Approximate and exact modeling of optical trapping

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ABSTRACT

Approximate methods such a Rayleigh scattering and geometric optics have been widely used for the calculation of forces in optical tweezers. We investigate their applicability and usefulness, comparing results using these approximate methods with exact calculations.

Keywords: Optical tweezers, gradient force, scattering force

1. INTRODUCTION

Simple approximate methods of calculation of optical forces have been traditionally widely employed for the modelling of optical trapping. However, the two major approximate methods, geometric optics and Rayleigh scattering, are only accurate for particles much larger or much smaller than the wavelength of the trapping beam, respectively, while the particles typically trapped in optical tweezers are on the order of a wavelength or a few wavelengths in size, and lie between these regimes of applicability. Alternatively, one can carry out exact calculations, determining the scattering of the trapping beam by the particle, and hence the optical force, based on either the Maxwell equations or the vector Helmholtz equation While in the early days of optical tweezers, the computational challenge posed by exact calculation of the optical force was formidable, rapid growth in readily available computational power, and software making it accessible, has reduced computational practicality as a motivation for using approximate methods. However, they continue to be used, and it is therefore important to understand the limitations of these approximate methods. In particular, methods such as geometric optics can be quantitatively wrong, and omit important physical effects, even when one expects to be in the regime of applicability. We discuss the advantages and limitations of approximate and exact methods of calculating optical forces in the modelling of optical tweezers. Despite the problems and perils of the approximate methods, they retain strong explanatory power, and can remain useful for qualitative explanation even in the presence of quantitative failure.

2. RAYLEIGH APPROXIMATION

The Rayleigh and geometric optics approximations are often presented as small and large particle approximations, respectively. This is, of course, largely true, but it is not a complete account. Therefore, we will briefly review both approximations, and their relationship with exact theory for optical trapping. We will, apart from the final discussion, only consider spherical particles, so a suitable exact theory is provided by Lorenz–Mie theory, or more precisely, generalized Lorenz–Mie theory, the extension of the classic Lorenz–Mie theory from plane wave illumination to arbitrary illumination.

We can take two distinct approaches to the Rayleigh approximation. We can first consider the electrostatic problem of the induced dipole moment of a sphere in a uniform applied field. This is well known as an exam question in electromagnetic courses, with an equally well known—and simple—analytical result: a dipole moment of

$$\mathbf{d} = 4\pi n_{\mathrm{med}}^2 \epsilon_0 r^3 \left(\frac{m^2 - 1}{m^2 + 2} \right) \mathbf{E} \tag{1}$$

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where $\mathbf{E}$ is the applied electric field, n_{med} is the refractive index of the surrounding medium, and m is the relative refractive index of the particle, with $m = n_{\text{part}}/n_{\text{med}}$. The force acting on this induced dipole due to a non-uniform field is[1]

$$\mathbf{F}_{\text{grad}} = \pi n_{\text{med}}^2 \epsilon_0 r^3 \left(\frac{m^2 - 1}{m^2 + 2} \right) \nabla |\mathbf{E}|^2. \tag{2}$$

For a sufficiently small sphere, this result will also hold for a time-varying field. In this case, this force is proportional to the gradient of the irradiance I,

$$\mathbf{F}_{\text{grad}} = \frac{2\pi n_{\text{med}} r^3}{c} \left(\frac{m^2 - 1}{m^2 + 2} \right) \nabla I. \tag{3}$$

While this requires a non-uniform field, if the particle in the optical trap is much smaller than the wavelength of the trapping beam, the field will be approximately uniform field, and the gradient force (3) provides an excellent approximation for the force.

For a static field were static, equation (3) is the total force. However, a time-varying field will result in, first, polarization currents due to the changing induced dipole moment, and, second, a magnetic field as part of the applied time-varying electromagnetic field. This results in an additional force on the dipole. The simplest approach to this is to consider the particle as a short electric dipole antenna. The equivalent circuit element for an infinitely small induced dipole moment is a pure reactance, with the current a quarter wave out of phase, which is the result we obtain from the dipole moment (1). In this case, there are no energy losses. A finite oscillating dipole moment, on the other hand, radiates with finite power, and is represented by an impedance consisting of the above reactance and the radiation resistance of the antenna (and any Ohmic resistance, if there is absorption in the sphere). gives an effective complex polarizability,[2]

$$\alpha_{\text{eff}} = \alpha_0 / (1 - 2\mathrm{i} k^3 \alpha_0 / 3) \tag{4}$$

where α_0 is the original uncorrected polarizability. Note that a similar complex polarizability (but with different scaling with the size of the sphere) also results if the sphere possesses a complex refractive index (i.e., if the sphere is absorbing). The additional force due to this resistive component is[1]

$$F_{\text{scat}} = \frac{8\pi n_{\text{med}} k^4 r^6}{c} \left(\frac{m^2 - 1}{m^2 + 2} \right)^2 I. \tag{5}$$

This force is usually called the *scattering force*. As noted above, the scattering force is similar in effect to absorption forces, with one chief difference: the scattering force acting on a re-radiating sphere is proportional to the square of the volume (ie, proportional to r^6), while the absorption force on a small absorbing sphere is proportional to the volume (proportional to r^3). If a sphere is small enough, the scattering force will be much smaller than the gradient force, and the effect of re-radiation can be neglected.

We can also view the Rayleigh approximation as a limiting case of generalized Lorenz–Mie theory. In Lorenz–Mie theory, the incident and scattered electromagnetic waves as written as sums of their multipole components (that is, in terms of a basis of vector spherical wavefunctions (VSWFs)). The incident field is

$$\mathbf{E}_{\text{inc}} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} a_{nm} \mathrm{M}_{nm}^{(3)} + b_{nm} \mathrm{N}_{nm}^{(3)}, \tag{6}$$

and the scattered field is

$$\mathbf{E}_{\text{scat}} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} p_{nm} \mathrm{M}_{nm}^{(1)} + q_{nm} \mathrm{N}_{nm}^{(1)} \tag{7}$$

where n is the radial mode index, m is the azimuthal mode index, a_{nm}, b_{nm}, p_{nm} and q_{nm} are the multipole coefficients, or mode amplitudes, of the incident and scattered fields, and $\mathrm{M}_{nm}^{(3)}$, $\mathrm{N}_{nm}^{(3)}$, $\mathrm{M}_{nm}^{(1)}$ and $\mathrm{N}_{nm}^{(1)}$ are the vector spherical wavefunctions of the third and first type respectively. Due to the orthogonality of the vector spherical wavefunctions over a sphere, there is no coupling between modes, and there is a simple linear relationship between the incident and scattered amplitudes,

$$p_{nm} = a_n a_{nm} \tag{8}$$
$$q_{nm} = b_n b_{nm}, \tag{9}$$

where a_n and b_n are the Mie scattering coefficients. (For a more general scatterer, there is coupling between modes, and the above relationship becomes

$$p_{n'm'} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} A_{n'm'nm} a_{nm} + B_{n'm'nm} b_{nm} \tag{10}$$
$$q_{n'm'} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} C_{n'm'nm} a_{nm} + D_{n'm'nm} b_{nm}. \tag{11}$$

This can be compactly written as a matrix–vector product by writing the incident and scattered mode amplitudes as column vectors $\mathbf{a}$ and $\mathbf{p}$, giving

$$\mathbf{p} = \mathbf{T}\mathbf{a}, \tag{12}$$

where $\mathbf{T}$ is the T-matrix (or transition matrix, or system transfer matrix). This is the T-matrix formulation of scattering.) While the above expressions for the fields involve infinite sums, these sums can be truncated at a finite $n_{\max}$ approximately equal to the size parameter of the sphere (kr, the product of the wavenumber and the radius)—for spheres on the order of the wavelength in size, only a modest number of terms are required.

Here, the Rayleigh approximation is simply that the only significant Mie coefficients are the electric dipole coefficients, b_1. (The b_n coeffients for $n > 1$ are for higher-order electric multipoles; the a_n coefficients are for magnetic multipoles.)

This second approach gives a clear indication of when the Rayleigh approximation will begin to fail: when the magnetic dipole moments and electric quadrupole moments (and higher multipole moments as well) cease to be negligibly small. We will see two levels of failure—a quantitative error when these higher moments begin to contribute to the forces, and a complete failure when they become dominant. The relevant Mie coefficients are shown as a function of sphere radius in figure 1.

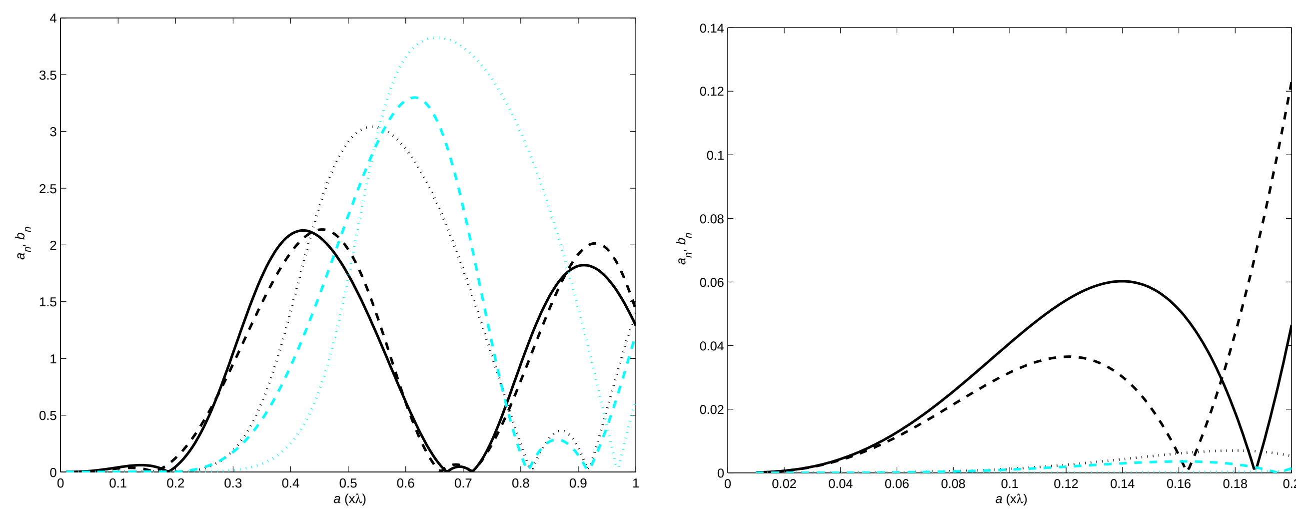

Figure 1. Mie coefficients. The absolute values of the lowest order Mie coefficients are shown as a function of sphere radius. The electric dipole coefficient is shown in solid black, the higher order electric multipole coefficients are dotted (black, $n = 2$, and cyan/gray, $n = 3$), and magnetic multipoles are dashed (black, $n = 1$, and cyan/gray $n = 2$). The right-hand plot shows the left-most fifth of the left-hand plot in more detail.

From this, we can see that the Rayleigh approximation should be accurate for $a < \lambda/10$, which is the usual criterion for accurate applicability of the Rayleigh approximation. This does not directly tell us how accurate force calculations will be. It should be noted that the momentum flux of the incoming and outgoing light depends on interference between different multipole moments;[3,4] in the Rayleigh limit, the interference between the electric dipole and quadrupole terms will be the most important. Therefore, it is useful to directly calculate the force. Both the exact force and the Rayleigh-limit force can be calculated using the T-matrix method.[4] For a particle at the focal point of the beam, the gradient force will be zero, and the entire force will be the scattering force. For a small radial displacement from this position, the radial restoring force will be purely due to the gradient force, since the scattering force will be parallel to the beam axis. This allows us to investigate the accuracy of both the scattering force (shown in figure 2) and gradient force (shown in figure 3) in a simple manner.

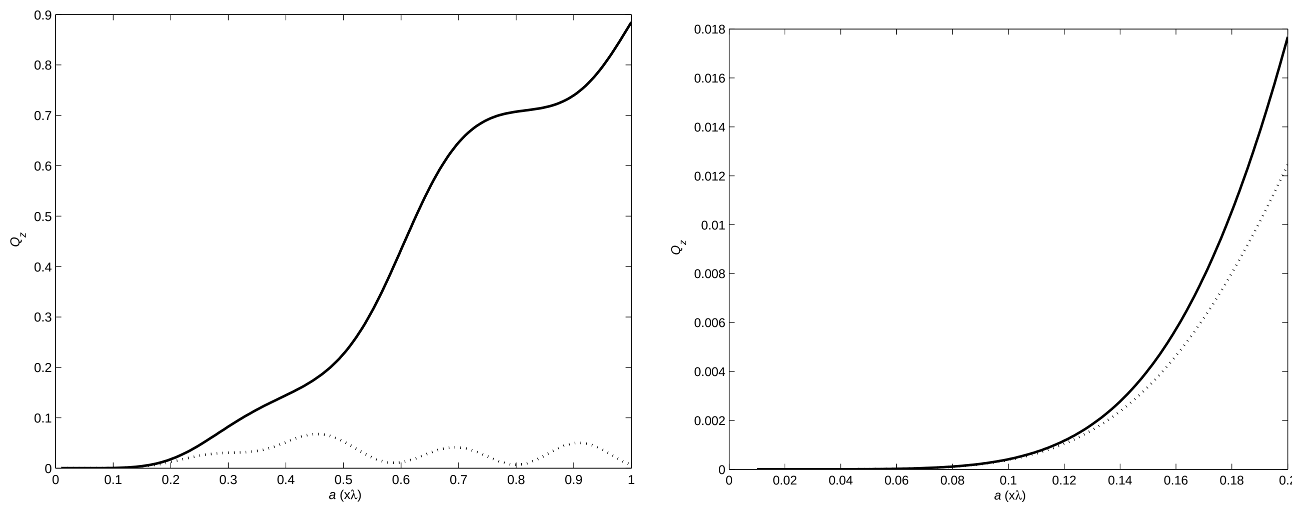

Figure 2. Scattering force. The scattering force efficiency acting on a polystyrene particle at the focus of an optical trap, with the beam focused by an NA $= 1.25$ objective, is shown. The solid line shows the force in the Rayleigh approximation, and the dotted line shows the exact result calculated using GLMT/T-matrix method.

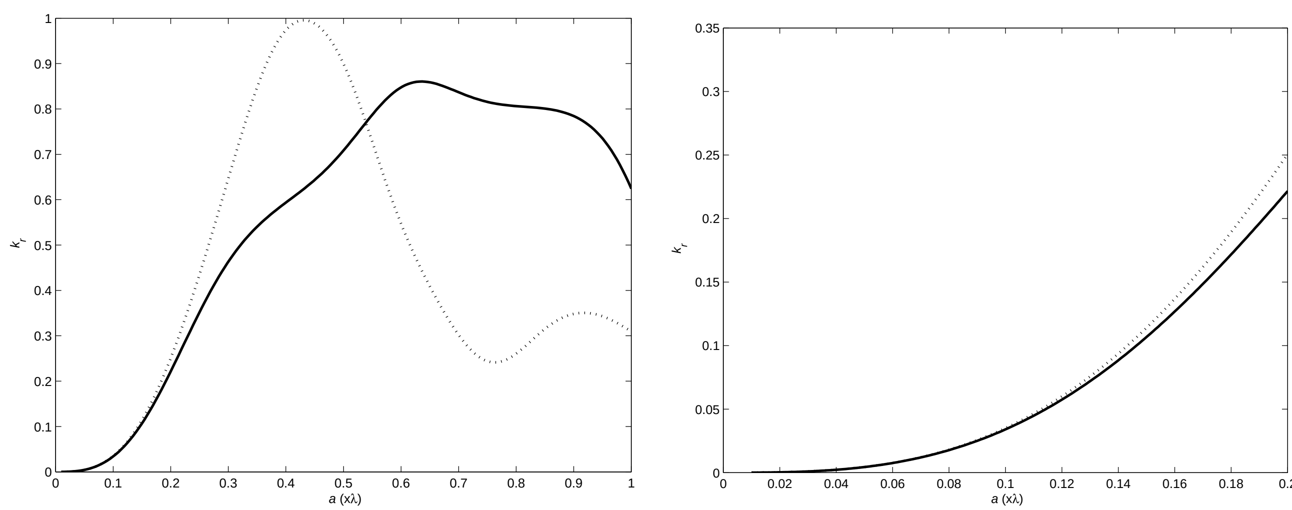

Figure 3. Gradient force. The normalised radial spring constant in the focal plane of an optical trap, with the beam focused by an NA $= 1.25$ objective, acting on a polystyrene particle is shown. The radial forces in the focal plane are due to the gradient force only, since the scattering force is purely axial in this plane.

From this, we can see that the Rayleigh approximation is accurate, with acceptably small quantitative error, for particles up to approximately $\lambda/4$ in radius. This is somewhat larger than we might expect from the usual $\lambda/4$ rule-of-thumb. For particles within the $\lambda/10$ size range, the accuracy is very good, with the curves in figures 2 and 3 being almost indistinguishable. For particles larger than $\lambda/4$ in radius, the accuracy rapidly becomes much worse, and the Rayleigh approximation cannot be regarded as even qualitatively useful past $\lambda/2$.

A key point to note is that calculation of the forces in the Rayleigh limit requires calculation of the fields. This needs to be performed explicitly if the direct formulae for the gradient and scattering forces, equations (3) and (5), are used. It is also included implicitly in a GLMT/T-matrix method calculation. For a spherical particle, this calculation of the field is the most demanding computational task—the Mie coefficients are given by a simple analytical formula.[4] Therefore, in the general case, there is very little computational gain from using the Rayleigh approximation. However, it can be possible to approximate the trapping field, with a consequent analytical result for the forces. For example, if the trapping beam is not too tightly focused, it may be possible to approximate it using the paraxial formula, or at least low-order corrections to the paraxial formula.[5,6]

Furthermore, the analytical results, as expressed in equations (3) and (5) for the forces, clearly show the scaling of these forces with both size and relative refractive index. This is perhaps the most valuable contribution from the Rayleigh approximation.

3. GEOMETRIC OPTICS

While the theoretical benefit of the Rayleigh approximation is clear, with the identification of gradient and scattering forces, the situation is less clear with the geometric optics approximation. We can distinguish between two distinct forces when a ray interacts with a surface—reflection forces, and refraction forces. This invites an identification between reflection forces and the scattering force, and refraction forces and the gradient force.[7] However, for any given ray, it is possible for the ray to undergo both refraction and reflection as it passes through the trapped particle, preventing a clear separation of these forces. However, it is reasonable to label the force due to any ray that has been reflected, whether or not it has also undergone refraction, as a reflection force, especially since the reflection coefficient is relatively small due to the small refractive index contrast between the trapped particle and the surrounding medium (if the reflectivity is not small, the particle is typically not trapped, as the reflection forces push it out of the trap).

The geometric optics approximation is often described as a large particle approximation. That the particle be large is indeed a requirement, but we also require radii of curvature of the surface of the particle to be large compared to the wavelength, and so on. We will note an important additional requirement later, but for the moment, we can see that these conditions will be satisfied by a spherical particle that is large compared to the wavelength.

For such a particle, it is straightforward to calculate the same forces as calculated in figures 2 3. For the scattering force acting on a particle at the focus of the trapping beam, the rays all meet the particle surface at normal incidence. If we make the approximation of only including single reflections from the first and second surface, the scattering force will be

$$\mathbf{F}_{\mathrm{scat}} = 4R\mathbf{p} = 4\left(\frac{m-1}{m+1}\right)^2 \mathbf{p}, \tag{13}$$

where $\mathbf{p}$ is the momentum flux of the beam (which will be less than nP/c which we would have for a parallel beam of power P, due to the convergence of the beam), and R is the Fresnel reflection coefficient at normal incidence. (For simplicity, this assumes that the power incident on the first and second surfaces is the same; this over-estimates the reflection force by 3%.) The momentum flux can be calculated numerically.

The radial spring constant can also be simply calculated. Each surface will cause the center of the beam to deviate away from the original beam axis, by an amount depending on the radial displacement of the particle from the axis and the optical power of the curved surface. Neglecting spherical aberration, the power of each surface of the sphere is given by $P_{\mathrm{opt}} = (n_{\mathrm{particle}} - n_{\mathrm{medium}})$, and the radial spring constant will be

$$k_r = \frac{F_r}{x} = 2\frac{P_{\mathrm{opt}}}{n_{\mathrm{medium}}}|\mathbf{p}| = 2\frac{m-1}{a}|\mathbf{p}|, \tag{14}$$

where x is the radial displacement of the sphere from the beam axis, and a is the radius of the sphere. (For simplicity, the reduction in power due to reflection is neglected. This will result in an overestimate of the spring constant of approximately 3%.)

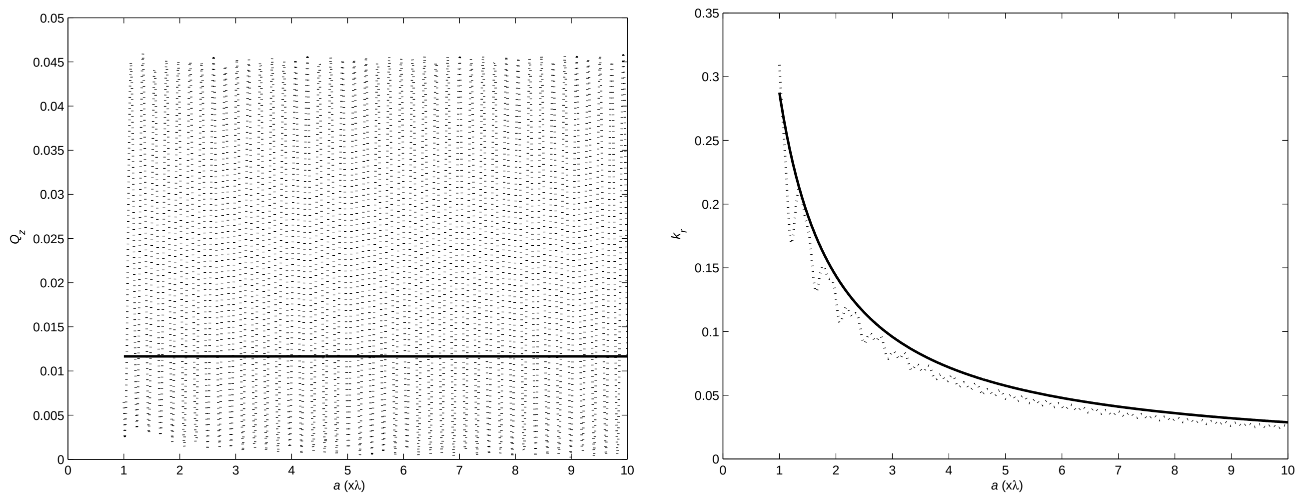

Figure 4. Geometric optics scattering (left) and gradient (right) force. The axial force efficiency on a particle at the focus is shown on the left, comparing the geometric optics result (solid) with the exact Mie theory result (dotted). On the right, the normalised radial spring constant in the focal plane is shown. The optical trap is formed by a beam focused by an NA = 1.25 objective, acting on a polystyrene particle.

The forces as calculated using geometric optics and Mie theory are compared in figure 4. We immediately see that for the scattering force, the geometric optics result only gives an average result. This is because the reflectivity of the sphere strongly depends on its radius.[8] This is the spherical equivalent of the variation in reflectivity of a thin film due to interference between light reflected from the first and second interfaces. This strongly affects the scattering force from large spheres,[8,9] and consequently affects the equilbrium position of trapped particles along the beam axis. Since the geometric optics approximation neglects such interference effects, the geometric optics calculation completely fails to predict this effect, even for large spheres where the approximation is usually assumed to be accurate.

This is the first additional condition we find for geometric optics to be accurate: interference effects must be negligible. The failure to predict the strong variation of scattering force with size due to interference is not entirely a bad thing. The effect seen in figure 4 is for a perfect sphere, and this is an idealization that is often not matched by the actual particle within the trap. For a less perfectly spherical large particle, the optical path length for different rays can easily vary by a wavelength, which would result in an averaging of such interference effects in practice. Thus, the geometric optics result can more accurately model the real particle, by automatically including this averaging.[10]

The gradient force, on the other hand, is only weakly affected by the interference effects on the reflectivity. This is because even the maximum reflectivity is small, and the transmitted power only varies by a small amount. As a result, the geometric optics gradient force is a good prediction of the exact gradient force. Interesting, this is true even for spheres well below the sizes often considered to be necessary for accuracy of the geometric optics approximation (typically $a \approx 5\lambda$ or greater).

From this, we can see that the geometric optics approximation can give quantitatively accurate results for some elements of optical trapping, but gives poor results for others. One important parameter of optical traps that is poorly predicted is the axial trap strength—even when other results, such as the spring constant and radial trap strength, are given accurately, the axial trap strength (i.e., the maximum restoring force in the direction opposite to the beam propagation direction, which is an important parameter since this is usually the weakest direction of trapping) can be incorrectly given by a factor of 2 by geometric optics.[11,12]

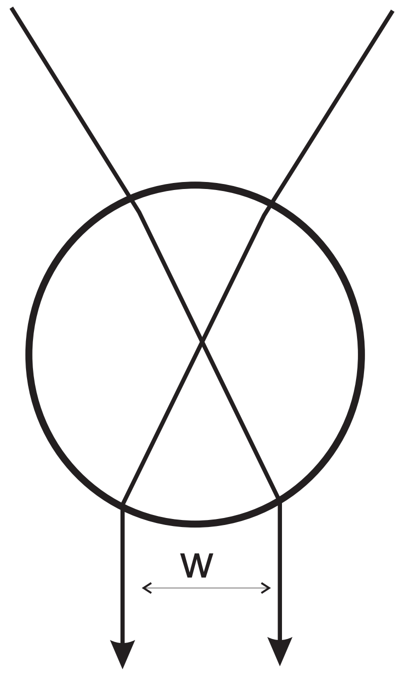

Figure 5. Geometric optics prediction of axial trap strength. The maximum axial restoring force against the direction of propagation occurs when the transmitted beam emerges as paralel as possible. If the beam width w of the emergent beam is not sufficiently large compared to the wavelength, the beam will be divergent, rather than parallel, even if the indicative rays emerge parallel.

The maximum axial restoring force in this direction occurs when the transmitted beam is made as parallel as possible. This is shown in figure 5. However, the emergent transmitted beam is of finite width, and will not be parallel—it will always be divergent. Therefore, the trap strength will generally be overestimated, perhaps greatly so, by geometric optics.

This is a special case of a more general failure of geometric optics—the focal region of the beam is not accurately represented. As the most obvious example of this, geometric optics predicts a focal spot of zero width and infinite irradiance, which we do not obtain in reality. This is the second addition condition for applicability of the geometric optics approximation. Surfaces which interact with the rays must lie where the focused beam is accurately modeled by rays. That is, all such surfaces must lie in the far-field of the beam, away from the focus, where the wavefronts are spherical and the angular variation of intensity does not change with propagation. This is an important difference between geometric optics modeling of the interaction of an object with a focused beam and with a plane wave—in the latter case, this condition is automatically satisfied everywhere. With a focused beam, we must make sure that no surface is near the focus. Unfortunately, the maximum axial restoring force often occurs when the near surface is near the focus, and the axial trap strength is poorly predicted.

4. DISCUSSION

We have seen that the quantitative accuracy of the common approximate methods for calculating forces in optical tweezers, the Rayleigh approximation and geometric optics, is poor outside their regimes of accuracy. Unfortunately, particles commonly trapped in optical tweezers—polymer or silica microspheres of a wavelength or a few wavelengths in size—fall between both approximations. Nonetheless, both approximations provide insight into the processes involved in optical trapping.

The Rayleigh approximation provides simple and clear results for the scaling of gradient, scattering, and absorption forces for small particles, and, if a suitable approximation for the trapping field can be made, can allow analytical formulae for these forces. This possibility of analytical results, even if only approximate due to simplification of the beam, is perhaps the most useful contribution to the computation of forces from the Rayleigh approximation, as well as being useful for understanding the physical processes acting in optical tweezers.

With the geometric optics approximation, we see that good quantitative results can be obtained even for particles smaller than the usually accepted regime of applicability of the approximation. On the other hand, we find an additional condition of applicability, that all surfaces of the particle must be away from the focus.

However, we also find that exact methods of calculating the optical forces grow linearly with particle size, or worse (sometimes much worse!), while the computational demands of geometric optics are independent of particle size. Therefore, geometric optics remains a potentially valuable computational tool, making some calculations of interest feasible, or feasible in the absence of a supercomputer, even if some caution is required.

In addition, geometric optics provides an averaging over interference effects due to particle size that can either cause the model to fail, or can be highly beneficial, depending on the situation.

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