Optical trapping of nonspherical particles in the T-matrix formalism

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Abstract: The theory of the trapping of nonspherical particles in the focal region of a high-numerical-aperture optical system is formulated in the framework of the transition matrix approach. Both the case of an unaberrated lens and the case of an aberrated one are considered. The theory is applied to single latex spheres of various sizes and, when the results are compared with the available experimental data, a fair agreement is attained. The theory is also applied to binary clusters of spheres of latex with a diameter of 220 nm in various orientations. Although, in this case we have no experimental data to which our results can be compared, we get useful indications for the trapping of nonspherical particles. In particular, we find substantial agreement with recent results on the trapping of prolate spheroids in aberrated gaussian fields [S. H. Simpson and S. Hanna, J. Opt. Soc. Am. A **24**, 430 (2007)].

OCIS codes: (290.0290) Scattering; (260.2110) Electromagnetic theory; (260.2160) Energy transfer; (140.7010) Laser trapping.

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1. Introduction

Optical trapping of particles is a consequence of the radiation force that stems from the conservation of electromagnetic momentum [1]. Indeed, when a laser beam is focalized by a lens of high numerical aperture, the configuration of the field may be such that the radiation force exerted on particles traps the latter within the focal region. This possibility led Ashkin et al. [2, 3] to the practical realization of trapping of small particles.

The configuration of the field in the focal region, in the absence of any particle, can be calculated, as done by Richards and Wolf [4] for the case of an aplanatic lens, by superposition of plane waves representing the rays that actually traverse the exit pupil. Once the field is known the radiation force exerted on any particle can be calculated by resorting to the theorem of conservation of the linear momentum for the combined system of field and particles. Although the resulting expression of the radiation force requires considering the Maxwell stress tensor [1], the literature reports several procedures to avoid using it when dealing with the optical trapping [5, 6]. For instance, one could calculate the Lorenz force density exerted on a particle by the focal field. This approach when applied to the problem at hand has to face some difficulty such as a reliable consideration of the charges induced in the particles [7]. Sometimes, the Lorenz force is calculated by assuming that the dielectric properties of the particles are adequately given by the polarizability [8]. Strictly speaking, this assumption applies to small dielectric spheres and prevents dealing with nonspherical particles or with particles whose refractive index relative to that of the surrounding medium is far from unity.

In this paper we reformulate the theory of optical trapping of nonspherical particles making full use of the Maxwell stress tensor. To this end we establish a complete formalism exploiting the multipole expansion of the fields in the framework of the transition matrix approach [9], that, in principle, does not require that the particles be spherical or small with respect to the wavelength, and implies the only approximation of truncating the multipole expansions after a number of terms suitable to get the convergence of the calculations. The formalism that we are going to establish is easily applicable to trapping of clusters of spherical scatterers. We already used the transition matrix approach just to calculate the radiation force on nonspherical particles [10]. Nevertheless, since in Ref. [10] the incident field was restricted to single plane waves, for the present purposes it is convenient to rewrite the main formulas of the theory in a

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form suitable to be extended to the superposition of plane waves that describes an optical beam focalized by a lens. Anyway, the formalisms based on the T-matrix seem to become more and more appreciated: e.g., in a recent paper the trapping force on dielectric ellipsoids has been calculated through the transition matrix approach [11].

2. Radiation force exerted by plane waves

In this section we review the theory of the radiation force exerted by a plane wave on a non-spherical particle of arbitrary size. Since our purpose is to extend the theory to the case of a laser beam focalized by a suitable lens, it is convenient to choose a frame of reference that makes this extension as simple as possible. To this end we define a frame of reference Σ whose origin O coincides with the focus of the lens and whose z axis is parallel to the optical axis. Let us attach to the particle a frame of reference Σ' whose origin O' lies inside the particle and whose axes are parallel to the axes of Σ. The vector position of O' with respect to Σ is $\mathbf{R}_{O'}$ (see Fig. 1). We assume that all the fields depend on time through the factor $\exp(-i\omega t)$ that is omitted throughout. Then, the force that the radiation exerts on the particle is given by the integral [1]

$$\mathbf{F}_{\mathrm{Rad}} = r'^2 \int_{\Omega'} \hat{\mathbf{r}}' \cdot \langle \mathsf{T}_{\mathrm{M}} \rangle \, \mathrm{d}\Omega' \,, \tag{1}$$

where the integration is over the full solid angle, r' is the radius of a large sphere with center at $\mathbf{R}_{O'}$ surrounding the particle, and

$$\langle \mathsf{T}_{\mathrm{M}} \rangle = \frac{1}{8\pi} \mathrm{Re}\left[n^2 \mathbf{E}' \otimes \mathbf{E}'^* + \mathbf{B}' \otimes \mathbf{B}'^* - \frac{1}{2} (n^2 |\mathbf{E}'|^2 + |\mathbf{B}'|^2) \mathsf{I} \right] \tag{2}$$

is the time averaged Maxwell stress tensor. In Eq. (2), the fields $\mathbf{E}'$ and $\mathbf{B}'$ are considered in the frame Σ', $\otimes$ denotes dyadic product, the asterisk indicates complex conjugation, and I is the unit dyadic. Of course, the fields that enter the definition of $\langle \mathsf{T}_{\mathrm{M}} \rangle$ are the superposition of the incident and of the scattered field.

We now assume that the field incident on the particle is the polarized plane wave

$$\mathbf{E}_{\mathrm{I}} = E_0 \hat{\mathbf{u}} e^{i\mathbf{k}\cdot\mathbf{r}} = E_0 \hat{\mathbf{u}} e^{i\mathbf{k}\cdot(\mathbf{r}'+\mathbf{R}_{O'})} = E_0' \hat{\mathbf{u}} e^{i\mathbf{k}\cdot\mathbf{r}'} = \mathbf{E}_{\mathrm{I}}' \tag{3}$$

of wavevector $\mathbf{k} = \hat{\mathbf{k}} n k_{\mathrm{V}}$, where $\hat{\mathbf{k}}$ is the unit vector in the direction of incidence, n is the refractive index of the surrounding medium, $k_{\mathrm{V}} = \omega/c$ and $\hat{\mathbf{u}}$ is the (unit) polarization vector.

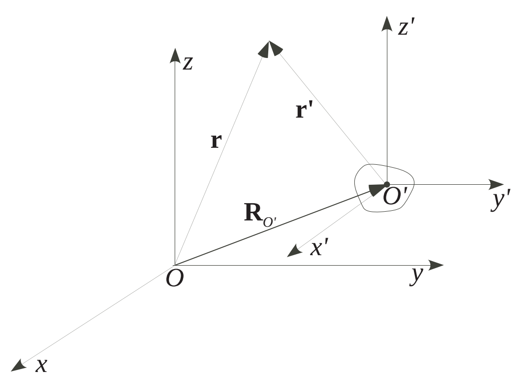

Fig. 1. Coordinate system we adopt to describe the radiation force on a particle at O'. The focus of the optical system coincides with O and the optical axis coincides with the z axis.

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Obviously, $|E_0'|^2 = |E_0|^2$ in Eq. (3). In view of our choice of the incident field, the integral in Eq. (1) can be calculated by resorting to the asymptotic expansion of a plane wave [12]

$$\mathbf{E}_\mathrm{I}' = E_0'\hat{\mathbf{u}}\frac{2\pi i}{r'k}\left[\delta(\hat{\mathbf{k}}+\hat{\mathbf{r}}')\exp(-ikr') - \delta(\hat{\mathbf{k}}-\hat{\mathbf{r}}')\exp(ikr')\right] .$$

Then, a straightforward calculation leads to the conclusion that the first two terms, i.e. the dyadic products, in the expression of $\langle \mathsf{T}_\mathrm{M}\rangle$ give a vanishing contribution to the radiation force [13]. In Appendix A we will prove this result through a different approach that applies even to the case in which the incident field is not a single plane wave. Anyway, the component of the radiation force along the direction characterized by the unit vector $\hat{\mathbf{v}}_\zeta$ turns out to be

$$F_{\mathrm{Rad}\,\zeta} = -\frac{r'^2}{16\pi}\mathrm{Re}\int_{\Omega'}(\hat{\mathbf{r}}'\cdot\hat{\mathbf{v}}_\zeta)\left[n^2(|\mathbf{E}_\mathrm{S}'|^2 + 2\mathbf{E}_\mathrm{I}'^*\cdot\mathbf{E}_\mathrm{S}') + (|\mathbf{B}_\mathrm{S}'|^2 + 2\mathbf{B}_\mathrm{I}'^*\cdot\mathbf{B}_\mathrm{S}')\right]\mathrm{d}\Omega' , \qquad (4)$$

where $\mathbf{E}_\mathrm{S}'$ and $\mathbf{B}_\mathrm{S}'$ are the fields scattered by the particle. Obviously, since the incident field is a plane wave, the integral (4) gets no contribution from the terms $\mathbf{E}_\mathrm{I}'\cdot\mathbf{E}_\mathrm{I}'^*$, and $\mathbf{B}_\mathrm{I}'\cdot\mathbf{B}_\mathrm{I}'^*$ that, accordingly, have been omitted. However, it is less obvious that the integral (4) gets no contribution from the same terms even when the incident field is a superposition of plane waves with different directions of propagation. This statement will be proved in Appendix A.

At this stage let us recall that the multipole expansion of the electric field of a plane wave and of the corresponding scattered wave is [14]

$$\mathbf{E}_\mathrm{I} = E_0\sum_{plm}\mathbf{J}_{lm}^{(p)}W_{\mathrm{I}lm}^{(p)} , \qquad (5)$$

$$\mathbf{E}_\mathrm{S} = E_0\sum_{plm}\mathbf{H}_{lm}^{(p)}A_{lm}^{(p)} , \qquad (6)$$

whence the multipole expansion of the magnetic field can be inferred through the equation

$$\mathbf{B} = -\frac{i}{k_\mathrm{v}}\nabla\times\mathbf{E} .$$

In Eqs. (5) and (6) we define the multipole fields

$$\mathbf{J}_{lm}^{(1)} = j_l(kr)\mathbf{X}_{lm}(\hat{\mathbf{r}}) , \quad \mathbf{J}_{lm}^{(2)} = \frac{1}{k}\nabla\times\mathbf{J}_{lm}^{(1)} ,$$

where the $\mathbf{X}_{lm}$ are vector spherical harmonics [1], and the multipole fields $\mathbf{H}_{lm}^{(p)}$ that are identical to the $\mathbf{J}_{lm}^{(p)}$ except for the substitution of the Hankel function of the first kind $h_l(kr)$ in place of the spherical Bessel functions $j_l(kr)$. The $\mathbf{J}$ fields are everywhere regular whereas the $\mathbf{H}$ fields satisfy the radiation condition at infinity. The superscript $p = 1,\ 2$ distinguish the magnetic multipole fields from the electric ones, respectively. The amplitudes $W_{\mathrm{I}lm}^{(p)}$ take into account both the direction of propagation and the polarization of the incident field and are defined as

$$W_{\mathrm{I}lm}^{(p)} = W_{lm}^{(p)}(\hat{\mathbf{u}},\hat{\mathbf{k}}) = 4\pi i^{p+l-1}\hat{\mathbf{u}}\cdot\mathbf{Z}_{lm}^{(p)}(\hat{\mathbf{k}}) ,$$

where

$$\mathbf{Z}_{lm}^{(1)} = \mathbf{X}_{lm}(\hat{\mathbf{k}}), \quad \mathbf{Z}_{lm}^{(2)} = \mathbf{X}_{lm}(\hat{\mathbf{k}})\times\hat{\mathbf{k}}$$

are transverse harmonics [15]. The amplitudes of the scattered field can be calculated by imposing the customary boundary conditions across the surface of the particle and are related to those of the incident field by

$$A_{lm}^{(p)} = \sum_{p'l'm'}\mathscr{S}_{lml'm'}^{(pp')}W_{\mathrm{I}l'm'}^{(p')} \qquad (7)$$

which defines the elements of the transition matrix of the particle [9]. Now, the particles we are going to deal with either actually are, or can be modeled as aggregates of spheres. We calculate $\mathscr{S}^{(pp')}_{lml'm'}$ for such aggregates always starting with the inversion of the matrix of the linear system that is obtained by imposing to the fields the boundary conditions across each of the spherical surfaces [16, 17]. The order of the matrix to be inverted is $2Nl_{\mathrm{M}}(l_{\mathrm{M}}+2)$, where N is the number of the spheres of the aggregate and l_{M} is the maximum value of l to be retained in the multipole expansions of the fields (5) and (6) in order to get convergence for the quantities of interest. The convergence of such kind of calculations is studied in Ref. [16]. A comprehensive treatment of all the abovementioned topics related to the calculation of the transition matrix can be found in Ref. [14, 18].

The transition matrix depends on the orientation of the particle but, once its elements are calculated in a given frame of reference, they turn out to be independent both on the direction of propagation and on the polarization of the incident field.

In our previous paper on radiation force [10] we started from the result obtained by Mishchenko [19] through the use of the optical theorem. Here, we found more convenient to perform the integration in Eq. (4) using the asymptotic expansion of the multipole fields [14] up to terms which give a contribution of order $1/r$. Actually, these expansions for the incident and the scattered field give

$$\mathbf{E}'_{\mathrm{I}} \to E'_0 \sum_{plm} \mathbf{Z}^{(p)}_{lm}(\hat{\mathbf{r}}') W^{(p)}_{\mathrm{I}lm} \frac{(-)^{p-1}}{kr'} \sin[kr' - (l+1-p)\pi/2] \,, \tag{8a}$$

$$\mathbf{E}'_{\mathrm{S}} \to E'_0 \sum_{plm} \mathbf{Z}^{(p)}_{lm}(\hat{\mathbf{r}}') A^{(p)}_{lm} \frac{\exp(ikr')}{kr'} i^{-l-p} \tag{8b}$$

which, when substituted into Eq. (4), yield the result

$$\begin{aligned} F_{\mathrm{Rad}\,\zeta} = &- \frac{|E_0|^2}{16\pi k_{\mathrm{v}}^2} \mathrm{Re}\left[\sum_{plm} \sum_{p'l'm'} \left(A^{(p)*}_{lm} A^{(p')}_{l'm'} + A^{(p'')*}_{lm} A^{(p''')}_{l'm'} \right) i^{l-l'} I^{(pp')}_{\zeta\, lml'm'} \right] \\ &- \frac{2|E_0|^2}{16\pi k_{\mathrm{v}}^2} \mathrm{Re}\left[\sum_{plm} \sum_{p'l'm'} \left(W^{(p)*}_{\mathrm{I}lm} A^{(p')}_{l'm'} + W^{(p'')*}_{\mathrm{I}lm} A^{(p''')}_{l'm'} \right) \right. \\ &\left. \times \sin[kr - (l-1+p)\pi/2] e^{ikr} (-i)^{l+p} i^{l-l'} I^{(pp')}_{\zeta\, lml'm'} \right] \\ &= -F^{(\mathrm{Sca})}_{\mathrm{Rad}\,\zeta} + F^{(\mathrm{Ext})}_{\mathrm{Rad}\,\zeta} \,, \end{aligned} \tag{9}$$

with $p'' \neq p$ and $p''' \neq p'$. In Eq. (9)

$$I^{(pp')}_{\zeta\, lml'm'} = \int_{\Omega'} (\hat{\mathbf{r}}' \cdot \hat{\mathbf{v}}_\zeta) i^{p-p'} \mathbf{Z}^{(p)*}_{lm}(\hat{\mathbf{r}}') \cdot \mathbf{Z}^{(p')}_{l'm'}(\hat{\mathbf{r}}') \, \mathrm{d}\Omega' = \frac{4\pi}{3} \sum_{\mu} Y^*_{1\mu}(\hat{\mathbf{v}}_\zeta) K^{(pp')}_{\mu;lml'm'} \,. \tag{10}$$

In turn $Y_{1\mu}(\hat{\mathbf{v}}_\zeta)$ in Eq. (10) denotes spherical harmonics whose arguments are the polar angles of $\hat{\mathbf{v}}_\zeta$, and

$$K^{(pp')}_{\mu;lml'm'} = \int_{\Omega'} \hat{\mathbf{r}}' i^{p-p'} \mathbf{Z}^{(p)*}_{lm}(\hat{\mathbf{r}}') \cdot \mathbf{Z}^{(p')}_{l'm'}(\hat{\mathbf{r}}') \, \mathrm{d}\Omega' \,. \tag{11}$$

The integrals (11) can be performed in closed form [10, 14] with the result

$$K^{(pp')}_{\mu;lml'm'} = 16\pi^2 \sqrt{\frac{3}{4\pi}} C(1,l',l;\mu,m',m) i^{l-l'} O^{(pp')}_{ll'} \,, \tag{12}$$

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where $C(1,l',l;\mu,m',m)$ denotes Clebsch-Gordan coefficients [20] and

$$O_{ll}^{(pp')} = -\frac{1}{\sqrt{l(l+1)}}(1-\delta_{pp'}) ,$$
$$O_{l,l-1}^{(pp')} = \sqrt{\frac{(l-1)(l+1)}{l(2l+1)}}\delta_{pp'} ,$$
$$O_{l,l+1}^{(pp')} = -\sqrt{\frac{l(l+2)}{(l+1)(2l+1)}}\delta_{pp'} .$$

We stress that Eq. (12) is correct, unlike the formula reported in [14] which contains a misprint [18]. The K-integrals have the symmetry properties

$$K_{\zeta\, lml'm'}^{(11)} = K_{\zeta\, lml'm'}^{(22)}, \quad K_{\zeta\, lml'm'}^{(12)} = K_{\zeta\, lml'm'}^{(21)} ,$$

which help us to get a more compact expression for $F_{\mathrm{Rad}\,\zeta}^{(\mathrm{Sca})}$ and $F_{\mathrm{Rad}\,\zeta}^{(\mathrm{Ext})}$. In fact, from Eq. (9) we get

$$F_{\mathrm{Rad}\,\zeta}^{(\mathrm{Sca})} = \frac{2|E_0|^2}{16\pi k_\mathrm{v}^2}\mathrm{Re}\sum_{plm}\sum_{p'l'm'} A_{lm}^{(p)*} A_{l'm'}^{(p')} i^{l-l'} I_{\zeta\, lml'm'}^{(pp')} , \tag{13a}$$

$$F_{\mathrm{Rad}\,\zeta}^{(\mathrm{Ext})} = -\frac{2|E_0|^2}{16\pi k_\mathrm{v}^2}\mathrm{Re}\sum_{plm}\sum_{p'l'm'} W_{\mathrm{I}lm}^{(p)*} A_{l'm'}^{(p')} i^{l-l'} I_{\zeta\, lml'm'}^{(pp')} , \tag{13b}$$

where the amplitudes of the scattered field $A_{lm}^{(p)}$ are given by Eq. (7) in terms of the elements of the transition matrix.

We notice that even though the radiation force has been separated into two contributions, there is no similarity with the customary separation into a field gradient contribution and a scattering contribution. The separation effected in Eqs. (13a) and (13b) can be tracked back to Eq. (4) which, due to the structure of the Maxwell stress tensor, includes $|\mathbf{E}'_\mathrm{S}|^2$ and $\mathbf{E}'^*_\mathrm{I}\cdot\mathbf{E}'_\mathrm{S}$ as well as the corresponding terms from the magnetic field. When these terms are expanded as a series of multipole fields we just get $F_{\mathrm{Rad}\,\zeta}^{(\mathrm{Sca})}$, that depends on the amplitudes of the scattered multipole fields, and $F_{\mathrm{Rad}\,\zeta}^{(\mathrm{Ext})}$ that depends on the amplitudes both of the incident and of the scattered multipole fields. As a result, $F_{\mathrm{Rad}\,\zeta}^{(\mathrm{Sca})}$ and $F_{\mathrm{Rad}\,\zeta}^{(\mathrm{Ext})}$ can be somehow related to the scattering and to the extinction cross section of the particle, respectively. Thus, according to the last line of Eq. (9), the radiation force can be related to the absorption cross section, i.e. to the absorptivity of the particle. Note that similar considerations hold true also for the radiation torque [21], and in particular for a spherical scatterer the torque exerted by an elliptically polarized plane wave can be explicitly written in terms of the difference of the extinction and of the scattering cross section [22].

3. Radiation force from a focalized laser beam

Let us now show how the teory of Sect. 2 can be extended to the case of a laser beam focalized by an aplanatic lens. However, let us first recall that in Sect. 2 we stressed the vanishing of the contribution to the radiation force from the terms $\mathbf{E}_\mathrm{I}\cdot\mathbf{E}_\mathrm{I}^*$ and $\mathbf{B}_\mathrm{I}\cdot\mathbf{B}_\mathrm{I}^*$. In fact, in Appendix A we show that the contribution from these terms vanishes even when the incident field is not a single plane wave but a superposition of plane waves of the kind described below.

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Let us consider a lens of focal length f, whose exit pupil has the radius $f \sin\vartheta_{\mathrm{Max}}$; of course, ϑ_{Max} is the angle under which the radius of the exit pupil is seen from the focus and is thus related to the numerical aperture of the lens by

$$\mathrm{NA} = n \sin\vartheta_{\mathrm{Max}} ,$$

where n is the refractive index of the medium that fills the image space. We consider the focalization of a gaussian TEM_{00} beam. Then, according to Novotny and Hecht [23], the field at any point within the focal region can be written in the paraxial approximation and using the angular spectrum representation as

$$\mathbf{E}(\mathbf{r}) = \int_{k_x^2+k_y^2 \le k_\perp^2} E_{\mathrm{PW}}(\hat{\mathbf{k}})\hat{\mathbf{u}}_{\hat{\mathbf{k}}} e^{i\mathbf{k}\cdot\mathbf{r}}\, \mathrm{d}\hat{k}_x \mathrm{d}\hat{k}_y , \tag{14}$$

where $k_\perp = k \sin\vartheta_{\mathrm{Max}}$, $\mathbf{k}$ has polar angles $\vartheta_{\mathbf{k}}$ and $\varphi_{\mathbf{k}}$, $\hat{\mathbf{u}}_{\hat{\mathbf{k}}} = \hat{\mathbf{u}}(\vartheta_{\mathbf{k}}, \varphi_{\mathbf{k}})$; the limits of integration ensure that only the rays that actually traverse the exit pupil of the optical system are considered. In Eq. (14)

$$E_{\mathrm{PW}}(\hat{\mathbf{k}}) = E_0\, i f \frac{e^{ikf}}{2\pi k}\sqrt{\frac{n_{\mathrm{I}}}{n}}\,(\cos\vartheta_{\mathbf{k}})^{-1/2} f_w ,$$

where n_{I} is the refractive index of the object space and f_w is the apodization function

$$f_w = \exp\left[-\frac{1}{f_0^2}\frac{\sin^2\vartheta_{\mathbf{k}}}{\sin^2\vartheta_{\mathrm{Max}}}\right] . \tag{15}$$

In the preceding equation f_0 is the filling factor which for a beam with waist radius w_0 is

$$f_0 = \frac{w_0}{f \sin\vartheta_{\mathrm{Max}}}.$$

The apodization function (15) is common also to the higher gaussian modes TEM_{10} and TEM_{01}, and when $f_w = 1$, i.e., for $w_0 \to \infty$, one recovers the description of the field of Richards and Wolf [4].

Often, the image space is not filled by a single homogeneous medium but rather by two homogeneous media, of refractive indexes n and n_{F}, separated by a plane interface orthogonal to the optical axis. We assume the interface to be located at $z_0 = -d$ between the exit pupil and the nominal focus. Hereafter, the quantities considered in the region $z > z_0$ will be characterized by the index F, even when, strictly speaking, this notation would not be necessary. For instance, since k_x and k_y are unaffected by the refraction, we have $k_x = k_{\mathrm{F}x}$ and $k_y = k_{\mathrm{F}y}$, and thus also $k_\perp = k_{\mathrm{F}\perp}$. On the contrary, k_z is affected by the refraction according to

$$k_{\mathrm{F}z} = \left(k_{\mathrm{F}}^2 - k_x^2 - k_y^2\right)^{1/2} = \left[\left(\frac{n_{\mathrm{F}}}{n}\right)^2 k^2 - k_x^2 - k_y^2\right]^{1/2}.$$

The refraction of the rays through the interface introduces a spherical aberration and a polarization-dependent transmission that can be taken into account by the Fresnel coefficients T_η [1]; $\eta = 1$ stands for polarization parallel and $\eta = 2$ for polarization perpendicular to the plane of incidence that, for each ray, is defined by the $\mathbf{k}$ or by the $\mathbf{k}_{\mathrm{F}}$ vector, and the z axis (optical axis). The decomposition of the polarization vectors of each of the plane waves in Eq. (14) into their components parallel and perpendicular to the plane of incidence can be effected by introducing for each plane of incidence a pair of unit vectors $\hat{\mathbf{u}}_{\eta\hat{\mathbf{k}}}$. Thus, we have

$$\hat{\mathbf{u}}_{\hat{\mathbf{k}}} = \sum_\eta (\hat{\mathbf{u}}_{\hat{\mathbf{k}}} \cdot \hat{\mathbf{u}}_{\eta\mathbf{k}})\hat{\mathbf{u}}_{\eta\mathbf{k}} = \sum_\eta c_\eta \hat{\mathbf{u}}_{\eta\hat{\mathbf{k}}} \tag{16}$$

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and, the refraction through the interface yields

$$\mathbf{E}(\mathbf{r}) = \int_{k_{\mathrm{F}x}^2+k_{\mathrm{F}y}^2\le k_{\mathrm{F}\perp}^2} E_{\mathrm{FPW}}(\hat{\mathbf{k}}_{\mathrm{F}}) \sum_\eta c_\eta T_\eta(\vartheta_{\mathbf{k}}) \hat{\mathbf{u}}_{\eta\hat{\mathbf{k}}_{\mathrm{F}}} e^{i\mathbf{k}_{\mathrm{F}}\cdot\mathbf{r}} \,\mathrm{d}\hat{k}_{\mathrm{F}x}\mathrm{d}\hat{k}_{\mathrm{F}y} , \tag{17}$$

where

$$E_{\mathrm{FPW}}(\hat{\mathbf{k}}_{\mathrm{F}}) = \exp[-id(k_z - k_{\mathrm{F}z})] E_{\mathrm{PW}}(\hat{\mathbf{k}}) .$$

We stress that, although $\vartheta_{\mathbf{k}}$ appears in place of $\vartheta_{\mathbf{k}\mathrm{F}}$ in Eq. (17), Snell's law grants an immediate relation between these angles. Moreover, the same law makes the apodization function (15) insensitive to the use of $\vartheta_{\mathbf{k}}$ or of $\vartheta_{\mathbf{k}\mathrm{F}}$.

To complete the expression of the field we need to specify the coefficients c_η in Eq. (16) for a given choice of the state of polarization. We assume that the TEM_{00} mode we deal with, before being refracted and focalized, is polarized along the x axis, i.e., its polarization vector has vanishing y component. This choice coincides with that of Rohrbach [8]. According to the considerations of Novotny and Hecht [23] and in agreement with the definitions of Mansuripur [24] for the polarization of refracted beams, it is an easy matter to see that [23]

$$c_1 = \cos\varphi_{\mathbf{k}}, \quad \text{and} \quad c_2 = -\sin\varphi_{\mathbf{k}} .$$

We are now able to calculate the radiation force that the field exerts on a particle at O'. To this end we rewrite Eq. (17) as

$$\mathbf{E}'(\mathbf{r}') = \int_{k_{\mathrm{F}x}^2+k_{\mathrm{F}y}^2\le k_{\mathrm{F}\perp}^2} E_{\mathrm{FPW}}(\hat{\mathbf{k}}_{\mathrm{F}}) e^{i\mathbf{k}_{\mathrm{F}}\cdot\mathbf{R}_{O'}} \sum_\eta c_\eta T_\eta(\vartheta_{\mathbf{k}}) \hat{\mathbf{u}}_{\eta\hat{\mathbf{k}}_{\mathrm{F}}} e^{i\mathbf{k}_{\mathrm{F}}\cdot\mathbf{r}'} \,\mathrm{d}\hat{k}_{\mathrm{F}x}\mathrm{d}\hat{k}_{\mathrm{F}y} , \tag{18}$$

and perform the multipole expansion

$$\hat{\mathbf{u}}_{\eta\hat{\mathbf{k}}_{\mathrm{F}}} e^{i\mathbf{k}_{\mathrm{F}}\cdot\mathbf{r}'} = \sum_{plm} \mathbf{J}_{lm}^{(p)}(\mathbf{r}', k_{\mathrm{F}}) W_{lm}^{(p)}(\hat{\mathbf{u}}_{\eta\hat{\mathbf{k}}_{\mathrm{F}}}, \hat{\mathbf{k}}_{\mathrm{F}}) .$$

Since the $\mathbf{J}$ multipole fields depend on the magnitude of $\mathbf{k}_{\mathrm{F}}$ only, they can be carried outside the integral with the result

$$\mathbf{E}' = \sum_{plm} \mathbf{J}_{lm}^{(p)}(\mathbf{r}', k_{\mathrm{F}}) \mathscr{W}_{lm}^{(p)}(\mathbf{R}_{O'}) , \tag{19}$$

where

$$\mathscr{W}_{lm}^{(p)}(\mathbf{R}_{O'}) = \sum_\eta c_\eta \int_{k_{\mathrm{F}x}^2+k_{\mathrm{F}y}^2\le k_{\mathrm{F}\perp}^2} E_{\mathrm{FPW}}(\hat{\mathbf{k}}_{\mathrm{F}}) e^{i\mathbf{k}_{\mathrm{F}}\cdot\mathbf{R}_{O'}} T_\eta(\vartheta_{\mathbf{k}}) W_{lm}^{(p)}(\hat{\mathbf{u}}_{\eta\hat{\mathbf{k}}_{\mathrm{F}}}, \hat{\mathbf{k}}_{\mathrm{F}}) \,\mathrm{d}\hat{k}_{\mathrm{F}x}\mathrm{d}\hat{k}_{\mathrm{F}y} . \tag{20}$$

Of course, Eq. (19) refers to the case in which there is a plane of separation between two media of different refractive index, so that the consequent refraction must be taken into account. It is an easy matter to show that, when $n_{\mathrm{F}} \to n$, Eq. (19) simplifies into

$$\mathbf{E}' = \sum_{plm} \mathbf{J}_{lm}^{(p)}(\mathbf{r}', k) \mathscr{W}_{lm}^{(p)}(\mathbf{R}_{O'}) , \tag{21}$$

where

$$\mathscr{W}_{lm}^{(p)}(\mathbf{R}_{O'}) = \int_{k_x^2+k_y^2\le k_\perp^2} E_{\mathrm{PW}}(\hat{\mathbf{k}}) e^{i\mathbf{k}\cdot\mathbf{R}_{O'}} W_{lm}^{(p)}(\hat{\mathbf{u}}_{\hat{\mathbf{k}}}, \hat{\mathbf{k}}) \,\mathrm{d}\hat{k}_x\mathrm{d}\hat{k}_y . \tag{22}$$

According to the case we deal with, Eqs. (19) and (21) show that the multipole expansion of the field in the focal region resembles the expansion of a plane wave, whose amplitudes $\mathscr{W}_{lm}^{(p)}(\mathbf{R}_{O'})$, according to Eqs. (20) or (22) depend on the position of the particle. Thus, when calculating the

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radiation force exerted on a particle, we only have to substitute the newly defined amplitudes $\mathscr{W}_{lm}^{(p)}$ into Eq. (7) to get the amplitudes of the scattered field $\mathscr{A}_{lm}^{(p)}$, and into Eq. (13b) to get $F_{\mathrm{Rad}\,\zeta}^{(\mathrm{Ext})}$. In practice, the required result is still given by Eqs. (13a) and (13b) provided that

$$E_0' W_{1lm}^{(p)} \to \mathscr{W}_{lm}^{(p)}(\mathbf{R}_{O'})\,, \quad E_0' A_{lm}^{(p)} \to \mathscr{A}_{lm}^{(p)}\,.$$

The preceding considerations highlight the importance of the quantities $\mathscr{W}_{lm}^{(p)}(\mathbf{R}_{O'})$ that describe the lens, as they depend on the characteristics of the latter. Then, the integrals (20) and (22) can be calculated numerically once for all at the nodes of a suitably chosen grid for a given lens and stored for further use. However, the indispensible ingredient for describing the trapping of particles by means of Eqs. (13) is the knowledge of the field scattered by the particles themselves, i.e., the knowledge of the multipole amplitudes $\mathscr{A}_{lm}^{(p)}$. In this paper we preferred to resort to the transition matrix, Eq. (7), but let us stress that the $\mathscr{A}_{lm}^{(p)}$ amplitudes can be calculated also by other methods such as those devised by Chew [25] and by Xu [26]

Finally, we recall that, for computational reasons, the multipole expansion of the fields must be truncated. Therefore, wherever in Eqs. (5) through (21) sums over the multipole order l and/or l' appear, it must be understood that the sums were actually performed up to $l, l' = l_{\mathrm{M}}$ where l_{M} is large enough to ensure fair convergence of all the quantities of interest.

4. Applications

The theory expounded so far has been applied to the calculation of the trapping position of homogeneous spheres of latex ($n_{\mathrm{p}} = 1.57$) of various sizes as well as of aggregates of two mutually conntacting spheres of latex with a diameter $d = 220\,\mathrm{nm}$. In order to be able to compare our results with the experimental data existing in the literature we assumed an aplanatic optical system with numerical aperture $\mathrm{NA} = 1.2$ both in case the image space is filled of water with refractive index $n = 1.33$ and in case the exit pupil is immersed in oil with refractive index $n = 1.52$ whereas the trapping particle is immersed in water. These media are separated by a cover slip orthogonal to the optical axis located at $D = -20\,\mu\mathrm{m}$ with respect to the origin at the nominal focus of the lens. Since $\mathrm{NA} < 1.33$ no plane wave is totally reflected at the separation interface. As the presence of two media of different refractive indexes introduces a spherical aberration, the maximum field intensity occurs at a point at $\approx \Delta F = -4.0\,\mu\mathrm{m}$ with respect to the nominal focus. The incident field is assumed to be a TEM_{00} Gaussian beam, linearly polarized along the x axis, with filling factor $f_0 = 2$ and wavelength $\lambda_0 = 1060\,\mathrm{nm}$ in vacuo, i.e., $\lambda = 800\,\mathrm{nm}$ in water. In Fig. 2 we report the contur plot of the field intensity in the xz and in the yz plane both in the case of the unaberrated gaussian beam and of the aberrated beam. Note that in the latter case the origin of the z axis is shifted by $\Delta F = -4.0\,\mu\mathrm{m}$. A look to Fig. 2 shows the aberration actually manifests as a large shift of the field maximum and a more accentuated lack of cylindrical symmetry around the optical axis due to the linear polarization of the incident beam. These results are in substantial agreement with those reported by Rohrbach and Stelzer [27]

4.1. *Spherical particles*

We now go to consider the trapping of single spheres both in an unaberrated and in an aberrated field. In order to comply with the common usage of the experimentalists we define the so-called trapping efficiency as

$$\mathbf{Q}(\mathbf{r}) = \mathbf{F}_{\mathrm{Rad}}(\mathbf{r})\frac{c}{Pn}\,,$$

where P is the power of the trapping beam and n is the refractive index of the medium surrounding the particle. Thus, $n = 1.33$ in all the cases we deal with. The argument $\mathbf{r}$ denotes

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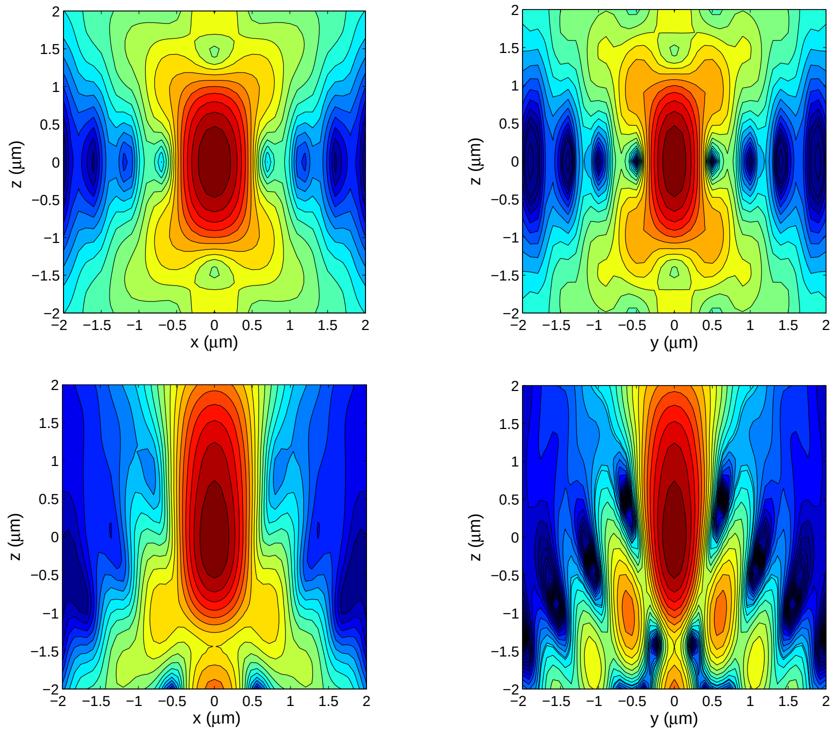

Fig. 2. Contour plot (log scale) of the intensity $|\mathbf{E}(\mathbf{r})|^2$ of the unaberrated gaussian (top panels) and aberrated gaussian field (lower panels) in the *xz* (left panels) and in the *yz* plane (right panels). The origin of the z axis in the lower panels is shifted by $\Delta F = -4.0\,\mu$m.

the position of the particles, i.e., the position of the center for single spheres, or the position of the point of mutual contact of the spheres of the binary aggregates. Of course, the trapping occurs at the point $\mathbf{r}_0 \equiv (x_0, y_0, z_0)$ in an unaberrated field ($\mathbf{r}_{0a} \equiv (x_{0a}, y_{0a}, z_{0a})$ in an aberrated field) where $\mathbf{Q}$ vanish with negative derivatives. Now, a look to Fig. 2 shows that, for evident symmetry reasons, the trapping point, if any, may occur on the optical axis only. Accordingly, in Fig. 3 we report the components $Q_x(x,0,z_0)$, $Q_y(0,y,z_0)$, and $Q_z(0,0,z)$ in the unaberrated field (left panels), as well as the corresponding functions for the aberrated field (right panels), for single spheres with diameter $d = 850$, 1030 and $1660\,$nm. Spheres with so large a diameter were chosen as representative examples of particles to which, according to our experience, the Rayleigh or the Born approximations do not apply. Note that in the right panels of Fig. 3 the origin of the z axis has been shifted by $\Delta F = -4.0\,\mu$m. Even a cursory look shows that all the spheres we considered undergo trapping on the optical axis. In fact, both $Q_x(x,0,z_0)$ and $Q_y(0,y,z_0)$ vanish on the optical axis. Moreover, $Q_z(0,0,z)$ satisfies the trapping condition at least at one value of z. Nevertheless, by examining the contour plot of the aberrated field we realized that that there exist a spot at $z \approx -2\,\mu$m in which the field reaches a second maximum (this spot is outside the lower boundary of Fig. 2). For this reason we calculated the trapping efficiency in the vicinity of this point in order to see whether or not trapping may occur. We found a negative answer, i.e. no trapping occurs either for a $d = 850\,$nm sphere or for spheres of larger diameter. Nevertheless, a weak trapping, i.e. the vanishing of Q_z with a small negative derivative, may occur for spheres of smaller diameter. As a result, we are led to conclude that the only stable trapping point is the one that appears in the right panels of Fig. 3. The values of

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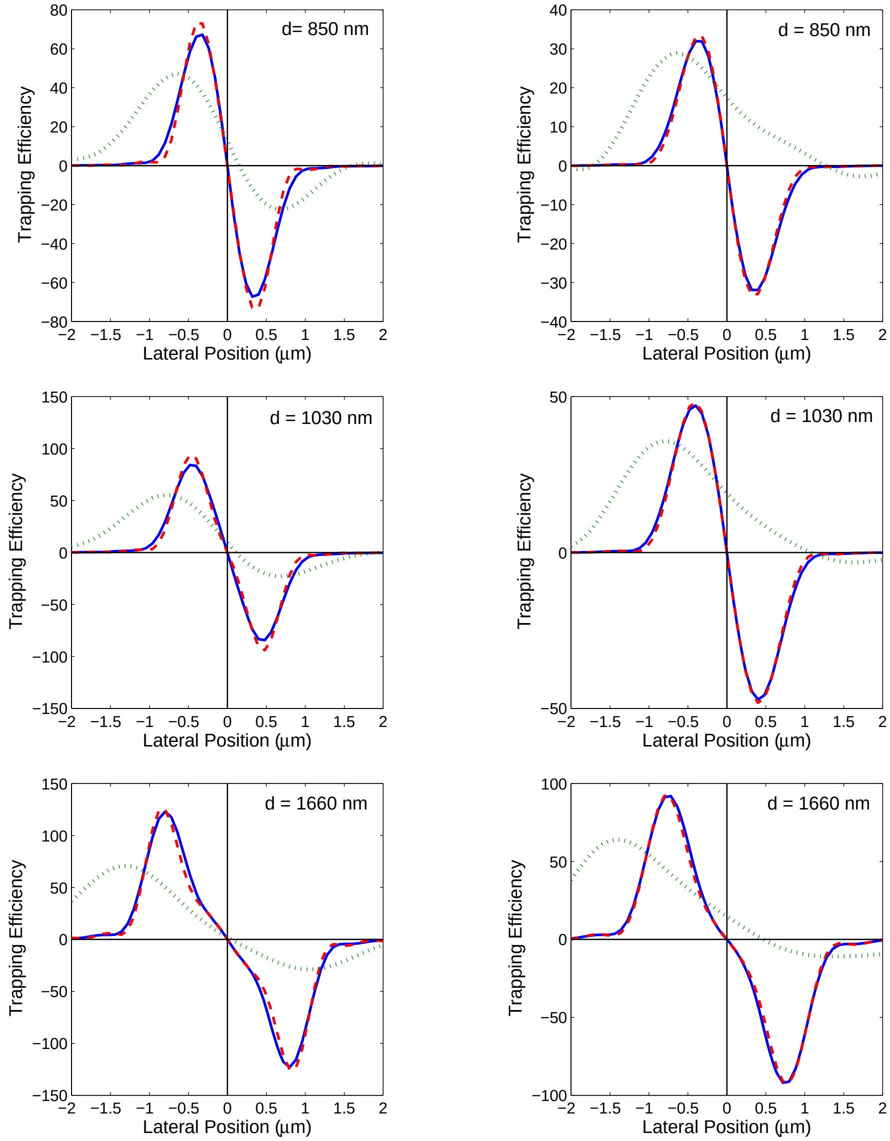

Fig. 3. $Q_x(x,0,z_0)$ (blue solid line), $Q_y(0,y,z_0)$ (red dashed line), and $Q_z(0,0,z)$ (green dotted line) for single spheres with diameter $d = 850$, 1030 and 1660 nm as a function of the position of their centers. Trapping both in unaberrated (left panels) and in aberrated beam (right panels) is considered. Note that the origin of the z axis in the right panels is shifted by $\Delta F = -4.0\,\mu$m.

Table 1. Calculated and experimental values of $s_l = 1 - \kappa_x/\kappa_y$ as well as the trapping position for the spheres we deal with in this paper

d (nm)	z_0 (nm)	s_l calc.	$z_{0\mathrm{a}}$ (nm)	$s_{l\mathrm{a}}$ calc.	s_l exp.	$s_{l\mathrm{a}}$ exp.
220	120	0.38	800	0.19	0.38	
530	200	0.27	1280	0.16	0.31	
690	240	0.11	1520	0.09	0.08	
850	120	−0.07	1200	0.05	0.03	
1030	80	−0.13	1040	−0.01	−0.12	
1280	0	−0.02	480	−0.30		−0.33
1500	40	0.20	560	−0.20		−0.18
1660	40	0.02	400	−0.10	−0.10	
1900	160	0.06	480	0.12		0.08

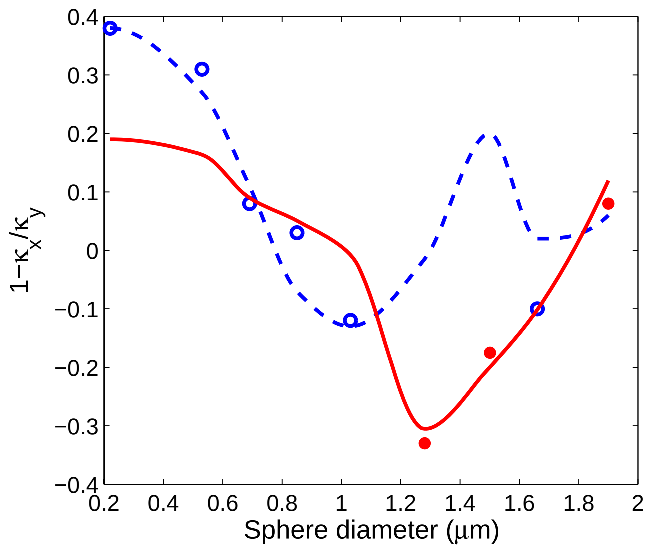

Fig. 4. Comparison of calculated asymmetry factors s_l (dashed blue line) and $s_{l\mathrm{a}}$ (solid red line) with experimental data of Rohrbach [8] (blue circles) and of Zakharian et al. [7] (red dots).

z at which the trapping occurs are reported both for unaberrated (z_0) and for the aberrated field ($z_{0\mathrm{a}}$) in Table 1.

Since the behaviour of the components of the trapping efficiency is almost linear in the vicinity of the trapping point, one is able to define the stiffness of the optical trap by introducing the constants κ_x, κ_y, and κ_z such that the components of the radiation force can be written as

$$F_x = -\kappa_x x, \quad F_y = -\kappa_y y, \quad F_z = -\kappa_z z$$

in the neighbourhood of the point where they vanish. A good parameter to be compared with the experimental data is the so-called stiffness asymmetry factor $s_l = 1 - \kappa_x/\kappa_y$ that we report in Table 1 both for the gaussian field (s_l) and for the aberrated field ($s_{l\mathrm{a}}$). The experimental values of the asymmetry factor were taken from the paper of Rohrbach [8] for the unaberrated field and from the paper of Zakharian et al. [7] for the aberrated field. We note that the size parameter $x = \pi nd/\lambda_0$ for the spheres considered in Table 1 goes from 0.6 to 5.61 in vacuo, i.e., from 0.80 to 7.46 in water, so that we had to use up to $l_{\mathrm{M}} = 12$ to get full convergence of all the calculated values [16]. Table 1 seems to show a fair agreement between theory and experiment. This agreement seems confirmed by Fig. 4, where we report the curves of the asymmetry factor calculated both for unaberrated and for the aberrated field, together with the experimental values for the spheres used by Rohrbach (circles) and by Zakharian et al. (dots). Nevertheless, we call the attention on the values of the asymmetry parameters for the spheres with $d = 850$ and 1660 nm. Actually these values are favourably located on at least one of the two theoretical curves we draw in Fig. 4. We stress, however, that Rohrbach declares the experimental values at $d = 850$ and 1660 nm as obtained in the absence of aberration [8], whereas in Fig. 4 they appear to be on the curve for the aberrated field. On the other hand, the experimental values for the spheres considered by Zakharian et al. appear very close to the curve for the aberrated field, according to what is declared in Ref. [7]. In this respect, it may be interesting to notice that the experimental values mentioned above are not located on the calculated curve that Zakharian et al. report in Fig. 12 of their paper [7]. This discrepancy, in our opinion, may be due to an inadequate consideration of the effect of aberration, and/or to the fact that with so large a diameter any approximation used to calculate the Lorenz force density does not apply. Moreover, the diameter of these spheres is larger than the size of the trap, that, according to Fig. 2, spans $\approx \lambda = 800$ nm according to Fig. 2, so that great care must be exercized both in computations and in the interpretation of the experimental data when dealing with such large objects.

4.2. *Binary clusters*

We now present our results for the trapping of binary clusters as an example of application of our formalism to nonspherical particles. The clusters are composed of two identical, mutually contacting spheres of latex with refractive index $n_{\mathrm{p}} = 1.57$ and diameter $d = 220$ nm. The frame Σ' attached to the cluster has its origin at the center of mass of the aggregate. In Fig. 5 we report our results for the trapping efficiency both in an unaberrated gaussian field (left panels) and in an aberrated one (right panels), for orientation of the axis of the cluster along the *x*, *y*, and *z* axis.

Table 2. Calculated values of $s_l = 1 - \kappa_x/\kappa_y$ for the unaberrated field and of $s_{l\mathrm{a}}$ for the aberrated field as well as the trapping position for the binary cluster we deal with in this paper

Cluster axis parallel to	z_0 (nm)	s_l	$z_{0\mathrm{a}}$ (nm)	$s_{l\mathrm{a}}$
x axis	240	0.46	1280	0.27
y axis	160	0.21	1200	0.09
z axis	40	0.42	160	0.26

The size we chose for the component spheres ensures that the whole cluster is contained within the trap, even when the axis of the aggregate is orthogonal to the optical axis. The trapping position both in unaberrated (z_0) and in aberrated field ($z_{0\mathrm{a}}$) and the corresponding calculated values of s_l and of $s_{l\mathrm{a}}$ are reported in Table 2. We immediately notice that the trapping position depends on the orientation of the cluster. The largest value of z_0 and of $z_{0\mathrm{a}}$ are achieved when the axis of the aggregate is parallel to the direction of polarization of the incident field,

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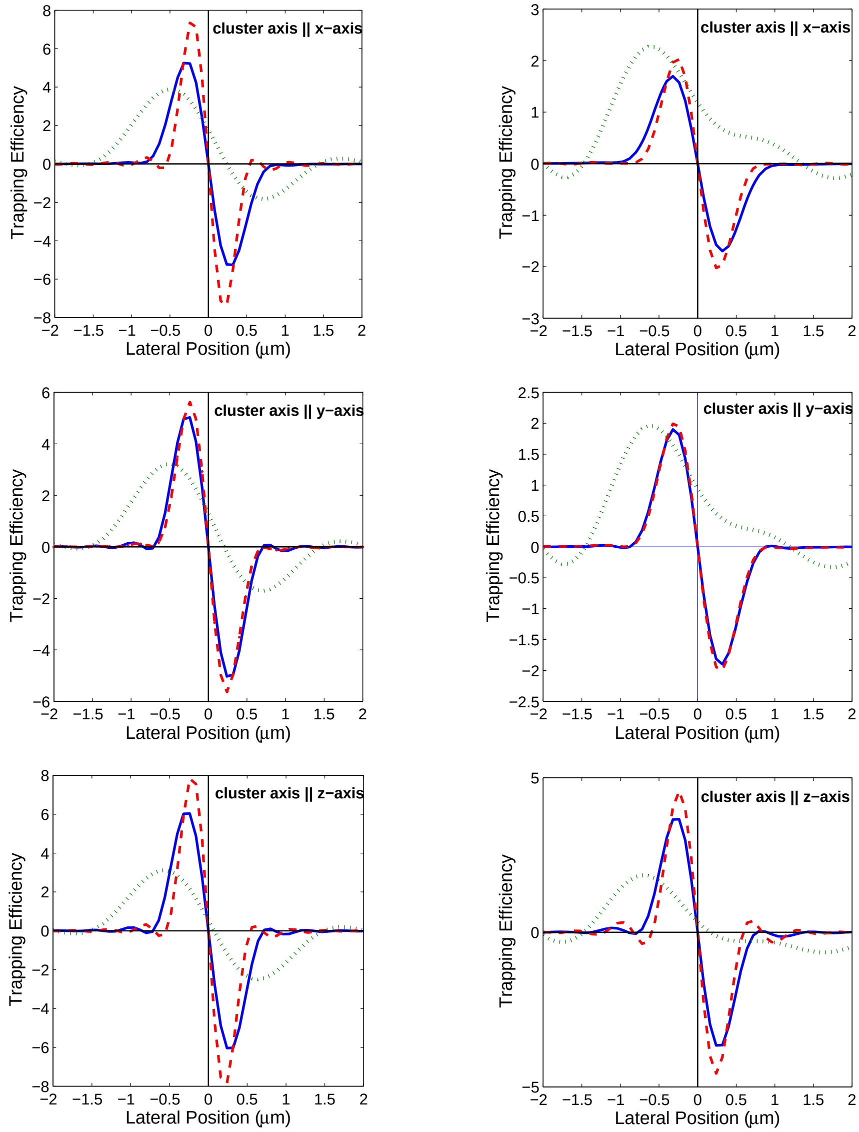

Fig. 5. $Q_x(x,0,z_0)$ (blue solid line), $Q_y(0,y,z_0)$ (red dashed line), and $Q_z(0,0,z)$ (green dotted line) for binary aggregates of latex with diameter $d = 220\,\mathrm{nm}$, as a function of the position of the contacting point. Trapping both in an unaberrated field (left panels) and in an aberrated field (right panels) is considered. In the right panels the origin of the z axis is shifted by $\Delta F = -4.0\,\mu\mathrm{m}$.

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which, we recall, is polarized along the x axis. In turn, the minimum value both of z_0 and of z_{0a} is achieved when the axis is parallel to the optical axis. This result is in substantial agreement with the results of Simpson and Hanna [11] for prolate sferoids.

Appendix A

As anticipated in Sect. 2, with the help of the asymptotic multipole expansions it is easily proved that the dyadic terms

$$\hat{\mathbf{r}}'\cdot\left[n^2(\mathbf{E}'\otimes\mathbf{E}'^*)+(\mathbf{B}'\otimes\mathbf{B}'^*)\right]=n^2\left(\hat{\mathbf{r}}'\cdot\mathbf{E}'\right)\mathbf{E}'+\left(\hat{\mathbf{r}}'\cdot\mathbf{B}'\right)\mathbf{B}'$$

give a vanishing contribution to the radiation force. In fact, a look to Eqs. (8a) and (8b) shows that the asymptotic multipole expansions of $\mathbf{E}'_{\mathrm{I}}$ and $\mathbf{E}'_{\mathrm{S}}$ contain the transverse harmonics $\mathbf{Z}^{(p)}_{lm}(\hat{\mathbf{r}}')$ which, according to their definition are orthogonal, in the ordinary vector sense, to $\hat{\mathbf{r}}'$. This decrees the vanishing of the contribution of the dyadic terms for whatever form of the incident amplitudes $W^{(p)}_{\mathrm{I}lm}$, even when the latter are substituted by the $\mathscr{W}^{(p)}_{lm}(\mathbf{R}_{O'})$.

Now, we show how it happens that the terms $\mathbf{E}'_{\mathrm{I}}\cdot\mathbf{E}'^*_{\mathrm{I}}$ and $\mathbf{B}'_{\mathrm{I}}\cdot\mathbf{B}'^*_{\mathrm{I}}$ give a vanishing contribution to the radiation force even when the incident field is not a single plane wave but rather a superposition of plane waves with the same magnitude of k but different direction of propagation, i.e., different $\hat{\mathbf{k}}$.

Let us thus assume that the incident electric field is a superposition of plane waves of the kind of Eq. (14). Thus a typical term that would enter Eq. (1) is

$$I_E=\mathrm{Re}\left[r'^2n^2\int_{\Omega'}\mathbf{E}'_{\mathrm{I}}(\hat{\mathbf{k}})\cdot\mathbf{E}'^*_{\mathrm{I}}(\hat{\mathbf{k}}')\hat{\mathbf{r}}'\,\mathrm{d}\Omega'\right]\ ,$$

where, according to Eq. (3), $\mathbf{E}'_{\mathrm{I}}(\hat{\mathbf{k}})=E'_{\mathrm{PW}}(\hat{\mathbf{k}})\hat{\mathbf{u}}_{\hat{\mathbf{k}}}\exp(i\mathbf{k}\cdot\mathbf{r}')=\mathbf{E}'_{\mathrm{PW}}(\hat{\mathbf{k}})\exp(i\mathbf{k}\cdot\mathbf{r}')$. An analogous term I_B comes from $\mathbf{B}_{\mathrm{I}}$. Since r' is large, we can use the asymptotic form of a plane wave [13, 12] so that I_E becomes

$$\begin{aligned}I_E=\mathrm{Re}\Big\{\frac{4\pi n^2}{k^2}\int_{\Omega'}&\mathbf{E}'_{\mathrm{PW}}(\hat{\mathbf{k}})\cdot\mathbf{E}'^*_{\mathrm{PW}}(\hat{\mathbf{k}}')\left[\delta(\hat{\mathbf{k}}+\hat{\mathbf{r}}')\exp(-ikr')-\delta(\hat{\mathbf{k}}-\hat{\mathbf{r}}')\exp(ikr')\right]\\&\times\left[\delta(\hat{\mathbf{k}}'+\hat{\mathbf{r}}')\exp(ikr')-\delta(\hat{\mathbf{k}}'-\hat{\mathbf{r}}')\exp(-ikr')\right]\hat{\mathbf{r}}'\,\mathrm{d}\Omega'\Big\}\ .\end{aligned}$$

Due to the properties of the δ-function, the result of the integration is

$$\begin{aligned}I_E=\mathrm{Re}\Big\{\frac{4\pi n^2}{k^2}&\mathbf{E}'_{\mathrm{PW}}(\hat{\mathbf{k}})\cdot\mathbf{E}'^*_{\mathrm{PW}}(\hat{\mathbf{k}}')\left[-\hat{\mathbf{k}}\delta(\hat{\mathbf{k}}-\hat{\mathbf{k}}')+\hat{\mathbf{k}}'\delta(\hat{\mathbf{k}}-\hat{\mathbf{k}}')\right.\\&\left.+\hat{\mathbf{k}}'\delta(\hat{\mathbf{k}}+\hat{\mathbf{k}}')\exp(2ikr')-\hat{\mathbf{k}}'\delta(\hat{\mathbf{k}}+\hat{\mathbf{k}}')\exp(-2ikr')\right]\Big\}\ .\end{aligned}$$

A quite similar expression, except for the absence of n, is obtained for I_B, so that collecting all the terms we get

$$\begin{aligned}I=&I_E+I_B\\=&\mathrm{Re}\Big\{\frac{4\pi}{k^2}\left[n^2\mathbf{E}'_{\mathrm{PW}}(\hat{\mathbf{k}})\cdot\mathbf{E}'^*_{\mathrm{PW}}(\hat{\mathbf{k}}')+\mathbf{B}'_{\mathrm{PW}}(\hat{\mathbf{k}})\cdot\mathbf{B}'^*_{\mathrm{PW}}(\hat{\mathbf{k}}')\right]\\&\times\hat{\mathbf{k}}'\delta(\hat{\mathbf{k}}+\hat{\mathbf{k}}')\left[\exp(2ikr')-\exp(-2ikr')\right]\Big\}\end{aligned}$$

which is easily seen to vanish, even when $\hat{\mathbf{k}}'=-\hat{\mathbf{k}}$, on account that

$$\mathbf{B}'_{\mathrm{PW}}(\hat{\mathbf{k}})=-in\hat{\mathbf{k}}\times\mathbf{E}'_{\mathrm{PW}}(\hat{\mathbf{k}})\ .$$

Similar conclusions can be easily reached when the lens is aberrated by a plane interface orthogonal to the optical axis separating two media of different refractive indexes.

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