Calculation and optical measurement of laser trapping forces on non-spherical particles

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Abstract

Optical trapping, where microscopic particles are trapped and manipulated by light is a powerful and widespread technique, with the single-beam gradient trap (also known as optical tweezers) in use for a large number of biological and other applications.

The forces and torques acting on a trapped particle result from the transfer of momentum and angular momentum from the trapping beam to the particle.

Despite the apparent simplicity of a laser trap, with a single particle in a single beam, exact calculation of the optical forces and torques acting on particles is difficult. Calculations can be performed using approximate methods, but are only applicable within their ranges of validity, such as for particles much larger than, or much smaller than, the trapping wavelength, and for spherical isotropic particles.

This leaves unfortunate gaps, since wavelength-scale particles are of great practical interest because they are readily and strongly trapped and are used to probe interesting microscopic and macroscopic phenomena, and non-spherical or anisotropic particles, biological, crystalline, or other, due to their frequent occurance in nature, and the possibility of rotating such objects or controlling or sensing their orientation.

The systematic application of electromagnetic scattering theory can provide a general theory of laser trapping, and render results missing from existing theory. We present here calculations of force and torque on a trapped particle obtained from this theory and discuss the possible applications, including the optical measurement of the force and torque.

Keywords: light scattering; optical forces; optical tweezers; laser micromanipulation
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1   Introduction

Optical trapping, which is the trapping and manipulation of microscopic particles by a focussed laser beam or beams, is a widely used and powerful tool. The most common optical trap, the single-beam gradient trap, commonly called *optical tweezers*, consists of a laser beam strongly focussed by a lens, typically a high-numerical aperture microscope objective, with the same microscope being used to view the trapped particles (see fig. 1) [1]. The trapped particle is usually in a liquid medium, on a microscope slide. Commonly used laser sources employed for trapping range from He-Ne lasers, through Ar ion and semiconductor lasers to TiS and NdYAG lasers. Varying laser powers are used in a broad range of applications of optical tweezers - from just a few milliwatts to hundreds of mW. For most of the lasers used, when the beam is passed through the objective lens, the focal spot of the trapping beam is of the order of a micron. The trapped objects can vary in size from hundreds of nanometres to hundreds of microns.
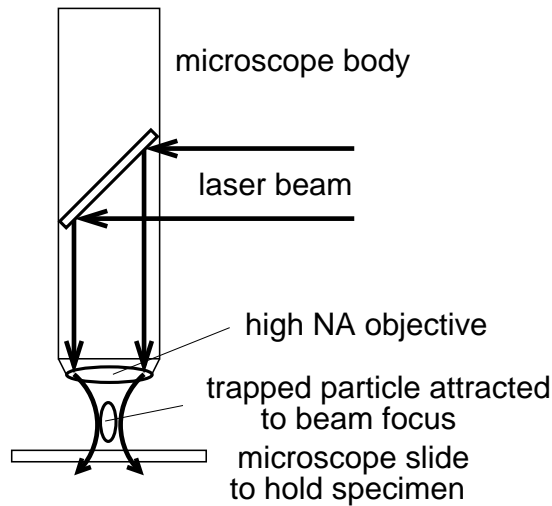
Figure 1: Schematic diagram of a typical optical tweezers setup

Although simple trapping and manipulation are sufficient for many applications, the use of optical trapping for quantitative research into physical, chemical, and biological processes, typically using a laser-trapped particle as a probe, requires accurate calculation of the optical forces and torques acting within the trap. The approximate methods commonly used for such calculations may prove inadequate for many applications [2]. An accurate quantitative theory of optical trapping not only allows such calculations to be performed, but also greatly extends the usefulness of techniques such as optical force and torque measurement and optical particle characterisation.

The concept of optical trapping is based on a gradient force causing small particles to be attracted to regions of high intensity in a tightly focussed laser beam [3]. Other optical forces, due to absorption, reflection, and scattering are termed scattering forces. Both the gradient and scattering forces result from the transfer of momentum from the trapping beam to the particle. Optical torques can also be produced by the transfer of angular momentum from the beam, which can result from birefringence, or particle shape, or absorption of a beam carrying non-zero angular momentum [4–7].

Although the optical forces and torques within a trap result in a straightforward manner from the change in momentum and angular momentum due to scattering processes, exact calculation is difficult, and a number of approximations are usually made. Approximate calculations use geometric optics for large particles (radius $a > 5\lambda$), or assume that a small particle ($a < \lambda/2$) acts as a Rayleigh scatterer or a point-like polarisable particle. This leaves a large range of particle sizes without adequate results; an unfortunate gap since particles of size comparable to the trapping wavelength are of great practical interest because they can be readily and strongly trapped, and can be used to probe interesting microscopic and mesoscopic phenomena. Reecnt theoretical efforts have individually eliminated some of the deficiencies due to the various approximations used, but there still exists no general correct theory [8–11].

The lack of suitable theory is even more acute when non-spherical or anisoropic particles are considered. Non-spherical paricles are of particular interest due to their suitability for use as microscopic probes, and their frequent occurence in nature, for example, biological structures and crystals are usually non-spherical, and are often anisotropic. The possibility of rotating or controlling the orientation of such particles greatly extends the range of manipulation possible within an optical trap, introducing new applications, such as, for example, the investigation of microscopic rotational dynamics [12].

These theoretical deficiencies can be overcome by considering the scattering processes responsible for optical trapping. There exists a well-developed body of work on electromagentic scattering which can be applied to laser trapping in order to determine the scattered fields, from which, in turn, the optical forces and torques can be found.

There are some examples in the literature of attempts to develop a general theory of optical trap-

ping. These are typically restricted to a limited range of particle types and sizes. The systematic application of scattering theory can eliminate these limitation, giving a general theory correct for all particles compositions, including transparent, conductive, absorbing, etc., all particle sizes and shapes, and for arbitrary trapping fields.

2 Light scattering in an optical trap

An optical trap in most ways presents a simple electromagnetic scattering problem, with usually only a single particle in a single orientation in the trap at any one time. The major problems are the representation of the beam, and the possibility that the particle is such that calculations will be difficult even for a single particle. A number of the available techniques require that the trapping beam (i.e. the incident field) be represented as a plane wave spectrum or in terms of vector spherical wavefunctions (VSWFs). The trapping beam is usually a strongly focussed (i.e. non-paraxial) Gaussian beam. An immediate problem is that the standard representations of Gaussian beams do not actually satisfy the Maxwell equations, leading to some difficulty in finding a plane wave or VSWF spectrum, though satisfactory methods exist [13–15]. Additionally, the trapping beam cannot actually be Gaussian, but will have been truncated at some point in the optical system. Non-Gaussian beams are also used for trapping, for example, Laguerre-Gaussian "donut" beams [16].

We can note that while the existence of a wide variety of techniques for the calculation of scattering is indicative of the lack of a universally superior method, each technique has its own particular advantages and disadvantages, and we can find a usable or even ideal method for any particular case. A brief survey of commonly used methods follows, focussing on application to trapping problems. Computer codes implementing many of these methods are available [17, 18].

In general, the solution of an electromagnetic scattering problem requires the solution of the Maxwell equations. Some geometries yield relatively simple solutions, more general cases require direct numerical solution of the Maxwell equations. The best known analytical method is Mie theory, restricted to scattering by a homogeneous isotropic sphere illuminated by a plane wave. Extensions of Mie theory, including the use of spheroidal expansions instead of spherical coordinates allow a broader, but still very limited, range of applicability. In general, numerical methods must still be used to obtain the final solutions in these cases [19].

Closely related to Mie theory is a family of numerical techniques where the incident and scattered fields are expressed in terms of VSWFs, and the expansion coefficients of the scattered field are found by the boundary conditions at the surface of the scatterer. These methods include the point matching method [20] and the T-matrix method [21, 22]. The T-matrix method is widely used, computationally efficient for axisymmetric particles, and a number of computer codes implementing this technique are freely available [17, 18, 23]. The T-matrix method is of particular interest, since, for a given scatterer and illuminating wavelength, the T-matrix only needs to be computed once, and can then be used for repeated calculations. A surface integral over the particle must be computed, but in the case of a rotationally symmetric particle, this integral reduces to one dimension [24].

These surface-based techniques are, in their simple forms, restricted to homogeneous particles, though extensions to layered particles exist [25]. Other surface methods include the generalised multipole technique [27] and the method of moments [19, 20, 28].

If the scattering particle is such that techniques such as those above cannot be used, there are a number of general techniques, in principle usable for any scattering problem. In general, these methods are computationally intensive [19, 20].

Since the Maxwell equations are a set of differential equations, finite difference or finite element methods can be used. The finite difference time domain method (FDTD) is widely used in computational electromagnetics, and can be applied to scattering problems [26]. A discrete grid of points in space is set up, and the fields at successive time steps are calculated. Since the discretisation in space must be much smaller than the wavelength ($\approx \lambda/20$), and a correspondingly small time step must be used, only a relatively small volume can be used for the calculation, so the boundary conditions at the edge of the computational volume must be carefully chosen, and if the far-field is desired, it must be found from the near-field via a suitable transformation. Finite element methods (FEM) can also

be used, again using spatial discretisation to obtain a numerical solution to the system of differential equations [29, 30]. Both of these methods a conceptually simple, and can represent a particle of any shape or composition, but are computationally intensive and require special care with the boundary conditions.

An alternative method is the disrete dipole approximation (DDA) where the particle itself is divided into small volumes, each of which can be treated as a simple dipole with a polarisability depending on the composition of the particle. An initial guess of the final field is iteratively improved until convergence is obtained [31, 32]. Computer codes implementing DDA are publicly available [17, 18, 33].

We can note that the characterisation of a laser trap will require repeated calculations with the same particle in different positions and orientations within the trap. Thus, the T-matrix method is attractive, since the T-matrix need only be found once. The T-matrix method requires that the incident beam be represented in terms of VSWFs; this can be done directly, or via an intermediate plane wave expansion. The need for repeated calculations makes the general methods (such as FDTD, FEM and DDA) less attractive since the entire calculation must be repeated if the incident beam is changed. In these cases, the total calculation required can be minimised by representing the trapping beam by a plane wave spectrum, and calculating the scattering for the different angles of plane wave illumination. This represents no greater computational effort than calculating the scattering for all orientations of the particle at a single location within the trap, and gives results that can be used to find the sccattering at all points and all orientations.

3 Calculation of forces

Once the scattering has been calculated, the resulting force and torque can be found from the field, by integrating around the particle. The momentum of an electromagnetic field is given by [34]

$$\mathbf{P}_{\text{field}} = \epsilon_0 \int_V \mathbf{E} \times \mathbf{B} d^3 x \tag{1}$$

and the angular momentum by

$$\mathbf{L}_{\text{field}} = \epsilon_0 \int_V \mathbf{x} \times (\mathbf{E} \times \mathbf{B}) d^3 x \tag{2}$$

If we have the far-field scattered field, which is an outgoing radiation field, we can choose a spherical surface for the integration, and the momentum and angular momentum fluxes are normal to the surface. Then, the field can be represented by the electric field alone, with two orthogonal components, with complex amplitudes E_θ and E_ϕ, $\mathbf{E}_\theta = E_\theta \hat{\theta}$ and $\mathbf{E}_\phi = E_\phi \hat{\phi}$, tangential to the surface of integration. The rate of transfer of linear and angular momentum per unit area can be found using [12]

$$\mathbf{P}_{\text{flux}} = \frac{\epsilon_0}{2} (E_\theta E_\theta^\star + E_\phi E_\phi^\star) \hat{\mathbf{n}} \tag{3}$$

and

$$\mathbf{L}_{\text{flux}} = \frac{ic\epsilon_0}{2\omega} (E_\theta E_\phi^\star - E_\theta^\star E_\phi) \hat{\mathbf{n}} \tag{4}$$

where $\hat{\mathbf{n}}$ is the unit vector normal to the surface of integration. Equation (3) can be readily recognised as the familiar result of the Poynting vector divided by c.

From the conservation of momentum and angular momentum, the integrated momentum and angular momentum fluxes give the force and torque acting on the trapped particle.

If the discrete dipole approximation (DDA) is used to calculate the scattering, the particle is represented by a number of dipoles, within a known field (after the scattering calculations have been performed). Therefore, the force and torque on each dipole can be found, giving the force and torque on the entire particle, and incidentally, the stresses within the particle. This allows the force and torque to be found without needing to integrate around the particle [35].

The basic methods can be summarised as:

- If the T-matrix method can be used:

    1. calculate T-matrix
    2. find VSWF representation of beam at the desired position within the trap, for the desired orientation
    3. find scattered field (in terms of VSWFs)
    4. integrate around particle

- If a general method must be used

    1. calculate plane wave scattering by the particle for all angles of incidence
    2. find plane wave spectrum of trapping beam at the desired position
    3. find the scattering for each spectral component, and combine to find the total scattered field
    4. integrate around particle

- If DDA is used

    1. find scattering at desired point
    2. find forces and torques on all dipoles, and combine to find the total force

Some sample force calculations are presented in figure 2. The trapped particle is a glass prolate spheroid ($n = 1.5 + 0.02i$), with $a = b = 0.5\mu$m and $c = 1.0\mu$m, trapped in water ($n = 1.33$) by a Gaussian beam of free space wavelength 1064nm, focussed to a spot width of 1μm. The T-matrix code developed by Mishchenko [23] was used to find the T-matrix an amplitude matrix. The trapping beam was decomposed into a plane wave spectrum consisting of 97 components. The size parameter of the particle is 4.95. The wavelength and beam profile and particle size, shape and composition were chosen to best model the most typical situation occurring in the experimental realisation of the technique.
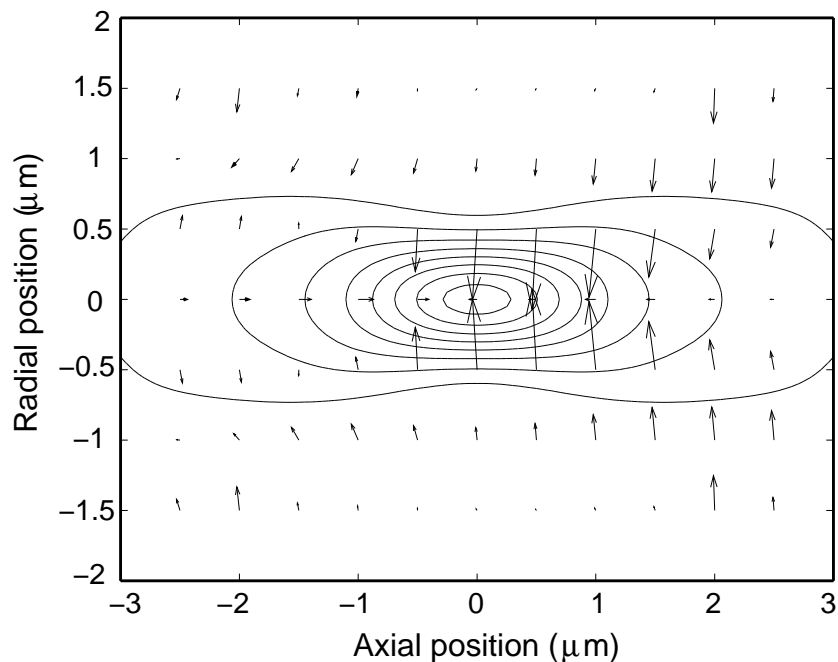

Figure 2: Optical force on spheroid

Figure 2 shows the forces exerted by the trapping beam, which is propagating from the left to the right, focussed to a small spot in the centre. The magnitude of the force is proportional to the length of the arrows, and the direction is the same as the direction of the arrows. The contours in the background are equal-intensity contours for the trapping beam. The trapping beam intensity falls of with increasing radial distance due to the narrow width of the beam. The intensity falls off axially due to the spreading of the beam. The strong radial trapping forces are clearly visible, and it can be seen that the forces are approximately normal to the intensity contours. Since the radial intensity gradient is so large, the radial forces are the largest optical forces acting on the particle. In the regions of low intensity (at the top and bottom of the middle of the graph), the forces are very small.

4 Optical measurement of forces and torques

The forces and torques acting on the trapped particle result from the scattering within the trap, and can be calculated if the scattered fields are known. So far, we have considered techniques for the calculation of the the scattered field. In many cases, this will not be possible, for example, if our particle is a biological structure within a living cell, with unknown optical properties, or a particle with known optical properties at an unknown position within the trap.

If the scattered radiation field can be experimentally measured, equations (3) and (4) can be used to find the force and torque by integrating over a surface around the particle. In principle, the required measurement of the scattered field is possible, but the application of this will be limited by a number of practical considerations, namely:

1. The normal method for measuring scattered light from trapped particles is to measure either the back-scattered light [36], or the forward scattered light [37, 38]. Back-scattering measurements usually record the total power received by the detector and do not give the directional resolution required for measuring the scattered field (which, in any case, would be virtually impossible to do with any accuracy after the return passage of the back-scattered light through the microscope optics). Forward scattering measurements usually use low resolution detectors, such as quadrant detectors, and do not make use of all the possible measurable information. It is generally impossible to collect all of the scattered light due to the spatial limitations imposed by a typical optical tweezers setup. To collect more than the forward scattered light emergent from the bottom of the trap will be very difficult. The placement of the detector(s) is limited by the design of the laser trap. Since the trapping cell, contained a microscope slide, will restrict collection of side-scattered light, and the focussing lens (the objective) will restrict the collection of back-scattered light, the detector must be placed below the trapping cell (see fig. 3). Since the detector must be capable of spatial resolution, and must be large enough to measure the forward-scattered light that passes through the trapping cell, a CCD array is ideal.
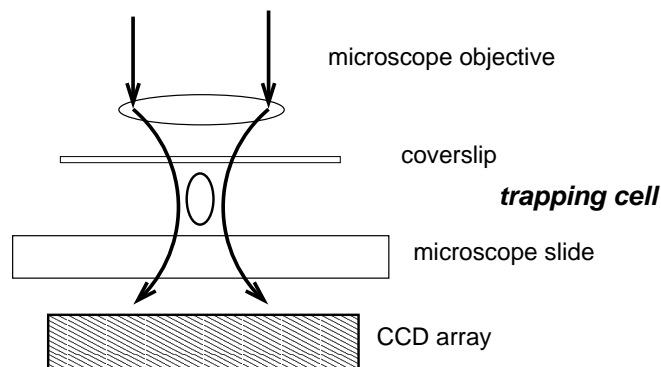

Figure 3: Optical trap with a CCD array to measure scattered light

A CCD array, by itself, is not sufficient to measure the field; only the intensity will be measured, and it will still be necessary to measure the state of polarisation. This can be done by

incorporating a polariser acting as an analyser (see fig. 4).

trapped particle

microscope slide

rotatable polariser
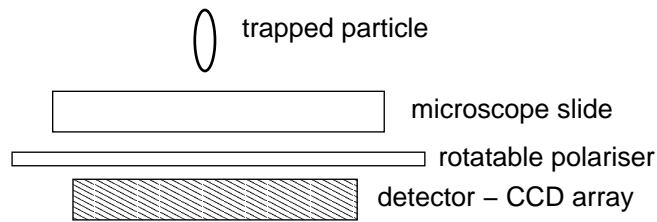
detector – CCD array

Figure 4: Using a polariser and CCD array to measure the polarisation state of light scattered by a trapped particle

2. The bottom of the trap will reflect and refract the scattered light. Since the scattered light is initially in a higher refractive index medium (the fluid within the trapping cell and the glass microscope slide), some of this light will be totally internally reflected, and will be unmeasurable (see fig. 5). For typical values of refractive index, the maximum scattering angle for which the light can be measured is approximately 45°. Reflection can also occur at interfaces internal to the trapping cell, although these will be smaller since the refractive index differences will be relatively small. The reflections that do occur will depend on the polarisation of the light. If too much light is scattered at large angles (and therefore unmeasurable), it will not be possible to accurately determine the optical force. Being restricted to measuring forward-scattered light will also make it difficult to measure torques other than that acting about the beam axis. The partial reflection of light that exits the trapping cell and is measured can, and in the interests of accuracy, should be compensated for.

trapped particle

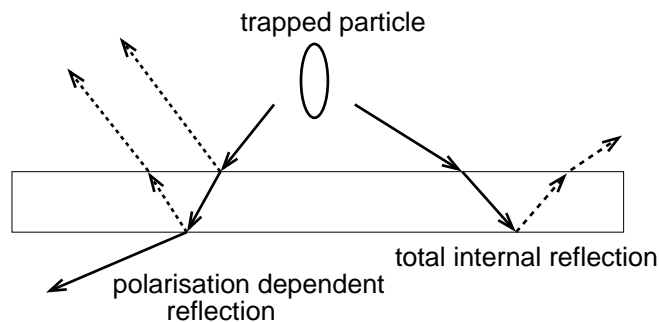total internal reflection

polarisation dependent
reflection

Figure 5: Total internal limits the maximum angle at which light can be scattered and still exit the trapping cell

3. The resolution and size of the detector will limit the measurements.

The restriction of the measurable scattering to the forward-scattered light limits the applicability of the technique. It remains useful, however, in the two cases of most interest, one case being organisms and biological structures, the second probe particles.

Organisms and biological structures in a trap will typically have unknown optical properties, and often have complex shapes. Thus, it will be necessary to measure the scattering since calculation will be impossible. Since such particles are optically soft (with a relative refractive index $m \approx 1$), very little light will be scattered at large angles, and the majority of the scattered light can be measured, and the force and torque acting on the particle determined with reasonable accuracy.

If the particle in the trap is not optically soft, with a large refractive index difference compared with the surrounding medium, it will not be possible to collect enough of the scattered light to accurately determine the force and torque in all cases. If, however, the particle in question is a probe particle of known size, shape, and optical properties, but at an unknown position within the trap,

the portion of the scattered light that is measured can be used to determine what the total scattering pattern must be. Thus, the position of the probe particle within the trap, and the optical force and torque acting on it, can be determined. In this way, the external non-optical forces acting on the probe particle can be determined [39].

A special case of the use of a trapped particle as a probe is the rotating probe particle, which can be used to measure the viscosity of a fluid, colloid, or suspension on a microscopic scale. The rotating particle will typically be birefringent, and will remain in the centre of the trap. The change in polarisation of the light on scattering will cause the particle to rotate. Both the optical torque acting on the particle and its rotation speed can be measured [12].

5 Conclusion

Approaching laser trapping as a scattering problem allows the calculation of forces and torques using electromagnetic scattering theory. Such calculations can be performed for all types of particles: transparent, abosorbing, conductive, reflective, anisotropic, complex shapes, etc. For particles for which efficient computational methods (such as the T-matrix method) can be used, calculations are fast and relatively simple, and can be performed on readily available PCs.

This means that the gap in previous calculations, where no adequate results were available for particles comparable in size to the trapping wavelength, can be closed.

Optical measurement of forces and torques acting on particles within the trap can also be performed, by measuring the scattered light. Apart from being free of the usual calibration difficulties for force measurement in optical traps, it can be used where traditional force measurements are impossible, such as measurement of the forces acting on structures within living cells.

Measurement of the scattered light from a known probe particle, coupled with calculation of the scattering in different positions of the trap, allows measurement of the position of, and force acting on, the probe particle. Thus, external non-optical forces can be determined. A special case of this, where the probe is a rotating trapped particle, is particularly simple, and the rotation speed and optical torque can be simultaneously measured.

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