Electromagnetic forces and torques in nanoparticles irradiated by a plane wave

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Optical tweezers and optical lattices are making it possible to control small particles by means of electromagnetic forces and torques. In this context, a method is presented in this work to calculate electromagnetic forces and torques for arbitrarily-shaped objects in the presence of other objects illuminated by a plane wave. The method is based upon an expansion of the electromagnetic field in terms of multipoles around each object, which are in turn used to derive forces and torques analytically. The calculation of multipole coefficients are obtained numerically by means of the boundary element method. Results are presented for both spherical and non-spherical objects.

INTRODUCTION

Electromagnetic forces produced by intense focused lasers acting on small particles have recently found application in trapping and manipulating small particles in optical tweezers [1, 2, 3, 4, 5]. Also, optically-powered rotors have been produced either by scattering of elliptically-polarized light [6] or by using particles of helical shape [7]. These are the counterpart of similar effects observed at the atomic and molecular levels, including molecular quantum rotors and motors [8, 9].

In this work, we calculate electromagnetic torques acting on elongated particles illuminated by a plane wave. We show that the magnitude of these quantities, as well as the sign of the torque, can be controlled by using the right polarization and wavelength for the external light. We use a multipole formalism to calculate both torques and forces, which can be applied to complex geometries involving more than one particle, as illustrated below for forces acting on metallic spheres in the presence of neighboring particles of different shapes.

For practical applications in the context of optical tweezers [8] and optical stretchers [10], an extension of the present study to include focused beams will be necessary, similar to the one carried out in Ref. [5], where gradient forces are essential to achieve trapping. Even in this case, one would expect that control over the orientation of small particles is attainable by choosing the right combination of polarization and wavelength. However, the present work can find some relevance in different situations: (1) to control the orientation of particles in free space by irradiating them with successive plane-wave pulses of appropriate strength, duration, wavelength, orientation, and polarization, specially if the absolute spatial position is not so relevant; (2) to explore the dynamics (both translational and rotational) of complex particles in inter-stellar environments; or (3) to control the orientation and position of particles trapped against a solid-fluid interface (the analysis becomes straightforward if the dielectric constant is approximately the same on either side of the interface), although friction and other interfacial forces can play a substantial role in this case.

The electromagnetic response of each of the particles considered in this work has been expressed in terms of their corresponding multipole t-matrix, which relates the coefficients of the multipole expansion of the induced electromagnetic field to those of the external field [11, 12]. These t-matrices are in turn obtained by solving Maxwell’s equations using the boundary element method [13, 14].

TORQUES ON NON-SPHERICAL PARTICLES

We begin by expressing the electromagnetic field acting on a given particle in terms of magnetic and electric multipoles in frequency space \( \omega \) as [11, 12, 15]

\[
E(\mathbf{r}, \omega) = \sum_{lm} \left[ \psi_{lm}^{M,\text{inc}} \mathbf{L} - \psi_{lm}^{E,\text{inc}} \frac{1}{k} \nabla \times \mathbf{L} \right] Y_{lm}(\hat{r}) \]

\[
+ \left[ \psi_{lm}^{M,\text{sc}} \mathbf{L} - \psi_{lm}^{E,\text{sc}} \frac{1}{k} \nabla \times \mathbf{L} \right] Y_{lm}(\hat{r}) \]

where \( \mathbf{L} = -i \mathbf{r} \times \nabla \) is the orbital angular-momentum operator, \( k = \omega/c \) is the momentum of the light, and the field has been separated in incident (inc) and scattered (sc) components. Assuming linear response, the coefficients of
proportionality between them are given by the scattering matrix $t$ according to

$$\psi^{\nu,\text{sc}}_{lm} = \sum_{l'm'} t^{\nu\nu'}_{lm,l'm'} \psi^{\nu'}_{l'm'} \psi^{\text{inc}}_{lm},$$

(2)

where $\nu$ runs over $M$ and $E$ components. The $t$ matrix is analytical for spherical particles $[11, 12]$ (Mie coefficients) and we have calculated it numerically using the boundary element method $[13, 14]$ for arbitrarily-shaped objects (whiskers and torii in the examples offered below).

The torque acting on the particle in the presence of this field is a quadratic, analytic function of these coefficients that can be obtained from the integral of the Maxwell stress tensor over a spherical surface $S$ of radius $R$ surrounding the object. The time-averaged torque reads $[16]$ 

$$G = -\frac{R^3}{4\pi} \int_S d\hat{R} [(\hat{R} \cdot E)(E \times \hat{R}) + (\hat{R} \cdot H)(H \times \hat{R})].$$

(3)

Then, calculating the magnetic field $H$ using Faraday’s law and inserting the resulting expression together with Eq. 1 into Eq. 3, one finds

$$G = \frac{1}{4\pi k^3} \sum_{l|m'|} l(l+1) \text{Re} \left[ \left\{ \frac{1}{2} \sqrt{(l+m+1)(l-m)} \delta_{m+1,m'} (\hat{x} - i\hat{y}) + \frac{1}{2} \sqrt{(l-m+1)(l+m)} \delta_{m-1,m'} (\hat{x} + i\hat{y}) + m \delta_{m,m'} \hat{z} \right\} \right.$$

$$\times \left[ \psi_{lm}^{E,\text{sc}} \psi_{l'm'}^{E,\text{sc}} + i \psi_{lm}^{M,\text{sc}} \psi_{l'm'}^{M,\text{sc}} + i \psi_{lm}^{E,\text{inc}} \psi_{l'm'}^{E,\text{inc}} + i \psi_{lm}^{M,\text{sc}} \psi_{l'm'}^{M,\text{inc}} \right].$$

(4)

Eq. 4 has been used here to obtain the torque acting on metallic and dielectric whiskers illuminated by a light plane wave, as shown in Fig. 1.
In the case of silver particles, the scattering cross section, which is directly obtained from the scattering amplitude, shows a pronounced resonance when the polarization of the external light is directed along the whisker [Fig. 1(a)]. The dielectric function of silver has been taken from optical data [17]. Part of the scattered light is absorbed by the metal (silver in this case), so that the total cross section (solid curve, obtained by using the optical theorem [13]) is actually larger than the elastic cross section (broken curve). The cross section for polarization perpendicular to the particle is negligible (by a factor of 40000 at the resonance) as compared with the case considered in Fig. 1(a).

The torque acting on this particle when it is illuminated by circularly-polarized light follows the same profile as the scattering cross section [Fig. 1(b)]. This torque is induced by the angular momentum carried by the external light, part of which is transferred to the particle [6].

A more interesting situation is presented when linearly-polarized light is used [Fig. 1(c)], in which case the particle tends to align itself parallel (perpendicular) to the polarization vector when light of wavelength below (above) the resonance is employed. Here, the torque scales with the sine of the angle between the polarization vector and the particle axis of symmetry. It should be noted that the torque takes non-negligible values well outside the absorption resonance, so that a sizable orientational effect can still be obtained while minimizing heat transfer to the particle (this arises from absorption of external light). Moreover, control over the particle orientation is possible by using the right combination of polarization and wavelength of the external light.

It is interesting to point out that the wavelength of the resonance depends on the length of the whisker, and this offers the possibility of manipulating separately whiskers of different lengths by tuning their respective resonances. For dielectric particles of with same shape [Fig. 1(d)-(f)], the value of the torque is one order of magnitude smaller and qualitatively very different as compared to the metallic particles discussed above. For instance, dielectric particles do not exhibit plasmon resonances, unlike metallic ones. Moreover, their total and elastic cross sections are identical, since a dielectric particle (real dielectric function) cannot dissipate energy, so that heating of the particle is avoided.

**THE EFFECT OF ENVIRONMENT ON ELECTROMAGNETIC FORCES**

For aggregates formed by several scattering objects, one can still use the multipole expansion of Eq. 1 around each of the objects. The scattered part of the self-consistent field around a given object labeled $\alpha$ is the sum of contributions coming from the other objects ($\beta \neq \alpha$) plus the scattering of the incident field. Both scattering at each object and propagation of the field between objects are linear operations (this would be different in non-linear materials), so that the self-consistent multipole coefficients satisfy the equation

$$
\psi_{\alpha}^{\text{sc}} = t_{\alpha} (\psi_{\alpha}^{\text{inc}} + \sum_{\beta \neq \alpha} H_{\alpha\beta} \psi_{\beta}^{\text{sc}}),
$$

where matrix notation has been used, that is, $\psi$ is actually a vector that contains all $M$, $E$, and $(l, m)$ components, and $t$ is the matrix of coefficients $t_{\alpha\beta}^{lm,l'm'}$, as defined in Eq. 2. Here, the matrix $H_{\alpha\beta}$ describes the propagation of the field from object $\beta$ to object $\alpha$, and it can be derived analytically in terms of the coordinates of the multipole origins for the different objects [11, 12]. Eq. 5 separates the geometrical configuration of the cluster, fully contained in $H_{\alpha\beta}$, from the actual shape and composition of the objects, which is entirely buried into $t_{\alpha}$. A similar approach can be also followed to treat two-dimensional geometries as well as photonic crystals consisting of periodic configurations of the objects [13, 14].

This multiple scattering formalism has been used to obtain Fig. 2, which shows the force acting on aluminum spheres of 55 nm in diameter when a nearby particle contributes as well to the scattering of the external field. The electromagnetic force has been calculated from the integral of Maxwell’s stress tensor [16], which results in an analytical but complicated expression in terms of the multipole coefficients. A Drude dielectric function has been used for aluminum, with a plasma energy of 15 eV and a damping of 1.06 eV. The self-consistent field has been obtained by using a method based upon multiple scattering of multipoles [11, 12]. A marked influence of the neighboring particle is observed on the force acting on the aluminum sphere, and the magnitude and even the sign of this force changes dramatically over the photon energies under consideration when choosing different particle shapes. This suggests the possibility of using neighboring effects to control the relative position of particles under the influence of external light. The polarization of the latter has been chosen to maximize these effects: a strong dipole-dipole interaction is triggered by the component of the electric field directed along the line that separates the centers of the objects, whereas the complementary polarization results in minor neighboring effects that originate in higher multiple contributions.
FIG. 2: Electromagnetic force acting on an aluminum sphere when it is illuminated in the presence of a nearby object. The light is linearly polarized, with the polarization vector contained in the plane of the insets.

CONCLUSIONS

Torques and forces acting on small particles under external illumination have been calculated in this work under illumination by a single plane wave. Electromagnetic torques acting on whiskers, both metallic and dielectric, have been shown to provide a possible tool for nanoparticle alignment. The magnitude of the torque for attainable light beam intensities is sufficiently large as to overcome other forces such as gravity and Brownian motion. Finally, the effect of neighboring particles on the electromagnetic force acting on small aluminum spheres has proven to be very large, suggesting a possible way to manipulate the relative orientation of neighboring objects under external illumination. The present study can be easily generalized to account for illumination under focused beams, which will be needed to discuss situations of practical interest in optical tweezers.

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