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Calculation of the radiation trapping force for laser tweezers by use of generalized Lorenz–Mie theory. II. On-axis trapping force

James A. Lock

The efficiency of trapping an on-axis spherical particle by use of laser tweezers for a particle size from the Rayleigh limit to the ray optics limit is calculated from generalized Lorenz–Mie light-scattering theory and the localized version of a Gaussian beam that has been truncated and focused by a high-numerical-aperture lens and that possesses spherical aberration as a result of its transmission through the wall of the sample cell. The results are compared with both the experimental trapping efficiency and the theoretical efficiency obtained from use of the localized version of a freely propagating focused Gaussian beam. The predicted trapping efficiency is found to decrease as a function of the depth of the spherical particle in the sample cell owing to an increasing amount of spherical aberration. The decrease in efficiency is also compared with experiment. © 2004 Optical Society of America

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1. Introduction

This paper is the second in a series whose purpose is to demonstrate that generalized Lorenz–Mie theory (GLMT) that uses the localized model of an incident beam provides an accurate and computationally practical way to calculate the radiation trapping force of a tightly focused beam of arbitrary profile incident upon a spherical particle of arbitrary size. In the first paper,[1] a description was given of localized beams of GLMT generalized to arbitrary profile and polarization state for incidence upon a spherical particle whose center lies on the beam axis. This is called the on-axis beam particle geometry. If the coordinate system is oriented such that the beam propagates along the positive z axis, the trapping force possesses only a z component, by symmetry. In this paper the radiation trapping force produced by such a beam is calculated for two different beam profiles and compared with experimental data. One of the beam profiles is theoretically simple but experimentally unrealistic. The other is theoretically more complicated but is a more realistic model of the experimental beam. Previously, wave theory calculations of the trapping force were used if the particle radius was less than ~0.5 μm and ray theory methods were used for particle radii greater than ~5.0 μm. The GLMT wave theory calculation reported here bridges this gap.

The body of this paper is organized as follows: In Section 2, the GLMT formula for the on-axis trapping force is expressed as an infinite series of partial wave contributions. The force depends on both the particle's transverse electric (TE) and transverse magnetic (TM) partial wave scattering amplitudes and the TE and TM partial wave shape coefficients of the incident beam. In Section 3, the formula for the trapping efficiency is obtained for the highly idealized case of a freely propagating Gaussian beam incident upon the particle. The Rayleigh and geometrical optics limits of the scattering efficiency for this beam are obtained and compared with the results derived by previous authors. The on-axis trapping efficiency predicted for this highly idealized beam is also compared with experimental data.[2,3] In Section 4, the formula for the trapping efficiency is obtained for the more experimentally realistic case of a Gaussian beam truncated and focused by a high-numerical-aperture (NA) oil-immersion microscope objective lens. The beam also possesses spherical aberration owing to its being transmitted through the glass wall of the water-filled sample cell. The trapping efficiency of this beam is

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compared both with the experimental data of Refs. 2 and 3 and with the prediction of the idealized focused Gaussian beam of Section 3. Finally, in Section 5 the results are summarized and the final conclusions are presented. The extension of the GLMT formalism to the x, y, and z components of the radiation trapping force for off-axis incidence of a tightly focused beam on a spherical particle, and to the optical torque on such a particle, will be treated separately.

2. On-Axis Radiation Trapping Force on a Spherical Particle

Consider an electromagnetic beam of frequency ω, free-space wavelength λ, free-space wave number $k = 2\pi/\lambda$, field strength E_0, and time dependence $\exp(-i\omega t)$, as in Ref. 1, propagating in a medium of refractive index n and incident upon a sphere of radius a and relative refractive index m with respect to the medium. The center of the particle coincides with the origin of an xyz rectangular coordinate system oriented such that the beam propagates in the positive z direction.

The symmetry axis of the beam is assumed to coincide with the z axis, making the beam's incidence on axis with respect to the particle. The on-axis beam is characterized by the partial wave TM and TE shape coefficients g_l and h_l, respectively, for $1 \leq l < \infty$. The radiation trapping force of such a beam on the particle has been calculated from Maxwell stress tensor[4] and the radiative momentum balance between the particle and the incoming and outgoing fields.[5,6] Both calculations give the same result, though a comparison of the final formulas of different authors is complicated by the fact that those authors use different systems of units[7] and different conventions for associated Legendre polynomials and spherical harmonics[8] and they absorb different multiplicative factors into g_l and h_l. With the intensity vector in SI units taken as

$$\mathbf{I} = (\mathbf{E}^* \times \mathbf{B})/\mu_0, \tag{1}$$

where μ_0 is the permeability of free space, and with associated Legendre polynomials as defined in Ref. 8, the z component of the radiation trapping force of the on-axis beam on the spherical particle is[4–6]

$$F_z = (n/c)(nE_0^2/\mu_0 c)(\pi/n^2k^2)\Sigma, \tag{2}$$

where

$$\Sigma = \sum_{l=1}^{\infty} [l(l+2)/(l+1)](g_l g_{l+1}^* U_l + g_l^* g_{l+1} U_l^* + h_l h_{l+1}^* V_l + h_l^* h_{l+1} V_l^*) + [(2l+1)/l(l+1)] \times (g_l h_l^* W_l + g_l^* h_l W_l^*), \tag{3}$$

with

$$U_l = a_l + a_{l+1}^* - 2a_l a_{l+1}^*, \tag{4a}$$

$$V_l = b_l + b_{l+1}^* - 2b_l b_{l+1}^*, \tag{4b}$$

$$W_l = a_l + b_l^* - 2a_l b_l^*. \tag{4c}$$

The Mie partial wave scattering amplitudes for the spherical particle of relative refractive index m with respect to the exterior medium of index n are[9]

$$a_l = [\Psi_l(X)\Psi_l'(Y) - m\Psi_l'(X)\Psi_l(Y)]/[\zeta_l(X)\Psi_l'(Y) - m\zeta_l'(X)\Psi_l(Y)], \tag{5a}$$

$$b_l = [m\Psi_l(X)\Psi_l'(Y) - \Psi_l'(X)\Psi_l(Y)]/[m\zeta_l(X)\Psi_l'(Y) - \zeta_l'(X)\Psi_l(Y)], \tag{5b}$$

where particle size parameter X is

$$X \equiv nka, \tag{6a}$$

$$Y \equiv mX, \tag{6b}$$

the Riccati–Bessel functions $\Psi_l(z)$ and $\zeta_l(z)$ are

$$\Psi_l(z) \equiv z j_l(z), \tag{7a}$$

$$\zeta_l(z) \equiv z h_l^{(1)}(z), \tag{7b}$$

and $j_l(z)$ and $h_l^{(1)}(z)$ are spherical Bessel and Hankel functions, respectively. From the radiative momentum balance point of view, the first two terms on the right-hand sides of Eqs. (4) are due to the momentum contained in the interference between the scattered fields and the outgoing portion of the beam fields, and the last term is due to the momentum of the scattered fields alone. For on-axis incidence of the beam on a spherical particle, the x and y components of the radiation force are zero, from symmetry. Radiation trapping efficiency Q is defined by

$$F_z \equiv (nP/c)Q, \tag{8}$$

where P is the beam power in the plane containing the center of the particle. For the freely propagating focused Gaussian beam of Section 3 below, this distinction is not important because conservation of energy requires that the power in all planes perpendicular to the z axis be identical. But, for the beam of Section 4 that is truncated and focused by a lens and then transmitted through a plane interface before arriving at the particle, P is the power transmitted through the interface and incident upon the particle, rather than the beam power incident upon the focusing lens.

3. Radiation Trapping by a Freely Propagating Focused Gaussian Beam

A. General Considerations

In this section the incident beam is taken to be the modified localized version of a freely propagating focused on-axis Gaussian beam propagating in the z direction and polarized in the x direction, as discussed in Ref. 1. It is tacitly assumed that this beam is produced by a Gaussian beam incident upon a focusing lens whose aperture is much larger than the beam width. None of the incident beam is cut off by the lens, no diffractive ringing is produced by the edge of the lens aperture, and no account is taken of the focused beam refracting at the surface of the sample cell. The Gaussian beam merely propagates undistorted in a single medium, converging to a focal waist and then reexpanding. The shape coefficients of the modified localized version of this beam are[1,10]

$$g_l = h_l = \exp(-inkz_0)\exp[-s_i^2(l+2)(l-1)/(1-2is_iz_0/w_i)]/(1-2is_iz_0/w_i), \tag{9}$$

where z_0 is the coordinate of the center of the beam's focal waist, with the center of the particle assumed to be at the origin. A negative value of z_0 means that the center of the particle is located past the center of the focal waist in the diverging portion of the beam. The field strength of the beam at the center of the beam's focal waist is E_0, the intended transverse $1/e$ electric field half-width at the center of the focal waist is w_i, and the intended beam confinement parameter is

$$s_i = 1/(nkw_i). \tag{10}$$

Numerical computations reported in Ref. 1 show that the localized beam generated by this set of coefficients has a nearly Gaussian transverse profile at the center of the focal waist, even for tight confinement, but has an actual $1/e$ electric field half-width w_a, where $w_a \gtrsim w_i$. The actual beam confinement parameter is

$$s_a = 1/(nkw_a), \tag{11}$$

and the beam power is approximately

$$P \approx (nE_0^2/\mu_0 c)(\pi w_a^2/2). \tag{12}$$

Substituting Eq. (12) into Eqs. (2) and (8) yields the trapping efficiency for this beam:

$$Q = 2s_a^2\Sigma. \tag{13}$$

For an incident beam directed vertically downward, as is usually the case, the particle is pushed in the direction of beam propagation when Q is positive and is not trapped. The particle is pulled upward by the beam and is trapped when Q is negative and when the radiation force balances gravity and bouyancy forces.

B. Rayleigh Scattering Limit

In the Rayleigh scattering limit the particle is sufficiently small that the beam's amplitude and phase are virtually constant over the particle volume. In this case, the particle acts as if it were in an instantaneously uniform field, and the resultant radiation force has two sources.[11–13] First, the particle acquires an induced electric dipole moment by its presence in the beam's electric field. The beam's electric field then exerts a force, called the gradient force, on the dipole moment that it has just induced. Second, the particle's induced electric dipole moment oscillates as a function of time at frequency ω and emits electric dipole radiation. Because the radiation carries away different amounts of momentum in different directions, the particle recoils in response, to conserve momentum. The effective force that produces the recoil is called the scattering force. The gradient-plus-scattering force on a particle in the Rayleigh limit is straightforwardly derived by electrodynamic methods to be[11–13]

$$\mathbf{F} = (n/c)(nE_0^2/\mu_0 c)(2\pi a^3)[(m^2-1)/(m^2+2)]\nabla(\mathbf{e}^*\cdot\mathbf{e})_{\text{particle}} + (n/c)(nE_0^2/\mu_0 c) \times (8\pi n^4k^4a^6/3)[(m^2-1)/(m^2+2)]^2(\mathbf{e}^*\times\mathbf{b})_{\text{particle}}, \tag{14}$$

where the beam fields have been factored as

$$\mathbf{E} = E_0\mathbf{e}, \tag{15a}$$

$$\mathbf{B} = (nE_0/c)\mathbf{b}. \tag{15b}$$

The first term in Eq. (14) is the gradient force, the second term is the scattering force, and the fields and their gradient are evaluated at the position of the particle.

The fields of a weakly confined on-axis freely propagating focused Gaussian beam with $s \ll 1$ are given analytically by[1]

$$\mathbf{e} = \mathbf{u}_x D\exp[ink(z-z_0)]\exp[-D(x^2+y^2)/w^2], \tag{16a}$$

$$\mathbf{b} = \mathbf{u}_y D\exp[ink(z-z_0)]\exp[-D(x^2+y^2)/w^2], \tag{16b}$$

where

$$D = 1/[1+2is(z-z_0)/w]. \tag{17}$$

The confinement of the beam is assumed to be sufficiently weak that there is no difference between the intended and the actual beam widths. Substituting Eqs. (16) and (17) into Eq. (14) and evaluating the fields and their gradient at the position of the particle yield for the radiation trapping efficiency of Eq. (8)

$$Q = 32X^3s^5[(m^2-1)/(m^2+2)](z_0/w)/(1+4s^2z_0^2/w^2)^2 + (16/3)X^6s^2[(m^2-1)/(m^2+2)]^2/(1+4s^2z_0^2/w^2), \tag{18}$$

where again the first term is due to the gradient force and the second term is due to the scattering force. The gradient force is always directed toward the center of the beam's focal waist. It is positive when $z_0 > 0$ and negative when $z_0 < 0$. The scattering force is always positive (i.e., in the direction of beam propagation) and is largest when the particle is in the strongest part of the beam, thus producing the strongest scattered electric dipole radiation and the strongest recoil. For strong focusing, the calculation of Q by use of Eq. (14) with the Davis–Barton fifth-order fields is complicated by the fact that the relation between $nE_0^2/\mu_0 c$ and P is more involved than for weak focusing [see Eq. (54) of Ref. 1] and that for $s \gtrsim 0.2$

additional terms beyond the fifth order are required for convergence.

In the Rayleigh scattering limit of the trapping force with the GLMT formalism, only the $l = 1$ partial wave contributes to Eq. (3). This can be seen from a comparison of the first few partial wave scattering amplitudes[14]:

$$a_1 = (-2i/3)[(m^2 - 1)/(m^2 + 2)]X^3 - (2i/5) \times [(m^2 - 1)(m^2 - 2)/(m^2 + 2)^2]X^5 + (4/9) \times [(m^2 - 1)/(m^2 + 2)]^2 X^6 + O(iX^7), \quad (19a)$$

$$b_1 = (-i/45)(m^2 - 1)X^5 + O(iX^7), \quad (19b)$$

$$a_2 = (-i/15)[(m^2 - 1)/(2m^2 + 3)]X^5 + O(iX^7), \quad (19c)$$

$$b_2 = O(iX^7). \quad (19d)$$

Amplitudes b_1 and a_2 provide $O(X^5)$ corrections to the imaginary part of a_1 and are thus ignored. The real part of a_1, which is $O(X^6)$, must be retained because of energy conservation among the incoming beam field, the outgoing beam field, and the $O(X^3)$ scattered field as expressed through the optical theorem.[15] Equation (3) then becomes

$$\Sigma = (3/2)(g_1 g_2{}^* a_1 + g_1{}^* g_2 a_1{}^* + g_1 h_1{}^* a_1 + g_1{}^* h_1 a_1{}^*). \quad (20)$$

Substitution of a_1 from Eq. (19a) and g_1, h_1, and g_2 for the localized version of the freely propagating Gaussian beam from Eq. (9) into Eq. (20) gives

$$\Sigma = X^3[(m^2 - 1)/(m^2 + 2)]\{2K \sin(\Theta) + (4/3)X^3[(m^2 - 1)/(m^2 + 2)][1 + K \cos(\Theta)]\}/(1 + 4s^2 z_0{}^2/w^2), \quad (21)$$

where

$$K \equiv \exp[-4s^2/(1 + 4s^2 z_0{}^2/w^2)], \quad (22)$$

$$\Theta \equiv 8s^3(z_0/w)/(1 + 4s^2 z_0{}^2/w^2). \quad (23)$$

In the $s \rightarrow 0$ weak-beam confinement limit, one has $K \approx 1$, $\cos(\Theta) \approx 1$, and $\sin(\Theta) \approx \Theta$. As a result, Eq. (21) becomes

$$\Sigma = 16s^3X^3[(m^2 - 1)/(m^2 + 2)](z_0/w)/(1 + 4s^2 z_0{}^2/w^2)^2 + (8/3)X^6[(m^2 - 1)/(m^2 + 2)]^2 /(1 + 4s^2 z_0{}^2/w^2). \quad (24)$$

Equation (24) for the gradient-plus-scattering force derived from GLMT with the localized version of a Gaussian beam and substituted into Eq. (13) then agrees with Eq. (18) derived from standard electrodynamic methods and the analytical formula for a mildly focused Gaussian beam. The gradient force arises from the imaginary part of a_1 in Eq. (20), and the scattering force arises from the real part. This agreement between the two methods of calculation demonstrates the validity of the GLMT formula with the localized version of the incident beam in the Rayleigh scattering and weak-beam confinement limits.

C. Geometrical Ray Scattering Limit

The calculation of the momentum transfer imparted to the particle from the incoming beam in the ray theory treatments of Refs. 16–18 differs from that of GLMT in the following ways: First, ray theory assumes that the incident beam is completely removed by the scattering process and is replaced by the externally reflected light, the transmitted light, and the light transmitted following all numbers of internal reflections. Second, the intensity of these scattering processes is added incoherently, rather than coherently, when one is obtaining the momentum transfer to the particle. In GLMT, however, the outgoing portion of the beam in the absence of the particle is retained, the scattering processes also include diffraction, they are added coherently, and interference of the different scattering processes with one another and with the outgoing portion of the beam are taken into account. Obtaining an exact comparison with wave theory in the small-wavelength limit requires coherent addition.[19,20] But under a number of circumstances unrelated to laser tweezers, such as integration over a polydispersion of particle sizes for scattering by cloud particles, fog particles, or a spray from a nozzle, incoherent addition can provide a reasonable approximation to the coherent sum.[21]

To compare GLMT with the ray theory results of Ref. 17 for a tightly focused Gaussian beam incident upon a large spherical particle, the trapping efficiency of Eqs. (3) and (13) was numerically computed for the modified localized version of a freely propagating focused Gaussian beam with $\lambda = 0.488$ μm, $n = 1.33$, $m = 1.2$, $a = 5.0$ μm, and $w_a = 0.20$ μm. From the beam reconstruction procedure described in Ref. 1 it was found that an intended width of the modified localized beam of $w_i = 0.172$ μm produced an actual $1/e^2$ intensity half-width at the center of the focal waist of $w_a = 0.20$ μm. The length of the focal waist of this beam is ~0.68 μm, which is only ~7% of the particle diameter. I calculated the minimum trapping efficiency from Eq. (13) for the incident Gaussian beam by keeping the particle position fixed at the origin and by varying z_0 moved the beam past the particle. For the ray theory calculation summarized in Fig. 2 of Ref. 17 the trapping efficiency is negative for -10.5 μm $\lesssim z_0 \lesssim -5.6$ μm and reaches a minimum value (corresponding to the strongest trapping) of $Q^{\min} \approx -0.023$ when the center of the beam's focal waist is located at $z_0{}^{\max} \approx -7.2$ μm, approximately half a radius outside the particle surface. In comparison, the GLMT calculation from Eqs. (3) and (13) gives a negative trapping efficiency for -8.5 μm $\lesssim z_0 \lesssim -2.3$ μm, and it reaches a minimum value of $Q^{\min} = -0.02626$ at $z_0 = -5.21$ μm, just outside the particle surface.

The difference between the results of GLMT and of the ray treatments decreases when the beam that is incident upon the particle is less tightly focused. For example, when $w_a = 0.30$ μm the ray calculation

Table 1. Contribution to Minimum Radiation Trapping Efficiency Q^{min} of External Reflection (ER), Transmission (T), and Transmission Followed by $p - 1$ Internal Reflections (IR^{p-1}) for the Localized Version of a Focused Gaussian Beam with $\lambda = 0.488$ μm, $n = 1.33$, $m = 1.2$, $a = 5.0$ μm, $w_i = 0.172$ μm, $w_a = 0.200$ μm, and $z_0^{max} = -5.21$ μm

Process	Contribution to Q^{min}	Coherent Sum
ER	+0.6589	+0.6589
T	−0.6863	−0.02888
IR^1	+0.00211	−0.02657
IR^2	+0.00010	−0.02607
IR^3	+0.00024	−0.02603
IR^4	+0.00033	−0.02605
IR^5	−0.00010	−0.02621
IR^{∞}		−0.02626

of Fig. 2 of Ref. 17 shows that the beam just barely fails to trap the particle, and the efficiency reaches a minimum value of $Q^{min} \approx +0.001$ at $z_0^{max} \approx -8.8$ μm. The GLMT calculation that uses a modified localized beam with $w_i = 0.284$ μm corresponding to $w_a = 0.30$ μm gives qualitatively similar results but with a slightly less positive trapping efficiency for all z_0. This causes a small region of very weak trapping, with the efficiency reaching a minimum value of $Q^{min} \approx -0.00045$ at $z_0^{max} \approx -7.47$ μm. Comparison of ray theory and GLMT yields a result that is closer still when $w_a = 0.40$ μm. The ray calculation of Fig. 2 of Ref. 17 gives $Q^{min} \approx +0.012$ at $z_0^{max} \approx -10.0$ μm, whereas the GLMT calculation that uses a modified localized beam with $w_i = 0.388$ μm that corresponds to $w_a = 0.40$ μm gives $Q^{min} \approx +0.01170$ at $z_0^{max} \approx -9.26$ μm.

The values of Q^{min} for ray theory and GLMT for each of the three beam cases examined above are surprisingly similar in light of the fact that ray theory (i) uses Eqs. (16), which are appropriate to a moderately focused beam but not to a tightly focused beam; (ii) adds the various scattered intensities incoherently and omits the momentum transfer that is due to the interference between the scattering processes; and (iii) is applied to a sphere of size parameter $X = 85.6$, which is below the region of quantitative validity of geometrical optics.[19,20] The difference between the ray theory and GLMT predictions for z_0^{max} is larger than for Q^{min}, indicating that z_0^{max} is much more sensitive to the scattering model used than is Q^{min}. The same result will be found in Subsection 4(b) below for the more experimentally realistic beam as well.

To determine the relative importance to trapping of external reflection plus diffraction, transmission, and transmission following $p - 1$ internal reflections, a Debye series expansion[22] of a_l and b_l in Eqs. (5) was undertaken, and the trapping efficiency was computed for the modified localized version of a freely propagating focused Gaussian beam with the same parameters as used above, $\lambda = 0.488$ μm, $n = 1.33$, $m = 1.2$, $a = 5.0$ μm, $w_i = 0.172$ μm, and $w_a = 0.2$ μm for a number of combinations of scattering processes. The results are listed in Table 1. The first column lists the scattering process and the second column gives the trapping efficiency at $z_0^{max} = -5.21$ μm if this process alone were occurring. The third column gives the trapping efficiency at $z_0 = -5.21$ μm that is due to the coherent sum of all the scattering processes from the top of the table to the term under consideration. The number in column 3 corresponding to IR (super infinity) is the total GLMT result reported above. As expected, external reflection and diffraction strongly push the particle away from the center of the focal waist, whereas transmission strongly pulls the particle back toward the center of the focal waist. These two large opposing effects cancel to within 4% in this case, producing the trapping. For the beam and particle parameters used here, the portion of the scattered light that comprises all the numbers of internal reflections before the light exits the particle contributes only ~10% to the trapping force. This is because of the small magnitude of the individual contributions and because the interference of these processes with the dominant external reflection-plus-transmission contribution is sometimes constructive and sometimes destructive.

D. Comparison with Experiment

The minimum value of trapping efficiency Q^{min} was calculated from Eqs. (3) and (13) for a modified localized freely propagating focused Gaussian beam for $\lambda = 1.06$ μm, $n = 1.33$, and $m = 1.57/1.33 = 1.18$, corresponding to polystyrene latex (PSL) spheres in water illuminated by a Nd:YAG laser. The sphere radius was taken to be in the range 0.25 μm $\le a \le$ 10.25 μm, spanning the region from just above the Rayleigh scattering limit to just below the geometrical optics limit. The actual $1/e$ beam waist was taken to be $w_a = 0.390$ μm for comparison with the experimental results of Table 2 of Ref. 2, where the particle was trapped against the top surface of the sample cell such that aberration of the beam on transmission into the sample cell was minimal. It was found by numerical computation that an intended width at the center of the focal waist of $w_i = 0.319$ μm produced an actual $1/e^2$ intensity half-width of $w_a = 0.390$ μm. The computed minimum trapping efficiency, the position of the center of the beam's focal waist for which it occurs, and the experimental value of Q^{min} from Ref. 2 are shown in Table 2. As suggested in Ref. 2, the GLMT results verify that the trapping force becomes independent of particle radius as the particle size approaches the geometric optics regime. But the approach is not monotonic. The greatest magnitude of the trapping efficiency occurs when the center of the beam's focal waist lies approximately on the particle surface. The exact physical mechanism that is responsible for this is not clear, but the behavior of Q^{min} is found to be nearly identical for the more experimentally realistic beam of Section 4 below. Table 2 illustrates that, over the entire particle size region examined, the calculated Gaussian beam GLMT trapping efficiency for this set of beam and particle parameters is approximately a factor of 2–3 below the experimental efficiency. Similar theoretical results were found for

Table 2. Minimum Value of Radiation Trapping Efficiency Q^{min} As a Function of Particle Radius a for the Localized Version of a Focused Gaussian Beam with $\lambda = 1.06$ μm, $n = 1.33$, $m = 1.18$, and $w_a = 0.390$ μm Incident upon the Particle[a]

a (μm)	$Q_{exp}^{min\ b}$	$Q^{min\ c}$	z_0^{max} (μm)	$\lvert z_0^{max}/a \rvert$
0.25		−0.0154	−0.38	1.52
0.50		−0.0364	−0.53	1.06
1.00		−0.0450	−1.05	1.05
2.504	−0.070 ± 0.015	−0.0400	−2.42	0.97
4.935	−0.077 ± 0.014	−0.0345	−4.60	0.93
7.500	−0.091 ± 0.015	−0.0346	−7.06	0.94
10.245	−0.100 ± 0.018	−0.0349	−9.51	0.93

[a]Position z_0^{max} is the location of the center of the focused Gaussian beam waist that corresponds to minimum trapping efficiency.
[b]Ref. 2.
[c]Eq. (13).

the more-realistic beam and are reported in more detail in Section 4.

The radiation trapping force was also computed for the freely propagating modified localized beam and a different refractive-index particle, i.e., $\lambda = 1.06$ μm, $n = 1.33$, $m = 1.45/1.33 = 1.09$, $a = 0.50$ μm, and $w_a = 0.390$ μm as in Table 1 of Ref. 2 For this case the authors of Ref. 2 had determined that GLMT that used a Davis–Barton fifth-order beam[23] rather than the modified localized beam of Eq. (9) gave $Q^{min} = -0.034$. Equations (3) and (13) with the modified localized beam gave $Q^{min} = -0.0331$, in good agreement with the Davis–Barton calculation of Ref. 2. This agreement provides another check of the validity of the GLMT formalism that used localized beams. But, although the two wave theory calculations agree, the experimental minimum efficiency in Table 1 of Ref. 2, with the particle again trapped against the top surface of the sample cell, is $Q^{min} = -0.006 \pm 0.001$. The calculated result for this case is more than a factor of 5.5 larger than the experimental result, whereas it was a factor of 2–3 below the experimental result cited in the previous paragraph for the larger particles with $m = 1.18$. As an aside, by using the more realistic beam of Section 4 with the current set of particle and beam parameters, one obtains $Q^{min} = -0.0277$, which is a factor of 4.6 larger than the experimental result. A comparison of the theoretical and experimental values of Q^{min} with the Rayleigh scattering prediction of Eq. (18) for this set of parameters is not appropriate because the beam under consideration is tightly focused whereas Eq. (18) assumes weak confinement, and the particle size parameter is $X = 3.9$, which is above the Rayleigh regime.

4. Radiation Trapping by a Gaussian Beam Truncated and Focused by a Lens and Transmitted through a Plane Interface

A. General Considerations

A freely propagating focused Gaussian beam is a relatively poor approximation to the actual experimental beam incident upon the particle. A better candidate beam[24–27] is both truncated and focused by a high-NA oil-immersion microscope objective lens of refractive index n_1. It also possesses spherical aberration owing to its transmission through the wall of the sample cell, e.g., a microscope coverslip also of index n_1, into the cell itself, which has index n_2. The localized version of a plane wave truncated and focused by a lens and transmitted through the interface was described and tested in the research reported in Ref. 1. Here, we consider a Gaussian beam of field strength E_0, electric field half-width W, and flat phase fronts polarized in the x direction and incident onto a lens of aperture radius A and focal length F. The beam overfills the focusing lens such that $W > A$. The center of the particle is still located at the origin of coordinates, the coordinate of the focal point of the lens in the absence of the interface is z_0, and the coordinate of the flat interface is d, where $d < z_0$. Using the method of Ref. 1 yields the following shape coefficients of the beam transmitted through the flat interface:

$$\begin{aligned} g_l = -in_1kF \int_0^\alpha & \sin(\theta_1)d\theta_1[\cos(\theta_1)]^{1/2} \\ & \times \exp\{i[n_2k\cos(\theta_2)(z-d) - n_1k\cos(\theta_1) \\ & \times (z_0-d)]\}(1/2)\exp[-(A/W)^2\tan^2(\theta_1)/\tan^2(\alpha)] \\ & \times \{[t_{TE} + t_{TM}\cos(\theta_2)]J_0[(n_1/n_2) \\ & \times (l+1/2)\sin(\theta_1)] + [t_{TE} - t_{TM}\cos(\theta_2)] \\ & \times J_2[(n_1/n_2)(l+1/2)\sin(\theta_1)]\}, \end{aligned} \tag{25a}$$

$$\begin{aligned} h_l = -in_1kF \int_0^\alpha & \sin(\theta_1)d\theta_1[\cos(\theta_1)]^{1/2} \\ & \times \exp\{i[n_2k\cos(\theta_2)(z-d) - n_1k\cos(\theta_1) \\ & \times (z_0-d)]\}(1/2)\exp[-(A/W)^2\tan^2(\theta_1)/\tan^2(\alpha)] \\ & \times \{[t_{TM} + t_{TE}\cos(\theta_2)]J_0[(n_1/n_2)(l+1/2)\sin(\theta_1)] \\ & + [t_{TM} - t_{TE}\cos(\theta_2)]J_2[(n_1/n_2) \\ & \times (l+1/2)\sin(\theta_1)]\}. \end{aligned} \tag{25b}$$

The NA of the lens is

$$NA = n_1 \sin(\alpha); \tag{26}$$

angle θ_1 in the medium of refractive index n_1 and angle θ_2 in the medium of refractive index n_2 are related by Snell's law:

$$n_1 \sin(\theta_1) = n_2 \sin(\theta_2); \tag{27}$$

J_0 and J_2 are Bessel functions; and the Fresnel electric field transmission coefficients are

$$t_{TE} = 2\cos(\theta_1)/[\cos(\theta_1) + (n_2/n_1)\cos(\theta_2)], \tag{28a}$$

$$t_{TM} = 2\cos(\theta_1)/[(n_2/n_1)\cos(\theta_1) + \cos(\theta_2)]. \tag{28b}$$

The beam shape coefficients of the beam while it is still in medium n_1 are given by[1,28,29] Eqs. (25), with $d = 0$, $n_2 = n_1$, and $\theta_2 = \theta_1$.

An important distinction in notation between a freely propagating focused Gaussian beam and a beam truncated and focused by a lens is that in the first case E_0 is the electric field strength at the center of the beam's focal waist whereas in the second case E_0 is the maximum field strength of the beam incident upon the lens. As derived in Ref. 1, if a plane wave were incident upon an oil-immersion lens of refractive index n_1, the power in the focal plane in medium n_1 would be

$$P \approx (n_1 E_0{}^2/\mu_0 c)\pi F^2 \sin^2(\alpha). \tag{29}$$

If a Gaussian beam of half-width W is incident upon the lens, the power in the focal plane in medium n_1 is obtained in a similar way by Taylor series expanding the Gaussian function, integrating[30] the fields over θ_1, and then integrating[31] the resultant intensity over the xy plane. The result is relation (29), multiplied by the factor

$$\begin{aligned} G(\alpha) = 1 &- (A/W)^2 \cos^2(\alpha) \\ &- (2/3)(A/W)^2 \sin^2(\alpha)\cos^2(\alpha) \\ &+ (2/3)(A/W)^4 \cos^4(\alpha) + \ldots . \end{aligned} \tag{30}$$

Equation (30) is rapidly convergent as long as $W \gtrsim A$, which is always the case when the incident beam overfills the microscope objective lens. Fraction T_{12} of this power transmitted from medium n_1 to medium n_2 at the flat surface of the sample cell is modeled in ray theory by

$$\begin{aligned} T_{12} = (n_2/2n_1) &\int_0^\alpha \sin(\theta_1)\mathrm{d}\theta_1 \cos(\theta_2)(t_{\mathrm{TE}}{}^2 + t_{\mathrm{TM}}{}^2) \\ &\times \exp[-2(A/W)^2\tan^2(\theta_1)/\tan^2(\alpha)] \\ &\Big/ \int_0^\alpha \sin(\theta_1)\mathrm{d}\theta_1 \cos(\theta_1) \\ &\times \exp[-2(A/W)^2\tan^2(\theta_1)/\tan^2(\alpha)]. \end{aligned} \tag{31}$$

The trapping efficiency of Eqs. (2) and (8) is then given by

$$Q = \Sigma/[n_1 n_2 k^2 F^2 \sin^2(\alpha) G(\alpha) T_{12}]. \tag{32}$$

This result is independent of focal length F because Σ in Eq. (3) is proportional to the product of two beam shape coefficients, and each coefficient in Eqs. (25) is proportional to F. The only lens parameters required for the calculation of Q are α and the ratio W/A. If lens aperture size A is known, the focal length is

$$F = A \tan(\alpha). \tag{33}$$

B. Comparison with Experiment

First, as a consistency check of the localized model of the truncated and focused beam, the transverse $1/e^2$ half-width w_a of the beam intensity in medium n_1 at the center of the focal waist was computed for $n_1 = 1.5$, $\lambda = 1.06$ μm, and $W/A = 1.5$ and was compared with the experimentally measured $1/e^2$ beam intensity half-width in Table 1 of Ref. 2. The sum over partial waves in the reconstructed localized beam was numerically evaluated as described in Ref. 1. The experimental results reported in Ref. 2 are $w_a = 0.39, 0.54, 0.53, 0.61$ μm (all ± 0.03 μm) for $\alpha = 60.0°$, 56.4°, 41.8°, 32.2°. The GLMT calculated widths are $w_a = 0.395, 0.403, 0.49, 0.60$ μm for the same angles α. Except for $\alpha = 56.4°$, the beam width computed from the localized approximation is in good agreement with the measured width. In addition, the GLMT localized beam width was found to depend only weakly on W as long as $W \gtrsim A$; again, inasmuch as the incident Gaussian beam overfills the microscope objective in experiments, this is always the case.

Table 3. Minimum Value of Radiation Trapping Efficiency $Q^{\min}$ As a Function of Particle Radius a for a Gaussian Beam Truncated and Focused by a Lens and Transmitted through a Flat Interface with λ = 1.06 μm, w_a = 0.390 μm, W/A = 1.5, α = 60°, n_1 = 1.5, n_2 = 1.33, and m = 1.18 Incident upon the Particle[a]

a (μm)	$Q_{\exp}{}^{\min\, b}$	$Q^{\min\, c}$	$z_0{}^{\mathrm{SA}}$ (μm)	$\lvert z_0{}^{\mathrm{SA}}/a\rvert$
0.25		−0.0099	−0.77	3.08
0.50		−0.0356	−0.59	1.18
1.00		−0.0406	−0.75	0.75
2.504	−0.070 ± 0.015	−0.0333	−1.65	0.66
4.935	−0.077 ± 0.014	−0.0246	−3.36	0.68
7.500	−0.091 ± 0.015	−0.0283	−5.17	0.69
10.245	−0.100 ± 0.018	−0.0287	−6.76	0.66

[a]Position $z_0{}^{\mathrm{SA}}$ is the location of the spherical aberration's principal diffraction maximum that corresponds to the minimum trapping efficiency.
[b]Ref. 2.
[c]Eq. (32).

Next, the trapping efficiency of Eq. (32) was computed for a Gaussian beam with $\lambda = 1.06$ μm incident upon and focused by a lens with $W/A = 1.5$, $\alpha = 60°$, and $n_1 = 1.5$, transmitted through a flat interface with medium $n_2 = 1.33$ on the other side, and finally incident upon a homogeneous spherical particle in medium n_2 with $m = 1.18$ and radius in the range 0.25 μm $\leq a \leq 10.245$ μm. The particle is assumed to be resting against the interface (i.e., the top surface of the sample cell) such that $d = -a$. Again, I found the minimum trapping efficiency by keeping the particle fixed at the origin and moving the beam past the particle by varying z_0. The upper limit of the sum over partial waves in Eq. (3) was taken to be the same as in a tradional Mie scattering program,[1] Bessel function J_0 was computed as in Ref. 32, and Bessel function J_2 was computed either by a Taylor series expansion or an asymptotic expansion, depending on the value of the argument.[33] The resultant value of $Q^{\min}$ is given in Table 3, along with the position of the spherical aberration's principal diffraction maximum on the z axis, $z_0{}^{\mathrm{SA}}$, for which $Q^{\min}$ occurs. This principal diffraction maximum is the first and strongest of a sequence of diffraction maxima on the z axis and is the aberrated remnant of the center of the beam's focal waist. The sequence of maxima is accompa-

Table 4. Minimum Value of Radiation Trapping Efficiency Q^{min} As a Function of Interface Position d for a Gaussian Beam Truncated and Focused by a Lens and Transmitted through a Flat Interface with $\lambda = 1.06$ μm, $W/A = 1.5$, $\alpha = 60°$, $n_1 = 1.5$, $n_2 = 1.33$, $m = 1.18$, and $a = 4.935$ μm[a]

d (μm)	Q_{exp}^{min} [b]	Ratio	Q^{min} [c]	Ratio	z_0^{SA} (μm)	$\lvert z_0^{SA}/a \rvert$
−4.935	−0.077 ± 0.014	1.000	−0.0246	1.000	−3.36	0.68
−10.0	−0.059 ± 0.011	0.766	−0.0196	0.797	−3.57	0.72
−15.0	−0.050 ± 0.010	0.649	−0.0161	0.654	−3.72	0.75
−20.0	−0.047 ± 0.009	0.610	−0.0133	0.541	−3.76	0.76
−25.0	−0.042 ± 0.008	0.545	−0.0111	0.451	−3.77	0.76
−30.0			−0.0093	0.378	−3.85	0.78
−35.0	−0.034 ± 0.007	0.441	−0.0078	0.317	−3.96	0.80
−40.0			−0.0065	0.264	−4.00	0.81
−50.0			−0.0044	0.179	−3.98	0.81
−60.0			−0.0027	0.110	−4.02	0.81
−70.0			−0.0014	0.057	−4.25	0.86
−80.0			−0.0003	0.012	−4.26	0.86
−90.0			+0.0007		−4.17	0.84
−100.0			+0.0014		−4.38	0.89

[a] Position z_0^{SA} is the location of the spherical aberration's principal diffraction maximum that corresponds to the minimum trapping efficiency. The two columns labeled Ratio are the ratio of the trapping efficiency of the previous column divided by the corresponding trapping efficiency at $d = -4.935$ μm.
[b] Ref. 2.
[c] Eq. (32).

nied by a series of spherical aberration diffraction rings about the z axis inside the so-called caustic horn in the short-wavelength limit. A cross section through this spherical aberration diffraction structure is shown in Fig. 9.3 of Ref. 34, in Figs. 3(a)–3(e) of Ref. 35, and in Ref. 36. I calculated position z_0^{SA} in Table 3 by using the beam reconstruction method of Ref. 1 and varying z_0 and d in concert. For $a = 0.25$ μm and $a = 0.50$ μm, z_0^{SA} turns out to be the position of the unaberrated center of the beam's focal waist because, for these two particle sizes, the beam focuses in the n_1 material before arriving at the surface of the sample cell.

Perhaps the most significant feature of Tables 2 and 3 is the fact that, for this set of particle and beam parameters, Q^{min} for the more experimentally realistic truncated, focused, and aberrated beam is only ~20% lower on average than that for the idealized freely propagating focused Gaussian beam, whereas both are approximately a factor of 2–3 below the experimental value of Q^{min}. As mentioned in Section 3, for $m = 1.45/1.33 = 1.09$ and $a = 0.50$ μm, Q^{min} for the more-realistic beam is a factor of 4.6 above the experimental value and again 20% below that of the freely propagating focused Gaussian beam. All the additional work that went in to modeling the more-realistic beam appears to not make a dramatic difference in Q^{min}. The position of the center of the beam's focal waist, or equivalently the position of the spherical aberration's principal diffraction maximum on the z axis, however, strongly depends on the beam model used. In Table 2, for a freely propagating focused beam, z_0^{max} varies from just outside the particle surface to just inside it. In Table 3, for the truncated, focused, and aberrated beam and $a \gtrsim 1$ μm, z_0^{SA} lies deeper inside the particle, at ~70% of the distance from the center to the particle surface. The fact that z_0^{SA} lies well inside the particle makes the particle prone to rapid local heating if it contains strongly absorbing impurities that by chance are located at or near z_0^{SA}. It must be noted, however, that location z_0^{SA} in Table 3 is the position of the principal diffraction maximum of the aberrated beam when its refraction from the medium of index n_2 into the particle is ignored. If one wanted to take this effect into account, one would have to add up the Mie interior partial wave scattering amplitudes c_l and d_l modulated by the beam shape coefficients. One can only qualitatively compare the experimental minimum trapping efficiency for the $a = 10.245$ μm particle with the prediction of ray theory because external reflection and transmission need to be added coherently and because the particle size parameter for this case is $X = 80.8$, which is again below the geometrical optics limit.

For the experiments reported in Ref. 3 the particle was held at $d = -9.0$ μm rather than against the top surface of the sample cell. The minimum trapping efficiency was calculated with the truncated, focused, and aberrated beam for $\lambda = 1.06$ μm, $W/A = 1.5$, $\alpha = 60°$, $n_1 = 1.5$, and $n_2 = 1.33$, for $m = 1.57/1.33 = 1.18$ and $a = 0.51$ μm corresponding to PSL spheres, and for $m = 1.51/1.33 = 1.135$, $a = 0.60$, 0.69, 0.75, 1.35, 1.70, 2.13 μm, corresponding to glass spheres. The results were compared with the experimental value for Q^{min} of Table 1 of Ref. 3. The theoretical value of Q^{min} was found to be 18% below that of the experimental value for $m = 1.18$, it was 7% above to 12% below the experimental result for $m = 1.135$ for the smallest three particle sizes, and it was approximately a factor of 2–7 below the experimental value for the largest three particle sizes. These results are similar to those of Ref. 2 described in the previous paragraph.

One aspect of the trapping that cannot be predicted by use of the freely propagating focused Gaussian beam model is the decrease in trapping efficiency as the particle lies deeper in the sample cell. This is a result of increased spherical aberration of the beam as $/d/$ increases.[35] To assess the ability of the truncated, focused, and aberrated beam model to describe this effect, I calculated the minimum trapping efficiency for $\lambda = 1.06$ μm, $W/A = 1.5$, $\alpha = 60°$, $n_1 = 1.5$, $n_2 = 1.33$, $m = 1.18$, $a = 4.935$ μm, and -100.0 μm $\leq d \leq -4.935$ μm. The results are given in Table 4, along with the experimental value for $Q^{\min}$ from Table 3 of Ref. 2 for these conditions. Also shown in Table 4 is the position z_0^{SA} of the spherical aberration's principal diffraction maximum corresponding to $Q^{\min}$. Trapping of the $a = 4.935$ μm particle is predicted to cease when the particle's center is 82.9 μm away from the interface. As the particle lies farther from the flat interface, the position of the spherical aberration's principal diffraction maximum slowly moves out from 68% of the distance between the particle center and its surface to 86% when trapping is lost at $d = -82.9$ μm. Though the theoretical value of $Q^{\min}$ remains a factor of ~3 lower than the experimental value, the calculated rate of decrease of $Q^{\min}$ as a function of d is only somewhat less than that of experiment.

To compare with the experimental results of Fig. 4 of Ref. 3 I computed the minimum trapping efficiency for the truncated, focused, and aberrated beam for $\lambda = 1.06$ μm, $W/A = 1.5$, $\alpha = 60°$, $n_1 = 1.5$, $n_2 = 1.33$, -53.0 μm $\leq d \leq -5.0$ μm, and either $m = 1.18$ and $a = 0.51$ μm or $m = 1.135$ and $a = 0.60$ μm. Though there is good agreement between theory and experiment for $d = -9.0$ μm for both particles, the truncated, focused, and aberrated beam predicts that the $m = 1.18$, $a = 0.51$ μm particle will cease being trapped at $d = -18$ μm while experimentally the particle remains trapped for $d \lesssim -44$ μm; for the $m = 1.135$, $a = 0.60$ μm particle, trapping is predicted to cease at $d = -50$ μm, whereas experimentally it remains trapped at $d \lesssim -79$ μm. Thus GLMT with the truncated, focused, and aberrated localized beam model does predict the falloff in the trapping efficiency that is due to increased spherical aberration as the particle lies deeper into the sample cell but somewhat overestimates the amount of spherical aberration that is present in the experimental beam.

5. Discussion and Conclusions

Although the beam-plus-particle parameter space for laser trapping calculations is large, the small sample of calculations reported here indicates that GLMT along with the localized model of the incident beam provides a reasonably accurate and practical theory with which to calculate the on-axis radiation trapping efficiency for a spherical particle from the Rayleigh scattering limit to the geometric optics limit. It was found that the predicted value of $Q^{\min}$ is relatively insensitive to the degree of realism of the beam model used but that the predicted positioning of the beam center with respect to the particle depends strongly on the beam model. In addition, the localized version of a truncated, focused, and aberrated beam models the spherical aberration produced by its transmission from medium n_1 to medium n_2 and the decrease in trapping efficiency as a function of depth in the sample cell produced by the increased spherical aberration. The principal mechanism that causes trapping is a delicate near cancellation of diffraction, external reflection, and transmission, with transmission following all numbers of internal reflections contributing only a small fraction of the total trapping efficiency.

Still, the fact that the theoretical minimum trapping efficiency is a factor of ~3 smaller to a factor of ~5 larger than the experimental efficiency requires further investigation. Modeling beam nonuniformities, misalignment, additional aberrations, particle inhomogeneities, deviations from sphericity, and complex refractive index will likely not make up the full difference, as the progression from the freely propagating focused Gaussian beam to the truncated, focused, and aberrated beam produced only a 20% change in $Q^{\min}$. The fact that the prediction of the truncated, focused, and aberrated beam is systematically 20% below that of the focused Gaussian beam is sensible and indicates that diffractive ringing of the focused beam produced by the lens aperture somewhat spoils the smoothness of focus enjoyed by the Gaussian beam model. Similarly, the fact that the calculated efficiency decreases faster as a function of d than is observed experimentally indicates that the model for spherical aberration used here overestimates the actual amount of aberration that is present in the experimental beam. A possible source of the difference between theory and experiment when the particle is near the top surface of the sample cell is the use of the Mie partial wave scattering amplitudes a_l and b_l of Eqs. (5), which assume the spherical particle is located in a homogeneous medium of infinite extent. It would be of interest to use partial wave scattering amplitudes that included multiple scattering contributions of repeated reflections of the beam between the particle and the flat interface, such as is studied in Refs. 37–40. Although the inclusion of repeated sphere–interface reflections may make a difference when the particle is near the top of the sample cell as in Tables 2 and 3, it is expected to not make much of a difference when the particle is deep in the sample cell as in Table 4. The fact that the calculated trapping efficiency sometimes lies below the experimental value, sometimes agrees with it, and sometimes lies above it possibly indicates a nonelectrodynamic cause of the difference. Thermal, convective, and residual electrostatic effects are worthy of additional study.

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