

## OPTICAL TRAPPING OF A CUBE

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### Abstract

The successful development and optimisation of optically-driven micromachines will be greatly enhanced by the ability to computationally model the optical forces and torques applied to such devices. In principle, this can be done by calculating the light-scattering properties of such devices. However, while fast methods exist for scattering calculations for spheres and axisymmetric particles, optically-driven micromachines will almost always be more geometrically complex. Fortunately, such micromachines will typically possess a high degree of symmetry, typically discrete rotational symmetry. Many current designs for optically-driven micromachines are also mirror-symmetric about a plane. We show how such symmetries can be used to reduce the computational time required by orders of magnitude. Similar improvements are also possible for other highly-symmetric objects such as crystals. We demonstrate the efficacy of such methods by modelling the optical trapping of a cube, and show that even simple shapes can function as optically-driven micromachines.

### Introduction

Optical tweezers (Ashkin *et al.* 1986) have been deployed for a variety of distinct uses: non-contact manipulation of microorganisms, the measurement of piconewton forces, and as a tool for the study of a range of microscopic systems, from colloids through to single molecules. One growing development is the exploitation of optical torque, which has already seen practical application (Bishop *et al.* 2004; Knöner *et al.* 2005). A major objective, towards which a number of groups are working, is the development of optically-driven micromachines (Nieminen *et al.* 2006). A serious impediment, however, is the difficulty of calculating the expected optical forces and torques for such micromachines.

The optical forces and torques in optical tweezers arise from scattering of the trapping beam by the particle. Therefore, the calculation of these forces and torques is essentially a problem in computational light scattering. As the particles involved have dimensions comparable to the wavelength of the light used, large and small particle approximations, such as geometric optics and Rayleigh scattering, respectively, are inapplicable. It is necessary to resort to solution of either the Maxwell equations. A wide range of methods are available for the solution of such scattering problems (Kahnert 2003), and, in principle, it should be possible to use any such method. However, when modelling optical trapping, one typically wishes to know how the force and torque vary with position, which required repeated calculations. One basic question is where in the trap does the particle rest when in equilibrium—to answer this might require a few dozen calculations of the force at different positions along the beam axis. To map the force and torque over a two-dimensional slice through an optical trap will require approximately a thousand separate calculations to achieve a reasonable resolution. When one considers the optical micromanipulation of a complex structure—such as an optically-driven micromachine—the orientation affects both the force and the torque, introducing even more degrees of freedom. Thus, a method that allows rapid repeated calculations is required for the modelling of optical micromanipulation.

Fortunately, such a method—the  $T$ -matrix method (Waterman 1971; Mishchenko *et al.* 2004)—is available. The  $T$ -matrix method is more properly a *description* of the scattering properties of a particle, rather than a method of calculating the scattering properties. The incident field can be expressed as a set of expansion coefficients  $a_n$  in terms of as a sufficiently complete basis set of functions  $\psi_n^{(\text{inc})}$ , where  $n$  is a mode index labelling the functions, each of which is a divergence-free solution of the Helmholtz equation:

$$U_{\text{inc}} = \sum_n^{\infty} a_n \psi_n^{(\text{inc})}. \quad (1)$$

Similarly, we can write the scattered wave, in terms of a basis set:  $\psi_k^{(\text{scat})}$ ,

$$U_{\text{scat}} = \sum_k^{\infty} p_k \psi_k^{(\text{scat})}, \quad (2)$$

where  $p_k$  are the expansion coefficients for the scattered wave. As long as the electromagnetic or optical properties of the scatterer are linear, the relationship between the two can be written as a simple matrix equation

$$p_k = \sum_n^{\infty} T_{kn} a_n \quad (3)$$

or, in more concise notation,

$$\mathbf{P} = \mathbf{T}\mathbf{A} \quad (4)$$

where  $T_{kn}$  are the elements of the  $T$ -matrix. Thus, the  $T$ -matrix formalism is a Hilbert basis description of the scattering properties of the particle, with the  $T$ -matrix depending only on the properties of the particle—its composition, size, shape, and orientation—and the wavelength, and is otherwise independent of the incident field. As a result, the  $T$ -matrix only needs to be calculated once for a particular particle, after which it can be used for rapid repeated calculations of the optical force and torque (Nieminen *et al.* 2004b).

In the simplest case, that of a homogeneous isotropic sphere, the  $T$ -matrix is given by the analytical Lorenz–Mie solution (Lorenz 1890; Mie 1908), while more complex cases require computational solution. For homogeneous isotropic axisymmetric particles of simple shape, such as spheroids or cylinders, this can be done very rapidly using the extended boundary condition method, also known as the null-field method (Tsang *et al.* 2001), since surface integrals over the particle reduce to one dimension. For more complex shapes, the computational time required increases greatly. However, symmetries such as discrete rotational symmetry or mirror symmetry can be used to reduce the time required (Kahnert 2005). Notably, these are exactly the symmetries typical of most optically-driven micromachine designs. We will proceed to use a cube as an example of such optimisation, and in the process show that even simple shapes can function as optically-driven micromachines.

### Exploiting the Symmetry of a Cube

For a compact scatterer, the  $T$ -matrix method is usually implemented with vector spherical wavefunctions (VSWFs) as the basis functions, which fall into two groups, TE and TM. These are usually written as  $\mathbf{M}_{nm}$  and  $\mathbf{N}_{nm}$ , respectively, where  $n$  is the radial mode index and  $m$  is the azimuthal mode index. The properties that are of importance when optimising the calculation of a  $T$ -matrix by exploiting the symmetry properties of a scatterer are the parity and rotational symmetries.

We employ a point-matching method that allows us to calculate the  $T$ -matrix column-by-column considering only a single incident VSWF at a time (Nieminen *et al.* 2004b). Each column requires the solution of an overdetermined linear system, and the time required by this is the dominant component in the overall computational time. Solution of linear systems typically scales as  $N^3$ , where  $N$  is the number of unknowns.

#### Parity

Each individual VSWF has either odd or even parity with respect to the  $xy$ -plane. That is, the magnitude of the electric field is symmetric relative to this plane, and the phase is either the same or differs by  $\pi$ , such that  $\mathbf{E}(x, y, z) = \mathbf{E}(x, y, -z)$  (even parity) or  $\mathbf{E}(x, y, z) = -\mathbf{E}(x, y, -z)$  (odd parity). TE VSWFs have odd parity when  $n + m$  is odd, and even otherwise. TM VSWFs have odd parity when  $n + m$  is even, and even otherwise. When the scatterer is mirror symmetric about the  $xy$ -plane, the parity of the incident field is unchanged on scattering, and thus the scattered field consists only of modes of the same parity as the incident field. Accordingly, only half of the total number of scattered field modes need to be included in the linear system, halving the number of unknowns,  $N$ , with a corresponding reduction in computational time.

### Rotational symmetry

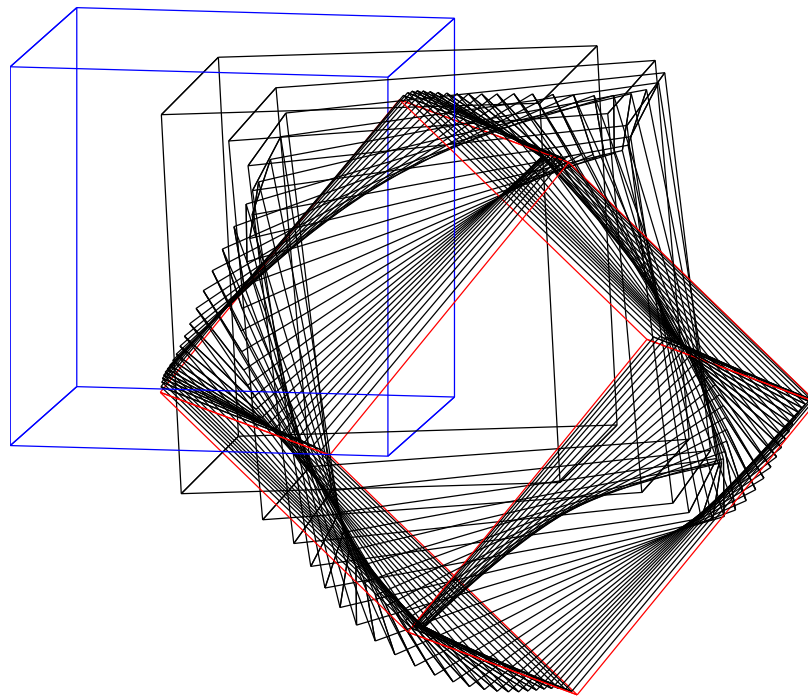
Each individual VSWF has an azimuthal dependence of  $\exp(im\phi)$ . If a scatterer possesses discrete rotational symmetry of order  $p$ , this effectively provides a periodic boundary condition, determining the periodicity with respect to the azimuthal angle  $\phi$  that the scattered field can possess. From Floquet's theorem, the allowed azimuthal mode indices for the scattered field are

$$m_{\text{scat}} = m_{\text{inc}} + ip \quad (5)$$

where  $i$  is an integer. This is analogous to the generation of a discrete spectrum of scattered plane waves by a grating. If the particle has no rotational symmetry (ie  $p = 1$ ), then coupling to all azimuthal modes occurs. For an axisymmetric particle,  $p = \infty$  and  $m_{\text{scat}} = m_{\text{inc}}$ , which is widely used when calculating scattering by such particles. For a cube,  $p = 4$ , and  $m_{\text{scat}} = m_{\text{inc}}, m_{\text{inc}} \pm 4, m_{\text{inc}} \pm 8, \dots$ . As a result, the number of unknown in the linear system is reduced to approximately 1/4.

Make use of both symmetries together reduces the number of unknowns by a factor of eight, with a considerable savings in computational time. For example, a cube with faces two wavelengths across required 30 minutes for the calculation of the  $T$ -matrix on a 32 bit single-processor 3GHz PC, as compared with 30 hours without the symmetry optimisations.

### Optical Trapping of a Cube

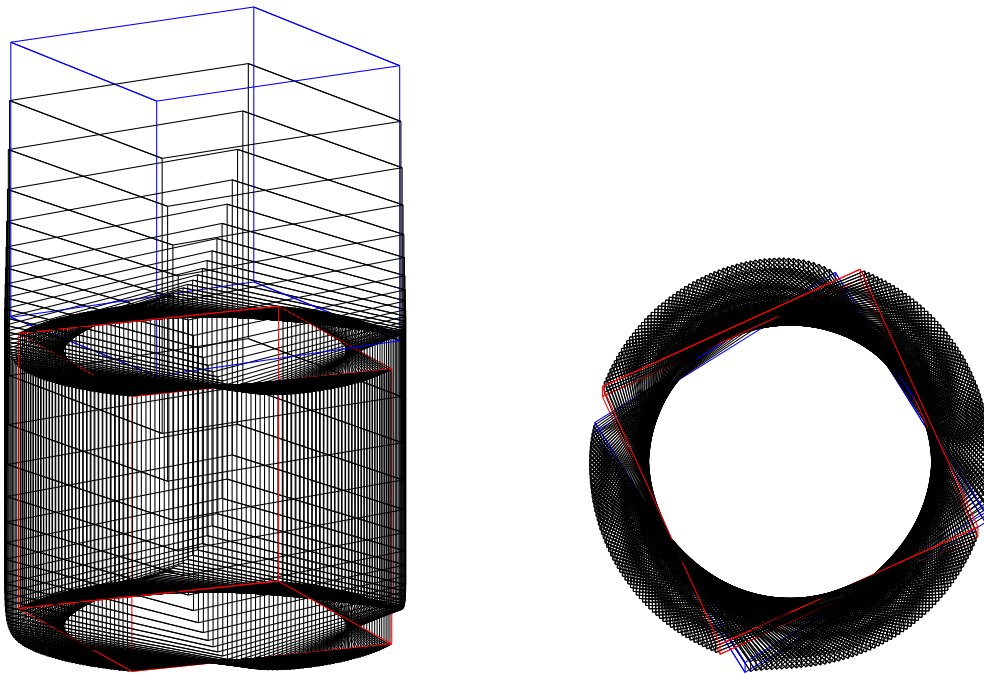


**Figure 1. Optical trapping of a cube**

Figure 1 shows the optical trapping of a cube. The initial position of the cube is shown by the blue frame, and the equilibrium position by the red frame. At each position, the optical force and torque are calculated, and the motion of the cube found. The cube is assumed to be moving at terminal speed at all times (the time constant for approach to terminal speed in optical tweezers is typically on the order of  $0.1 \mu\text{m}$  (Nieminen *et al.* 2001), which is much smaller than the time steps used to calculate the motion of the cube).

As the discrete rotational symmetry of a cube is typical of the rotational symmetry of optical driven micromachines (Nieminen *et al.* 2006), and the optical torque is determined by the rotational symmetry of a scatterer (Nieminen *et al.* 2004a), a cube can be expected to rotate when illuminated by a beam carrying angular momentum. To

test this, the cube is placed initially on the beam axis, at the focus of the beam. The beam is circularly polarised, and therefore carries spin angular momentum of  $\hbar$  per photon. As can be seen in figure 2, the cube is rapidly pushed into the equilibrium position along the beam axis, where it spins due to the transfer of angular momentum from the beam to the cube. Although the face-up position is an unstable equilibrium, any torque acting to bring the cube into the stable corner-up position seen in figure 1 is too small to have any visible effect over the duration of the simulation. The cube is shown both from the side and from below.



**Figure 2. Rotation of a cube**

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