-1,*} g_{n+1, TM}^{l-1}}{(n-|l-1|)!} \right) \right. \\ \left. - \frac{2n+1}{[n(n+1)]^2} c_n^* d_n S_n \left[(l+1) g_{n, TM}^{l+1,*} g_{n+1, TM}^{l+1} \frac{(n+|l+1|)!}{(n-|l+1|)!} - (l-1) g_{n, TM}^{l-1,*} g_{n+1, TM}^{l-1} \frac{(n+|l-1|)!}{(n-|l-1|)!} \right] \right\}. \quad (35)$$

229 which is the same as that given in Ref. [21]. Please note that a factor $1/2\pi$ is missing in Ref.
230 [21] due to a typo. Specifically, for a zeroth-order Bessel beam $l=0$, the BSCs satisfy:

$$231 \quad g_{n, TM}^1 = g_{n, TM}^{-1} = -ig_{n, TE}^{-1} = ig_{n, TE}^1 = \frac{g_n}{2}, \quad (36)$$

232 Eq. (35) then reduces to that given by Ambrosio in Ref. [10] considering that a time dependence
233 $\exp(i\omega t)$ was used there. Furthermore, if we set $\alpha=0^\circ$, the x -polarized Bessel beam reduces to
234 the case of a plane wave, where $g_n = 1.0$, then Eq. (35) reduces to that given by Mackowski
235 in Ref. [7] for a plane wave illumination.

236 Using the approach given in Ref. [33], the BSCs of a TM polarized circularly symmetric
237 Bessel beam with its beam center located at an arbitrary point (x_0, y_0, z_0) are:

$$238 \quad g_{n, TM}^{m, (TM \text{ mode})} = -g(\alpha) (-1)^{\frac{m-|m|}{2}} \frac{(n-m)!}{(n+|m|)!} e^{-ik_z z_0} J_{m-l}(k_\rho \rho_0) e^{i(l-m)\phi_0} i^{l-m} \tau_n^m(\cos \alpha) \quad (37)$$

$$239 \quad g_{n, TE}^{m, (TM \text{ mode})} = g(\alpha) (-1)^{\frac{m-|m|}{2}} \frac{(n-m)!}{(n+|m|)!} e^{-ik_z z_0} i^{l-m-1} J_{m-l}(k_\rho \rho_0) e^{i(l-m)\phi_0} m \tau_n^m(\cos \alpha) \quad (38)$$

240 where the superscript “TM mode” indicates the TM -polarization. Considering the relationship
241 between the electromagnetic field of TM -polarization and that of TE -polarization:

$$242 \quad \mathbf{E}^{TE \text{ mode}} / E_0 = \mathbf{B}^{TM \text{ mode}} / B_0, \quad \mathbf{B}^{TE \text{ mode}} / B_0 = -\mathbf{E}^{TM \text{ mode}} / E_0. \quad (39)$$

243 we have

$$244 \quad \begin{Bmatrix} g_{n, TM}^{m, (TE \text{ mode})} \\ g_{n, TE}^{m, (TE \text{ mode})} \end{Bmatrix} = \begin{Bmatrix} g_{n, TE}^{m, (TM \text{ mode})} \\ -g_{n, TM}^{m, (TM \text{ mode})} \end{Bmatrix} \quad (40)$$

245 where the superscript “TE mode” indicates the TE -polarization. For beam order $l=0$, the zero-
246 order Bessel beam in the TM mode and that in the TE mode is also known as radially polarized
247 and azimuthally polarized, respectively.

248 For an on-axis TM -polarization or TE -polarization Bessel beam, where $\rho_0 = 0$ and $\phi_0 = 0$,

249 all the BSCs are zero except $m=l$, we have:

$$250 \quad g_{n, TM}^{l, (TM \text{ mode})} = -g(\alpha) \frac{(n-l)!}{(n+|l|)!} e^{-ik_z z_0} \tau_n^l(\cos \alpha) \quad (41)$$

$$g_{n,TE}^{l,(TM \text{ mode})} = ig(\alpha) \frac{(n-l)!}{(n+|l|)!} e^{-ik_z z_0} l\pi_n^l(\cos \alpha) \quad (42)$$

Then we have $A_n^m = B_n^m = C_n^m = 0$, which results in $J_x = J_y = 0$. Inserting Eq. (41)-(42) into Eq. (11), the double summary reduces to a single summary of the series as:

$$J_z = -\frac{12nk}{|M|^2 x^3} \text{Im} \sum_{n=1}^{\infty} [D_n^l(S_n^* + \frac{n+1}{M} R_{n+1}) + E_n^l(-S_n + \frac{n+1}{M} R_n) + iF_n^l S_n] \quad (43)$$

3. Numerical results and discussions

Based on the theoretical derivations given in Section 2, a program was written in Fortran 90 to calculate each component of the asymmetry vector of a sphere illuminated by a circularly symmetric Bessel beam. To validate the correctness of our home-built code, the asymmetry factor J_z was calculated and displayed in Fig. 2(a) for a plane wave illumination. The curves in Fig. 2(a) are reproductions of those of Fig. 1, Fig. 2 in Ref. [7]. Perfect agreements between our results and those in Ref. [7] were achieved as expected since the plane wave illumination is a special case of Bessel beam illumination. Furthermore, ratio of photophoretic force to the weight of a glyceryl particle illuminated by a plane wave was calculated and displayed in Fig. 2(b). The parameters of the ambient atmospheric conditions and those of particles used in the simulations are listed in Table 1, which are the same as those given in the experiment implemented by Arnold and Lewitters [36]. Two kinds of complex refractive indices of the particle are considered, say $m_p = 1.57 + 0.0475i$ and $m_p = 1.57 + 0.38i$, which correspond to the wavelength of $\lambda = 10.63\mu\text{m}$ and $\lambda = 9.58\mu\text{m}$, respectively. As shown in Fig. 2(b), satisfactory agreements have been achieved between our results and those obtained by Mackowski [7], and the discrepancy is believed to results from certain differences in the thermal and hydrodynamic parameters used in the simulations. The agreements partially indicate the correctness of our theoretical derivations and our home-built code.

Table 1. Parameters of the ambient atmospheric conditions and those of particles used in the simulations

Particle density ρ_s	$1.2613 \times 10^3 \text{ kg / m}^3$	Temperature T_0	300K
Gas Viscosity η_g	$1.82 \times 10^{-5} \text{ Pa} \cdot \text{s}$	Light Intensity I_λ	$3.8 \times 10^3 \text{ W / m}^2$
Thermal conduction coefficient k_s	$0.28 \text{ W / (m} \cdot \text{K)}$	Pressure p	30Torr
Gas constant R	8.31	Mole mass of gas M	28.952 kg/mol

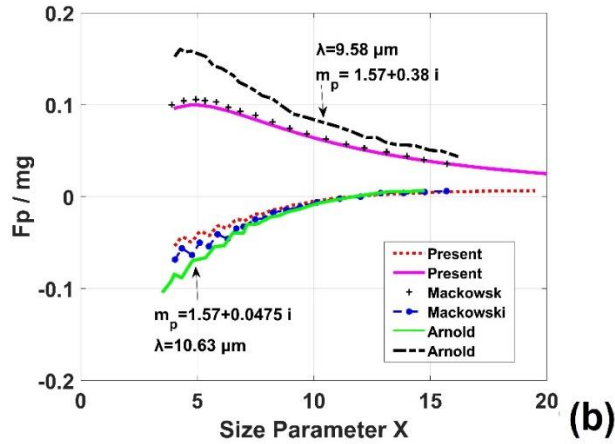
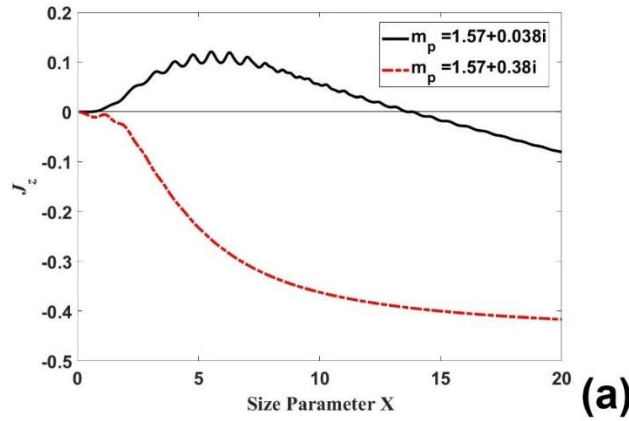


Fig. 2 .(a) photophoretic asymmetry factor J_z , which are reproductions of Fig. 1 and Fig. 2 in Ref. [7], and (b) ratio of photophoretic force to the weight of a glyceryl particle illuminated by a plane wave.

3.1 On-axis cases

For the on-axis case, only J_z is not zero, since we have $A_n^m = B_n^m = C_n^m = 0$, which results in $J_x = J_y = 0$. The J_z spectra (J_z versus the particle size parameter $x = 2\pi R / \lambda$) of a homogeneous sphere with different refractive indices illuminated by a zero-order Bessel beam of radial polarization and of azimuthal polarization are displayed in Fig. 3 and Fig. 4, respectively. Three different half-cone angles of Bessel beams are considered in the simulations to analyze the influence of half-cone angle on the J_z spectra.

As we can see from Fig. 3 and Fig. 4, the imaginary part of the refractive index plays a significant role in the behaviors of J_z spectra. For the cases under study, for particles with small absorptivity, for instance $\kappa = 0.01$ and $\kappa = 0.038$, we can observe positive J_z and thus negative photophoretic force for particles in a large range of size parameter. This range depends on the values of the half-cone angle and of the imaginary part of the refractive index. Generally speaking, the smaller the half-cone angle and the imaginary part of the refractive index, the

larger the size range for positive J_z . However, when the particle is highly absorbing, for instance $\kappa=0.38$ and $\kappa=1.0$, the size range for positive J_z is very limited and is not so sensitive to the change of the imaginary part of the refractive index or of the half-cone angle.

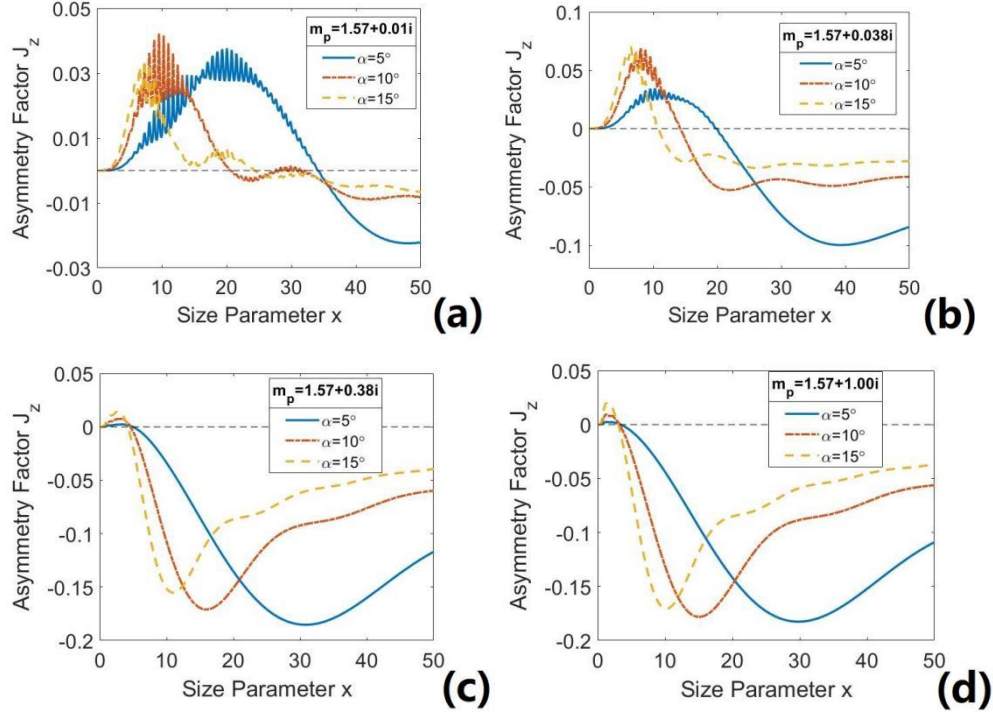


Fig. 3. J_z spectra for particles with different refractive indices in the case of a zero-order Bessel beam with different half-cone angles. (a) $m_p = 1.57 + 0.01i$; (b) $m_p = 1.57 + 0.038i$; (c) $m_p = 1.57 + 0.38i$; (d) $m_p = 1.57 + 1.0i$. The Bessel beam is radially polarized.

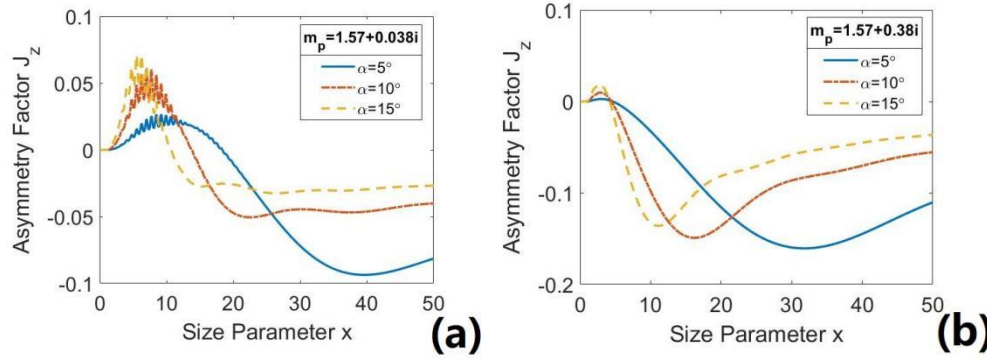
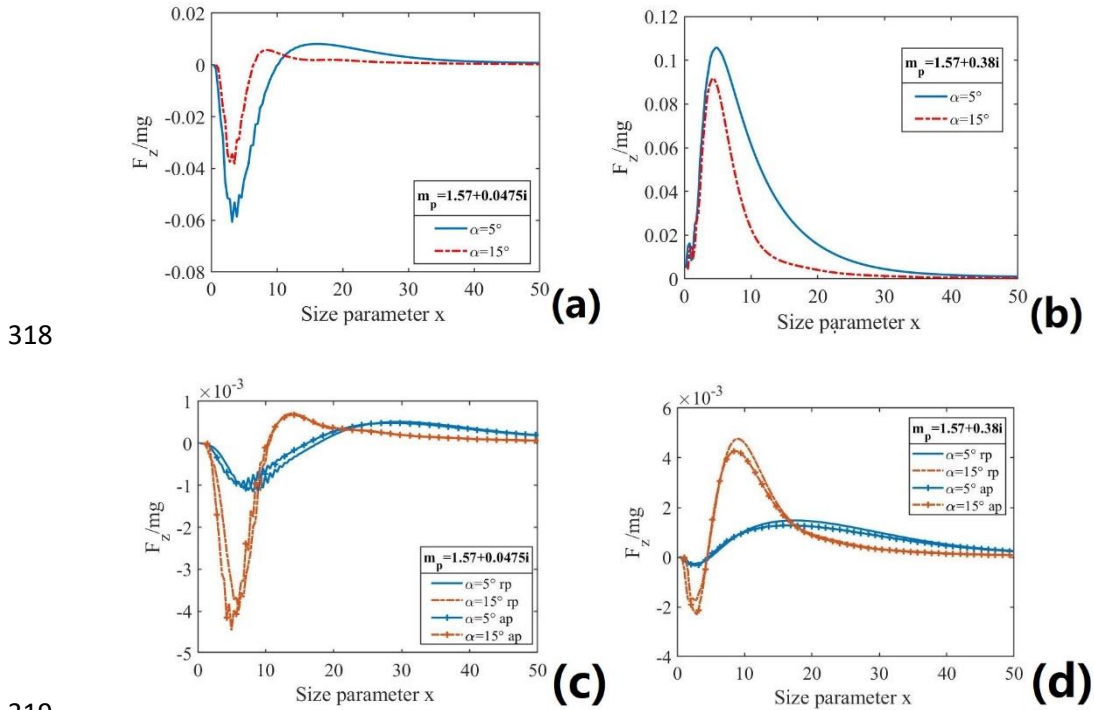


Fig. 4. J_z spectra for particles with different refractive indices in the case of a zero-order Bessel beam with different half-cone angles. (a) $m_p = 1.57 + 0.038i$; (b) $m_p = 1.57 + 0.38i$; The Bessel beam is azimuthally polarized.

When the imaginary part of the complex refractive index is relatively small, ripple structures can be observed in J_z for small size parameter, indicating a strong oscillation of the photophoretic force with the change of size parameter. This ripple structure fades away when the imaginary part of the complex refractive index increases or when the size parameter is large.

307 This ripple structure is believed to be related to the resonant modes in a weakly absorbing
 308 sphere, similarly to the ripple structures existing in extinction, scattering and absorption spectra.

309 As shown in Fig.3c and Fig.3d, when the imaginary part of the complex refractive index is
 310 relatively large, J_z spectra have similar profiles. The similarity between the profiles is because
 311 most of the incident light will be absorbed on the illuminated surface of the particle due to high
 312 absorptivity. Furthermore, an extreme minimum value of J_z can be found, which depends on
 313 the axicon angle, for instance, the extrema for both curves are around size parameters $x = 30$
 314 for axicon angle equal to 5° . It is interesting to find that positive J_z can also be found for high-
 315 absorbing particles when the particle is illuminated by a radially or azimuthally polarized
 316 Bessel beam. However, only negative J_z can be found in the case of x -polarized zero-order
 317 Bessel beam, as shown in Fig. 3(c)-(d) in [21].



320 Fig. 5. Ratios of photophoretic force to the weight of a glyceryl particle illuminated by a Bessel beam. (a)-(b) x-
 321 polarization; (c)-(d) radial polarization (rp) and azimuthal polarization (ap). Parameters of the ambient atmospheric
 322 conditions are the same as those listed in Table 1.

323 Making a comparison between Fig. 3 and Fig. 4, when the imaginary part of refractive index is
 324 the same, we can see that the J_z spectra pattern are slightly changed when the polarization
 325 varies from radial polarization to azimuthal polarization for the cases under study, although we
 326 should be aware that the absolute value of J_z depends on the polarization, resulting in a change
 327 of photophoretic force if the polarization is shifted. Ratios of longitudinal photophoretic force
 328 F_z to weight of a glyceryl particle illuminated by a Bessel beam have been calculated and

displayed in Fig. 5 for different polarizations. Two kinds of refractive indices of the particle $m_p = 1.57 + 0.0475i$ and $m_p = 1.57 + 0.38i$ have been considered, which correspond to the wavelength of $\lambda = 10.63\mu\text{m}$ and $\lambda = 9.58\mu\text{m}$, respectively. Parameters of the ambient atmosphere conditions are the same as those listed in Table 1.

Ignoring the ripple structure in the spectra, one extreme maximum and one extreme minimum can be observed in all the subfigures of Fig. 5, the corresponding size parameters depending on the value of the imaginary part of the refractive index and on the half-cone angle. As shown in Figs. 5(c) and (d), the spectra profiles of ratios of photophoretic force to the weight are quite similar for the radial polarization and the azimuthal polarization, although the internal field distributions inside of the sphere are quite different [37] in these two polarizations. It indicates that the longitudinal component of the asymmetry vector and the photophoretic force are mainly determined by the intensity profile of the incident beam in the case of a sphere illuminated by a circularly symmetric Bessel beam.

3.2 Off-axis cases

For the off-axis case, the photophoretic force has both a longitudinal and transverse component. The transverse component can be used to trap the particle inside the beam laterally, whereas the longitudinal component can be used to counterbalance the weight of particles. J_x spectra and J_z spectra (J versus the particle size parameter $x = 2\pi R / \lambda$) of a homogeneous sphere with different refractive indices illuminated by an off-axis zero-order Bessel beam are displayed in Fig. 6. Both radial polarization and x -polarization are considered.

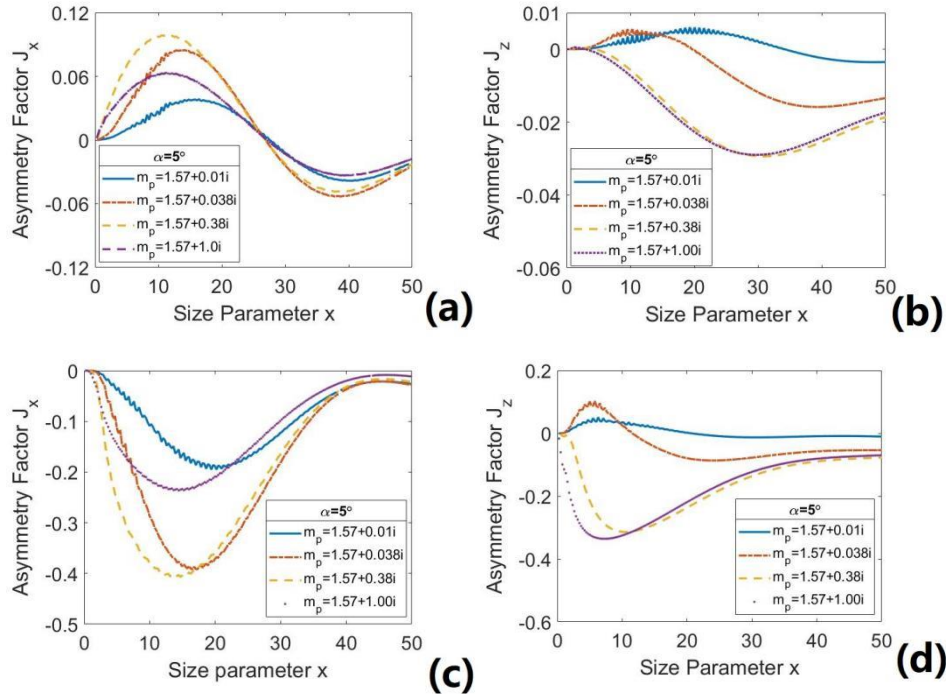


Fig. 6. J_x spectra and J_z spectra for different values of the imaginary part of refractive index. The particle is illuminated by an off-axis Bessel beam with beam center located at $X_0 = 2.5\mu\text{m}$. (a)-(b) radial polarization, (c)-(d) x-polarization.

As shown in Fig. 6, ripple structures can be observed in both J_x spectra and J_z spectra for particles with small absorptivity. This ripple structure starts to disappear for particles with large size parameter and strong absorptivity. Similar to the cases of on-axis illumination, positive J_z can be obtained when the absorption is small for both radial polarization and x-polarization, but only negative J_z exist for particles with strong absorption. As shown in Fig. 6(a), when a Bessel beam of radial polarization is assumed, the J_x is positive for small size parameters, indicating a restoring photophoretic force is exerted on the particle toward the beam center when the particle moves away from the beam center. This force increases with the increase of the particle size parameter during which positive part of the first lobe of the Bessel beam is covered by the particle step by step. Then J_x decreases and changes its sign from positive to negative when the particle is too large so that the first lobe of the Bessel beam was totally covered by the particle, and the photophoretic force starts to push the particle away from the beam center. However, when a Bessel beam of x-polarization is applied, as shown in Fig. 6(b), only negative J_z exist due to the fact that the maximum intensity is located at the beam center, so that the transverse photophoretic force will push the particle away from the beam center.

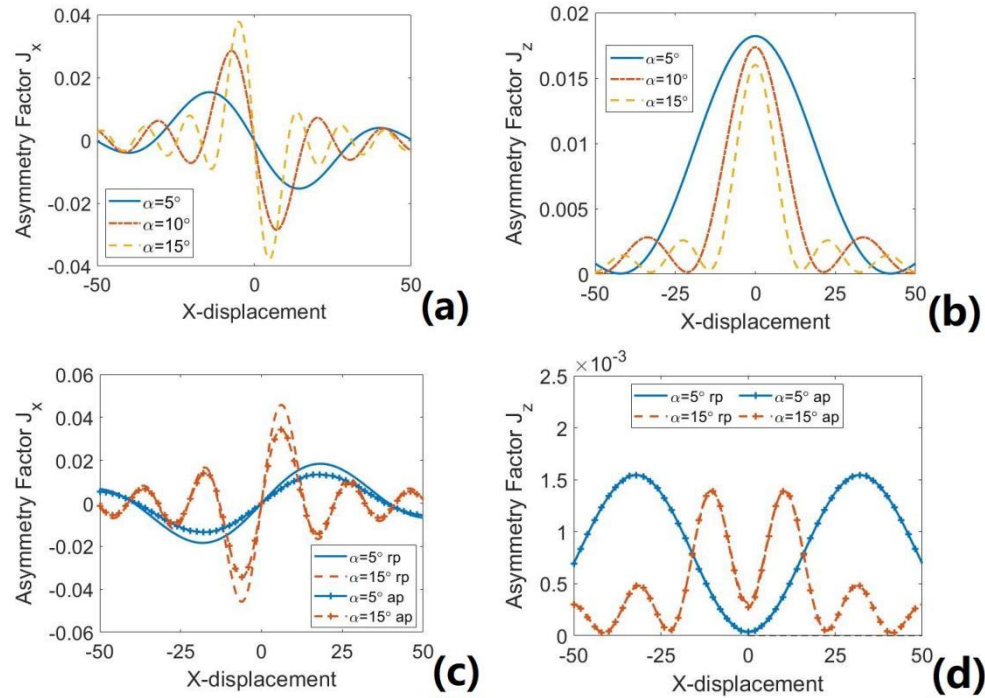


Fig. 7. Variations of J_x and J_z with particle location in the Bessel beam with different polarizations and different half-cone angles. (a)-(b) x-polarization; (c)-(d) radial polarization and azimuthal polarization. The radius of the

particle is $2.5\mu\text{m}$. The wavelength of the incident Bessel beam is $9.58\mu\text{m}$. The particle is assumed to move along X-axis. The refractive index is $m_p = 1.57 + 0.038i$.

To analyze the influence of particle locations on the photophoretic force, variations of J_x and J_z are predicted and displayed in Fig. 7 with the change of particle locations in the Bessel beam for different polarizations, including x -polarization, radial polarization, and azimuthal polarization. As shown in Fig. 7, all the J_z patterns are symmetric due to the circularly symmetric characteristics of Bessel beams. There is little difference in the J_z patterns between the radial polarization and azimuthal polarization. But the difference between the J_z profile of x -polarization and that of radial polarization is huge. As shown in Fig. 7(b), a maximum of J_z can be found when the particle sits at the center of the Bessel beam of x -polarization. The J_z decreases as the particle moves along x -axis away from the beam center. For the radial polarization and azimuthal polarization, the J_z has a minimum at the center of beam and then increases as the particle moves away from the beam center, as displayed in Fig. 7(d). The variations of J_z are similar to the variations of the transverse intensity profile of a Bessel beam, recalling that there is a maximum in the center of a Bessel beam of x -polarization, while a hollow center exists in the spatial intensity distribution of Bessel beam of radial polarization. It is also important to notice that the maximum value of J_z in x -polarization is around ten times larger than that in radial polarization.

The J_x profiles are antisymmetric with respect to $J_x = 0$ when the particle is located at the beam center. The J_x oscillates periodically as the particle moves transversely along X-axis, the period depends on the half-cone angle reflecting the transverse intensity distribution of the Bessel beam. Although there is little difference in the J_z patterns between the radial polarization and the azimuthal polarization, and that the J_x patterns for these two polarizations are similar, the amplitudes of J_x are different, indicating a different transverse trapping efficiency on particles by different polarizations.

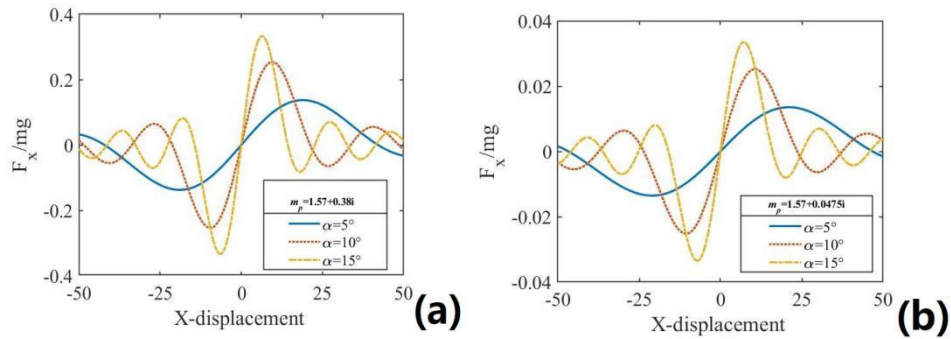


Fig. 8. Ratios of transverse component F_x of photophoretic force to the weight of a glyceryl particle illuminated by an off-axis Bessel beam of x -polarization. The radius of the particle is $2.5\mu\text{m}$.

To provide some references on the trapping efficiency of transverse component of photophoretic force, ratios of transverse component F_x of photophoretic force to the weight of a glyceryl particle have been calculated and displayed in Fig. 8 for x -polarization. Parameters of the ambient atmosphere conditions are the same as those listed in Table 1. As shown in Fig.

8, the imaginary part of refractive index has no influence on the ratio profile as the particle moves transversely. However, it plays a significant role on the absolute value of photophoretic force. The ratio of photophoretic force to weight can be different as high as ten times for a glyceryl particle with $m_p = 1.57 + 0.0475i$ and that with $m_p = 1.57 + 0.38i$. Similar behaviors being valid for radial polarization and azimuthal polarization, the results are not displayed.

4. Conclusions

In this paper, longitudinal and transverse photophoretic forces on a homogeneous sphere exerted by a zero-order Bessel beam with selective polarization are analyzed. The influences of particle size, absorptivity of the particle, half-cone angle and polarizations of the Bessel beam, and particle location in the laser beam on the asymmetry vector and on the photophoretic force are explored. The results show that ripple structures exist in both J_x spectra and J_z spectra for particles with small absorptivity. This ripple structure starts to disappear for particles with large size parameter and strong absorptivity. Due to the circularly symmetric characteristics of Bessel beams, all the J_z patterns are symmetric and the J_x patterns are anti-symmetric when the particle moves transversely away from the beam center. The J spectra of radial polarization are quite similar to that of azimuthal polarization, although big differences exist in the internal field distribution for these two polarizations, which indicates that the asymmetry vector and the photophoretic force are mainly determined by the intensity profile of the incident beam in the case of a sphere illuminated by a circularly symmetric Bessel beam. But it is worth mentioning that the amplitudes of J are different in different polarizations, indicating a different trapping efficiency on particles. The predicted dynamic behaviors of photophoretic force on the particle influenced by various parameters give important references to the manipulation of particles trapped in a structured beam and provide significant insights into the working mechanism underpinning the development of novel heat-mediated optical manipulation techniques, measurement of the refractive index of particle, and others.

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