Theory of Optical Trapping Forces: A Review

G.J. Sonek*,** and W. Wang*,**

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Optical trapping is a technique that uses focused laser light to confine, manipulate, and apply optical forces to a variety of microscopic objects including dielectric, metallic, and biological samples. In this paper, we review the basic principles of optical trapping and summarize some of the key results derived from ray-optic and wave-optic theories for trapping forces and their parametric dependence. The application of these theories to the study of low-index microparticles and different trapping geometries are also described.

Key Words: Optical tweezers, Gradient force, Gaussian beam, Rayleigh, Mie

1. Introduction

Optical laser trapping has established itself as a powerful tool for light micromanipulation and force transduction in applications that range from micro-chemistry and material engineering to DNA stretching and the study of cell signaling mechanisms. When a laser beam, such as that derived from a Nd:YAG (1064nm) or near infrared diode laser (e.g. 800nm), is focused to its diffraction limited spot size using a high numerical aperture lens, a single-beam gradient force trap (optical tweezers) is created\(^1\). It can be used to confine and manipulate a variety of microscopic objects including dielectric particles (e.g. latex microspheres, LiNbO\(_3\), SiO\(_2\)), metallic particles (e.g. gold, silver, bronze), and biological specimens (e.g. bacteria, viruses, cells)\(^1-6\). The magnitude and direction of the optical forces that are produced in materials of differing refractive index, polarizability, and geometry can therefore be studied.

To date, both wave-optic\(^7-13\) and ray-optic\(^2,13-15\) theories have been effectively used to predict the optical forces that are exerted on spherical microparticles in the Rayleigh (\(r \ll \lambda\)) and Mie (\(r \gg \lambda\)) regimes, where \(r\) is the particle radius and \(\lambda\) is the wavelength of light. More recent works have addressed the nature of trapping forces on non-spherical samples\(^7-13\), low-refractive index particles\(^5,17\), and in the regime intermediate to that of the Rayleigh and Mie regimes (\(r \lessgtr \lambda\))\(^18\). Regardless of the approach taken, basic theories seek to predict the trapping forces that are produced when a focused light beam interacts with a sample residing in a surrounding fluid medium (Fig. 1). The quantities of interest include the trapping position and range, and the axial and transverse trapping forces (or trapping efficiencies). These quantities depend on lens numerical aperture; sample size, shape, and refractive index; and laser wavelength, polarization, and beam profile. Experimentally, other factors can also impact the resulting forces\(^1,2,6,12,14,19-21\), including aberration\(^22\) and diffraction\(^23\) effects that exist in high numerical aperture focusing systems.

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\* Department of Electrical and Computer Engineering (University of California, Irvine, California 92697 USA)
\** Beckman Laser Institute and Medical Clinic (University of California, Irvine, California 92697 USA)
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2. Basics of optical laser trapping

Optical laser trapping can be understood in terms of the basic principle of the conservation of momentum. Photons carry momentum, and the interaction of light with matter results in change of photon momentum through the processes of reflection, refraction, scattering, and absorption. The corresponding forces, termed scattering and gradient forces, are the two specific force components that govern the trapping process. For a beam of incident power \( P \), and a surrounding medium of index \( n_1 \), the resulting optical forces are often expressed as \( F = Q n_1 P c \), where \( c \) is the speed of light, \( n_1 P c \) is the photon momentum, and \( Q \) is the trapping efficiency, a dimensionless parameter whose value varies between 0 and 2. Optical tweezers\(^1-2\), created with a single, highly focused laser beam, rely specifically on gradient forces and their dominance over the conventional scattering forces.

In the Rayleigh regime, a submicron- or nanometer-sized object can be represented as a point dipole scatterer. The scattering force, induced by surface reflections from the particle and internal absorption, is directed along the beam propagation direction. This component is directly proportional to the incident energy flux and the particle scattering cross-section. The latter term has a dependence on wavelength (\( \lambda \)) and particle size (\( r \)) that varies as \( r^6\lambda^4 \). Alternatively, the gradient force, arising from light-induced fluctuating electric dipoles within the sample, is proportional to the sample polarizability (having an \( r^3 \) dependence) and the energy density gradient (\( VE^2 \)). Stable trapping results when the gradient force dominates over the scattering force, i.e. when a restoring force exists to draw the sample towards the beam focus, rather then push it away in the direction of the propagating beam. The trapping effect is enhanced if the sample (e.g. dielectric, metallic) has a large polarizability, or if a large intensity gradient can be produced via high numerical aperture (N.A.) focusing optics.

In the Mie regime, the trapping forces can be analyzed by examining the change in momentum of propagating light rays, as illustrated in Fig. 2. For rays entering the back focal plane of an objective lens, a point focus \( f \) can be created within the sample of interest. We shall assume the particle has a refractive index \( n_2 \) that is greater than that of its surrounding medium \( n_1 \). When rays \( a \) and \( b \) refract at both the front and back surfaces of the sample (where reflection is neglected when relative refractive index \( n \) is close to 1.0), they experience a change in momentum. As a result of the momentum conservation principle, a force which is equal in magnitude but opposite in direction to the rate of change in the photon momentum is exerted on the particle. The change in momentum associated with ray \( a \) (\( \Delta P_a \)) gives rise to a force \( F_a \), while that of ray \( b \) (\( \Delta P_b \)) gives rise to the force \( F_b \). The vector sum of \( F_a \) and \( F_b \) yields a net force vector \( F \). For a particle whose center \( O \) is offset from the beam propagation axis in both axial and transverse directions, the resultant force has both axial and transverse components (\( F_{\text{Axial}} \) and \( F_{\text{Trans}} \)). Since the transverse force component always pulls the par-
particle towards the beam focus axis, a two-dimensional (transverse) trap is possible even with a low N.A. lens as long as the relative refractive index \( n \approx 1.05 \). The axial force component, however, pushes the particle away in the forward propagating direction when the convergence angle is small, and the scattering force dominates over the gradient force (Fig. 2(a)). As the convergence angle increases, the reflection and refraction processes give rise to increasing larger gradient forces. Only when the convergence angle is high enough, so that gradient force can overcome the scattering force, does the axial component pull the particle towards the beam focus to create a stable three-dimensional trap (Fig. 2(b)).

3. Theory of optical forces

To determine the magnitudes of the trapping forces and efficiencies in the Rayleigh, Mie, and intermediate regimes, a number of different theoretical approaches have been employed to date. However, ray-optics theory, based on geometrical optics and valid under the conditions that \( 2\pi r/\lambda >> 1 \) and \( 2\pi r/\omega_b >> 1 \) where \( \omega_b \) is the beam spot size, has been the most versatile for deriving qualitative and quantitative results.

In the Mie regime, the incident light beam can be decomposed into individual rays, each of which reflects and refracts at a dielectric interface to produce optical forces based on the change in light ray momentum\(^1,2,15\). The force due to a single incident ray of power \( P \) striking a dielectric sphere at an incident angle \( \theta \) and with incident momentum per second \( n_1P/c \), where \( n_1 \) is the index of the surrounding medium, is shown in Fig. 3. The total force on the sphere is the sum of the contributions due to the primary reflected ray of power \( PR \) and the multiply refracted rays with powers \( PT^2, PT^3R, ..., \) and \( PT^2R^n \), respectively. In the local \( \eta-\zeta \) coordinate system of the incident beam, the force on the sphere is given by:

\[
F_{\xi}F_{\zeta} = \frac{n_1P}{c} \left\{ \frac{1 + R\cos 2\theta}{T^2[\cos(2\theta - 2r) + R\cos 2\theta]} \right\}
\]  

(1)
\[ F_{\parallel} = F_{\perp} = \frac{n P}{c} \left\{ \frac{R \sin 2\theta}{1 + R^2 + 2 R \cos 2r} \right\} \]

where \( \theta \) and \( r \) are the angles of incidence and refraction, and \( R \) and \( T \) are polarization-dependent Fresnel reflection and refraction coefficients. The scattering and gradient force components \( F_s \) and \( F_g \) are defined as the \( F_{\parallel} \) and \( F_{\perp} \) components pointing in the directions parallel and perpendicular to the incident ray. The total force is obtained by summing the forces from all individual rays, where the total scattering and gradient forces are defined as the vector sums of the scattering and gradient components from each individual ray. This force is often expressed in terms of \( Q \), the trapping efficiency. By further introducing the concept of wave optics\(^{18}\), where each ray has its intensity, direction, and polarization defined with respect to the propagating wavefront of a Gaussian beam, it is also possible to estimate the trapping forces in the intermediate size regime \((\lambda/2 \leq r \leq 5\lambda)\).

The above analysis yields important results with respect to trapping position and range, spring constant, and refractive index dependence. To illustrate the general characteristics of the trapping process, the total axial trapping efficiency \( Q_t \), comprised of the scattering \( Q_s \) and gradient \( Q_g \) components, is shown as a function of \( S_z \) in Fig. 4. Here, it is assumed that the light beam is propagating in the +z direction, and the focus of the trapping beam is located a distance \( S_z \) above the center line of the particle. It is normalized with respect to the microsphere radius. In Fig. 4, positive axial forces are responsible for pushing the particle along the direction of light propagation, while negative forces pull the particle back towards the focal point. The results of Fig. 4 are derived for p-polarized light, a relative refractive index \( n = 1.20 \), and convergence angles of 20° (N.A. = 0.45) and 60° (N.A. = 1.15), which produce marginal trapping and very strong trapping effects, respectively.

Since the scattering force is symmetric with respect to \( S_z \) and always positive, it always pushes on the particle in the direction of beam propagation. Alternatively, the gradient force is anti-symmetric, acting as a spring that points along the electric field gradient and pulls the particle towards the focal point. For \( S_z < 0 \), both the scattering and gradient forces point in the same (+) direction and push the particle along the optical axis. At \( S_z = 0 \) (the geometric focus), the gradient force reverses direction. For \( S_z > 0 \), the gradient force points in a direction opposite to that of the scattering force. If the gradient force is sufficiently large so as to balance or overcome the scattering force, then stable trapping can occur. In the far field \((e.g.) |S_z| > 3\), however, the gradient forces become too weak to overcome the scattering forces, and no trapping is possible. Hence, particles can only be trapped when the gradient forces are greater in magnitude and opposite in direction to the scattering forces. A stable equilibrium (trapping) position \( Q = 0 \) is observed to occur at \( S_E = 0.06 \) (\( \phi = 60^\circ \)), where the particle is trapped just below the focal position.
point. As the convergence angle decreases to 20°, the trapping position shifts in the +z direction to $S_z = 1.40$, a location well outside the sphere. In addition, the region between the zero crossing points in the efficiency curve (shaded regions in Fig. 4) defines the “trapping range ($d_{TR}$”). It is within this region that particles will not be pushed out of the trap once they are captured. This range is seen to lie between $1.4 \leq S_z \leq 2.8$ when $\phi = 20^\circ$, and $0.06 \leq S_z \leq 2.0$ when $\phi = 60^\circ$. The strength of the optical trap is determined by the maximum magnitude of the force within the trapping range. The linearized slope of the force vs. displacement curve in the vicinity of the trapping position defines the effective spring constant of the trap. Axial spring constants generally increase monotonically with radius $r$, whereas they reach a maximum value in the transverse (lateral) case. As shown in Fig. 4, a large convergence angle creates a greater maximum trapping force, spring constant, and larger trapping range. For $r \geq 5 \mu m$ (ray-optics), the trapping range is nearly independent of particle size, while for $r = \lambda$ (intermediate), the primary equilibrium trapping position and trapping range can be estimated as: $S_z = 0.2 \mu m$ ($0.4mm < r < 3 \mu m$) and $d_{TR} \approx -0.26 \mu m + 1.48 \times r$ ($0.4mm < r < 5 \mu m$), respectively. From a combined ray-wave optics approach, recent results also show the existence of a second, but weaker, trapping region when $r \geq 3 \mu m$. This second trapping zone is predicted to be closer to the geometrical focal point (inside the sphere), and have a weaker spring constant. This result is consistent to that derived from wave optics alone when $r \geq 15 \mu m$.

The single-beam gradient force trap is a three-dimensional trap, having both axial and transverse restoring forces. Since the axial force primarily determines whether trapping can occur, it is the quantity of greatest interest for purposes of theoretical calculations. The parametric dependence of the axial trapping efficiency has been extensively studied. For example, the maximum axial trapping efficiency, calculated as a function of particle size in the Rayleigh and Mie regimes for a convergence angle of 60°, has a $r^3$ dependence for $r \leq 0.5 \mu m$, and a value that is nearly independent of $r$ for $r \geq 10 \mu m$ (Fig. 5). Other calculations have, in fact, reported an increase of up to 14% in the maximum axial trapping efficiency when $r$ is increased from 15mm to 20mm. In the intermediate range where $r$ is comparable to the wavelength $\lambda$, the axial efficiency has a dependence that varies monotonically between $r^0$ and $r^3$, while the transverse efficiency has a weaker dependence. In this regime, the transverse forces are predicted to be greater than the axial forces, with the ratio $F_{\text{Trans}}/F_{\text{Axial}}$ decreasing steadily as the particle size increases over the range $1/2 < r < 5 \mu m$. These predictions have been confirmed experimentally, where it has been empirically determined that $Q \sim r^2$ over the 0.6 - 2.2mm radius range.

From Eqs. (1) and (2), it is clear that the trapping forces depend intimately on the sample refractive index, polarization, and incident angle through the Fresnel refraction and reflection coefficients. When the relative refractive index $n$ is small, the force magnitude increases as $n$ increases. For larger $n$, however, the trapping force degrades because the dielectric microsphere behaves like a powerful lens and the scattering force component due to reflection increases faster than the gradient component does, resulting in a net force that pushes on the sample. Ray-optical calculations predict the best trapping performance to occur for the relative index $n = 1.3 - 1.4$5, while diffra-
tion theory predicts a maximum trapping force for \( n = 1.24^{9,9} \). For most samples of practical interest (e.g. latex microspheres, cells, microcrystallites), the relative index falls within the range \( 1.05 < n < 1.5 \) where efficient trapping can occur and there always exists a transverse restoring force that increases with relative index. Calculations have also considered the complex refractive index, and its affect on the resulting forces\(^{24} \). In addition, since the Fresnel coefficients differ slightly for s- and p-polarized light, the axial and transverse force components will be polarization-dependent as well. For example, in both the Rayleigh and Mie regimes, s-polarized light yields the larger transverse trapping force, being larger than the p-polarized force component by \( \approx 15\% \) when \( r \geq 10\mu m \), and \( \approx 5\% \) for \( r = 1\mu m \)\(^{13} \). In the intermediate regime (\( 0.5\mu m < r < 5\mu m \)), the transverse force parallel to the polarization is predicted to be larger than the transverse force perpendicular to the polarization by \( \approx 10\% \)\(^{18} \). Due to the existence of a polarizing angle, a much stronger polarization dependence for Gaussian beam forces has been conjectured\(^{1} \), but only over the region of \( S_2 \leq 1 \). With respect to numerical aperture (N.A.), it is clear that a larger numerical aperture produces a larger convergence angle, and this improves trapping performance by optimizing the gradient forces. Practically speaking, single-beam trapping can be achieved over the N.A. range of \( \approx 0.45 (\phi = 20^\circ) - 1.4 (\phi = 70^\circ) \), where the smallest N.A. produces marginal trapping, and the largest N.A. is expected to produce the best results, but often suffers from diffraction effects that impact the trapping of micron-sized samples.

The other parameters that affect trapping forces include the incident beam profile and wavelength. The Gaussian profile (TEM\(_{00}\)) clearly possesses an intensity gradient that can facilitate effective trapping and the production of rather large trapping forces (hundreds of piconewtons). As previously noted\(^{1,6,15} \), the axial (backward directed) force for a Gaussian beam is smaller than that for a uniform beam, since the Gaussian has less beam energy in the peripheral regions. A larger gradient force component can be produced by shifting the beam energy away from the beam axis, a process that can be achieved using a TEM\(_{01}\) mode profile, a modified vortex beam created using holographic or binary optical elements\(^{17,25} \), or a rapidly rotating caging beam\(^{26} \). Such beams are especially useful for trapping low-index particles or highly reflecting (e.g. metallic) samples. The wavelength dependence of trapping is dictated by the change in beam energy density and the dispersion characteristics of the sample under study. Since the Poynting vector and energy density scale as \((1/\lambda)^2 \), a shorter wavelength should produce a higher peak force. For example, by reducing the wavelength from 1064nm to 532nm, the maximum force increases by \( \approx 16\% \)\(^{9} \). Only recently has the complex refractive index contribution been accounted for in force calculations\(^{24} \). For normally dispersive media, a higher index at shorter wavelength should produce a larger axial trapping force. In reality, however, local absorption bands due to specific chromophores make some wavelengths less effective than others, primarily as a result of localized heating and an overall reduction in the gradient and scattering force components. Under certain circumstances, the role of other forces should also be considered, including those of gravity, radiometry, and Brownian motion.

4. Applications of trapping theory

The basic ray-optic and wave-optic trapping theories developed for spherical microparticles can be successfully applied to samples and traps having other geometrical shapes and configurations, respectively. While wave theory offers the most detailed description of the interaction between a focused laser beam and a particle of irregular shape\(^{16} \), the ray-optic approach offers an easier method for interpreting and quantifying the trapping forces. In this regard, ray optics has been used to study the trapping of low-index samples\(^{5,17} \), the performance of lensed fiber traps\(^{27} \), and the feasibility of such novel trapping geometries known as phase-conjugate traps\(^{28} \).

In the case of low-index particles, the gradient force generally acts to repel the sample out of the high in-
tensity region. However, by using a single, strongly focused stationary dark optical vortex beam (similar to a TEM$_{01}$ mode), it has been shown that hollow glass spheres functioning as low-index particles can be stably trapped$^{17}$. Here, in the vicinity of the vortex core, the large gradient force pushes the particle into the dark core. Hence, the core serves as a stable equilibrium position for small particle displacements and an unstable position for large transverse displacements when the particle moves out of the core. For a low-index particle in a strongly focused vortex, ray optics predicts that the equilibrium position will occur on the optical axis a short distance above the focal plane. Another interesting approach makes use of microfabricated ring-shaped low-index particles to study the trapping process$^{5}$. In this case, strong axial trapping is produced by a TEM$_{00}$ beam, a result of the fact that upward radiation pressure is induced when incident light rays strike the inner walls of the particle, while transmitted rays leave from the bottom of the sample and enter a higher index surrounding medium. Here, a ray-optics analysis correctly predicts the three-dimensional nature of the trap for the low-index micro-object.

Beyond single-beam gradient force trapping, the ray-optic theory is useful for predicting trapping forces in dual-beam as well as phase-conjugate optical traps. One example where trapping theory has been applied is in the study of the lensed, dual-fiber optical trap$^{27}$. Here, counter-propagating gaussian beams derived from low N.A. (0.20) lensed, single-mode fibers are used to confine and manipulate micron-sized samples. As an example, a vector plot of trapping efficiency in a dual-fiber trap for a 5μm diameter microsphere in the axial (z)-transverse (y) plane is shown in Fig. 6. As the gradient force pulls the particle closer to the fiber axis, the particle becomes more strongly affected by the axial scattering forces. Precisely along the z-axis, equal but oppositely directed scattering forces act on the sample to confine it to a stable equilibrium position. As another example, when a phase conjugate beam is used as one of the beams in a double-beam trapping geometry, a laser trap can be created that combines features of both optical trapping and optical phase conjugation (OPC)$^{28}$. OPC is a nonlinear process
which generates a reflected (phase conjugate) beam that precisely reverses the direction of propagation and recovers the overall phase or wavefront of the input beam in a time-reversed manner. OPC has some very unique image processing capabilities, including contrast reversal and motion detection, that make it attractive for integration with optical manipulation systems. A comparison of the trapping efficiencies derived from ray-optics for single beam gradient, phase conjugate dual-beam, and confocal dual-beam traps at the convergence angles of 20° and 60° is shown in Fig. 7. Here, it can be seen that the trapping efficiency is improved over the conventional gradient-force trapping geometry, primarily due to the cancellation of scattering forces and the reinforcement of the gradient forces. However, this advantage becomes less significant at higher lens N.A.s.

5. Conclusions

The various optical trapping theories employed to date provide an important and accurate prediction of the forces that can be generated in optical tweezers and modified-beam traps for a variety of sample types and shapes. As shown above, optical trapping offers a fascinating look into how the conservation of light momentum can be effectively used for confinement and manipulation of microparticles in the various particle size and wavelength regimes.

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