Optimization of an object shape
to achieve extremal axial optical force
in a standing wave

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ABSTRACT

We consider prolate objects of cylindrical symmetry with radius periodically modulated along the axial direction and we present a theoretical study of optimized objects shapes resulting in up to tenfold enhancement of the axial optical force in comparison with the original unmodulated object shape. We obtain analytical formulas for the axial optical force acting on low refractive index objects where the light scattering by the object is negligible. Numerical results based on the coupled dipole method support the previous simplified analytical conclusions and they are also presented for objects with higher refractive indices. The objects are trapped in a standing wave, that offers many useful advantages in comparison to single beam trapping, especially for submicrometer size particles. It provides axial force stronger by several orders of magnitude, much higher axial trap stiffness, and spatial confinement of particles with higher refractive index.

Keywords: optical force, nonspherical objects, analytical calculations, numerical computations, coupled dipole method

1. INTRODUCTION

Optical trapping of microobjects or nanoobjects is now well established micromanipulation technique that revolutionized various branches of physics, biology and engineering. Up to now majority of efforts has been devoted to the manipulations with spherical or close to spherical objects. The theoretical description of so called optical force is based on Lorenz-Mie scattering theory for single sphere or multiple Mie scattering theory for more considered spheres. Except spherical objects, also spheroidal or cylindrical ones are frequently considered theoretically. Optical forces acting on particles with more complex shapes must be calculated using numerical approaches - like coupled dipole method (CDM), finite element method (FEM) or finite-difference time-domain method (FDTD).

Previous studies revealed several advantages of optical trapping of smaller objects using a standing wave comparing to single beam trapping (optical tweezers). Extremal axial force and axial trap stiffness can be higher by several orders of magnitude and object confinement is possible with lower trapping power. Moreover, in contrast to single beam trap, particles with higher refractive index can be trapped. Therefore, we focused on the problem if the axial optical force can be even more enhanced by proper shape of prolate object which overlaps several periods of the standing wave intensity modulation. In this paper we focus on a prolate object of cylindrical symmetry with periodic modulation of its radius along axial axis and we consider two cases. In the first case the object is composed of several overlapping spheres (see Fig. 1-A) and in the second case the object coat is modulated sinusoidally (see Fig. 1-B). We expect that this object is placed into a standing wave so that its axial axis follows the axis of beams propagations. The depth of the radius modulation, its period, and overall length of the object is subject of changes to maximize the axial optical force.

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2. AXIAL OPTICAL FORCES ACTING UPON WEAKLY POLARIZABLE OBJECT

We assume that the radial extend of this object is much smaller comparing to radial variation of the illuminated beam. This allows us to expect an illuminating field in the form of a standing wave formed by an interference of counter-propagating plane waves of the same intensity $I_0$. Therefore the optical intensity $I$ of the standing wave has a form:

$$I(z) = 2I_0[1 + \cos(2kz)],$$

where $k = k_0n_2$ is the wavenumber in a surrounding medium (liquid) of refractive index $n_2$, and $k_0$ is the wavenumber in vacuum. We further assume that the refractive index of the object $n_1$ is slightly higher than the refractive index of the medium. Thus the presence of the object does not modify significantly the field distribution. Moreover, due to the counter-propagating geometry of the beams the radiation pressure (scattering force) coming from both beams can be omitted and only the spatial variation of the optical intensity determines the final optical force.$^{22,24}$ Therefore, the axial optical force $F_z(r_o)$ acting on an dielectric object placed at position $r_o$ can be expressed as

$$F_z(r_o) = \frac{\alpha n_2}{2c} \int_S I(r)n_z(r) \, dS,$$

where $S$ is the surface of the object, $c$ is the speed of the light in vacuum, and $n_z$ is the axial component of the outer normal unit vector to the surface $S$ at the position $r$. The object polarizability is $\alpha = (n_1/n_2)^2 - 1$.

In the rest of this article we will substitute Eq. (1) into Eq. (2) and for the surface integration and consequent analysis we will consider the two objects shapes shown in Fig. 1.

2.1 Cylinder

Let us start with the most simple case - a cylinder of length $L$ and radius $R$ oriented with its longitudinal axis parallel to the $z$ axis. Since $n_z = 0$ over the cylinder coat, the surface integration of Eq. (2) reduces only to the areas of cylinder bases placed at $z = z_A$ and $z = z_B$. Therefore the axial forces can be expressed as

$$F_{z_{\text{base}}}^{z_A} = -\frac{\alpha n_2}{2c}I(z_A)S_A,$$

$$F_{z_{\text{base}}}^{z_B} = +\frac{\alpha n_2}{2c}I(z_B)S_B,$$
where \( S_A \) or \( S_B \) denotes the area of the base at \( z_A \) or \( z_B \), respectively. Therefore the resulting optical force acting on the cylinder is equal to

\[
F_z = \frac{\alpha n_2}{2} \pi c 2 I_0 [- \cos(2kz_A) + \cos(2kz_B)] \pi R^2
= -2F_0 (kR)^2 \sin(kL) \sin(2kZ),
\]

where we used substitutions \( F_0 \) for the force amplitude and \( Z \) for the position of the cylinder centre:

\[
F_0 = \frac{\alpha n_2}{c} \frac{\pi}{k^2} I_0, \\
Z = \frac{z_A + z_B}{2}, \quad L = z_B - z_A.
\]

From Eq. (5) we can conclude several important rules. The larger \( R \) the bigger axial force. Further this force depends periodically on \( L \) but this periodic function does not change its amplitude with increasing \( L \). If \( \sin(kL) \) is positive (negative), the cylinder centre equilibrium position is placed at the intensity maximum (minimum) of the standing wave. However if \( \sin(kL) = 0 \) (i.e. cylinder length \( L \) is an integer multiple of \( \lambda/2 \), the cylinder moves freely along \( z \) axis because the acting longitudinal force is equal to zero for any cylinder positions.

### 3. SPHERICALLY MODULATED OBJECT

We deal here with the object composed of \( N \) identical overlapping spheres which are regularly displaced into a linear chain (see Fig. 1-A). The two outer spheres will be cropped by a plane perpendicular to the \( z \) axis. Therefore the object ends with two flat circular bases and positions of them can be changed by the parameter \( d \). The total force acting on the object is the sum of the force on the object \( coat \) and on its two plane \( bases \).

#### 3.1 Force on the object \( coat \)

Let us first consider a \( single cropped sphere \) of radius \( R \) centered at \( 0, 0, z_1 \). If the spherical polar coordinate \( \vartheta \) denotes an angle between \( \hat{z} \) and \( \mathbf{n}(r) \), then \( n_s = \cos \vartheta = (z - z_1)/R \). Differentiation of the last relation gives \( -\sin \vartheta \frac{d\vartheta}{dz} = dz/R \) and the polar surface element \( dS \) of the sphere can be expressed in the Cartesian coordinates using \( dS = [2\pi R^2 \sin \vartheta d\vartheta] = 2\pi R \, dz \). Therefore Eq. (2) can be rewritten to the following form:

\[
F_z(z_1) = \frac{\alpha n_2}{2} \pi c 2\int_{z_1}^{z_1} I(z)(z - z_1) \, dz,
\]

where \( z_a \) and \( z_b \) denote the axial positions of the planes cropping the sphere perpendicular to the optical axis. If Eq. (1) is substituted into Eq. (8) and the following substitution is used \( z_a = z_1 - D/2 \), \( z_b = z_1 + D/2 \), integration of Eq. (8) over one cropped sphere gives:

\[
F_z^{sph\, coat} = -F_0 G(kD) \sin(2kz_1), \\
G(kD) = \sin(kD) - kD \cos(kD).
\]

The force depends on the position of the object with respect to the standing wave by the term \( \sin(2kz_1) \) and on the geometry of the object through the factor \( G \) which is a periodic function of \( D/\lambda \) (see Fig. 2). The term \( G \) has extremal values at

\[
D = M\lambda/2; \quad M \text{ is integer},
\]

they increase linearly with \( M \) and the maximal force for this option is equal to

\[
F_z^{ex\, sph\, coat} = (-1)^M F_0 \pi M \sin(2kz_1).
\]

For \( D = 2R \) we obtain the known expression for a sphere placed into the standing wave.\(^{22}\)

However we study here an object composed of \( N \) such \( cropped spheres \) displaced \( D \) from the centres of each other. Therefore the total axial component of the optical force acting on such structure is equal to the sum of contributions done by Eq. (9) assuming that the centre of \( n \)-th cropped sphere \( z_n \) satisfies \( z_n = z_1 + (n - 1)D \).
with \( n = 1 \ldots N \). If we further define the centre of the object \( Z = (z_1 + z_N)/2 \), the total axial optical force acting on the object coat can be expressed:

\[
F_{z \text{coat}}^{N \text{sph}} = -F_0 T(kD, N) \sin(2kZ), \quad (13)
\]

\[
T(kD, N) = G(kD) \frac{\sin(NkD)}{\sin(kD)}, \quad (14)
\]

The term \( T \) plays the same role as \( G \) in Eq. (9) and determine if the object is localized in the standing wave with its centre at the fringe intensity maximum or minimum. There are many local extremes of the function \( T(kD, N) \) but only those are dominant that satisfy \( D = M\lambda/2 \) (see Fig. 3). Consequently, the related extremal values of the force (13) are

\[
F_{z \text{coat}}^{ex \text{N}\text{sph}} = (-1)^{MN} F_0 \frac{\pi MN}{2} \sin(2kZ) \quad (15)
\]

with \( M = 1, 2, \ldots M' \leq 4R/\lambda \) (bc. \( D \leq 2R \)). From Eq. (15) we can conclude that the force acting on the coat of fused spheres increases with the number of fused spheres \( N \) and surprisingly with the period \( D \) between spheres centres. Moreover, if the product \( MN \) is kept the same, the final force does not depend on the final shape of the object. Therefore \( N \) fused spheres with \( D = \lambda/2 \) will be pushed with the same maximal force as single cropped sphere with \( D = N\lambda/2 \). This force contribution from the object coat does not explicitly depend on the sphere radius \( R \) but the following must be satisfied \( D \leq 2R \).

This geometry can be made slightly more general if we assume that the original object bases placed at \( z_1 - \frac{D}{2} \) and \( z_N + \frac{D}{2} \) are shifted by a distance \( d \) into new positions \( z_A = z_1 - d \) and \( z_B = z_N + d \). This symmetrical extension on both sides keeps the object centre at \( Z = (z_A + z_B)/2 \). Therefore coat-force (13) must be added...
with two contributions obtained from Eq. (8) with integration limits \( \int_{z_A}^{z_1-D/2} \) and \( \int_{z_B}^{z_N+D/2} \), respectively. The sum of these two additional terms is equal to

\[
\Delta F^N_{z \text{coat}} = F_0 \left[ 2kd \cos(kL) - \sin(kL) + \sin(NkD) - kD \cos(NkD) \right] \sin(2kZ),
\]

\[
L = z_B - z_A = (N - 1)D + 2d,
\]  

where \( d \in (0; R) \) for \( N = 1 \) and \( d \in (-\frac{D}{2}; R) \) for \( N > 1 \), \( L \) is the length of the whole object.

Let us note that for unsymmetric displacements on both object ends it is not possible to separate the phase term \( \sin(2kZ) \) in Eq. (16).

### 3.2 Force on the bases

The total axial optical force acting on both plane circular bases located at \( z_A \) and \( z_B \) can be expressed using Eq. (5) as

\[
F^N_{z \text{bases}} = -2F_0 \left[ (kR)^2 - (kd)^2 \right] \sin(kL) \sin(2kZ),
\]

because we have \( S_A = S_B = \pi(R^2 - d^2) \).

### 3.3 Total force on the object

The total axial optical force is done as the sum of the forces acting on the object coat (Eq. (13), Eq. (16)) and on the object bases (Eq. (18)):

\[
F^N_{z \text{total}} = F^N_{z \text{coat}} + \Delta F^N_{z \text{coat}} + F^N_{z \text{bases}}.
\]  

It can be shown that if we fix \( R \) and \( N > 1 \), the extremal total force is obtained for

\[
D = M'\lambda/2, \quad M' = \max(M)
\]

\[
d = +\lambda/8, \quad M' \text{ is odd}
\]

\[
d = -\lambda/8, \quad M' \text{ is even}
\]

where \( M' \) is the greatest available integer \( M = M' \leq 4R/\lambda \) (see Eq. (15)). The corresponding extremal value of the total force is equal to

\[
F^N_{z \text{total}}(N, R) = (-1)^M N F_0 \left\{ 8\pi^2 \left( \frac{R}{\lambda} \right)^2 + 1 - \frac{\pi^2}{8} + \pi M'(N - 1) \right\} \sin(2kZ).
\]  

All these results are illustrated in Figs. (4, 5) which compare the total axial optical force as a function of sphere centre difference \( D/\lambda \) and sphere radius \( R/\lambda \) for bases displacements \( d = -\lambda/8, d = +\lambda/8, d = 0 \) and \( d = R \). White areas in the graphs correspond to impossible compositions of the object, due to the relevant inequalities noted in the graphs. Here we can see that maximal values of the force are taken near at \( D/\lambda = M/2 \) and always for \( d = \pm\lambda/8 \) depending on parity of \( M \), entirely according to the results mentioned above. Note that the extreme positions in Eq. (11) hold exactly for force acting on the coat in Eq. (13), but forces caused by the bases and their displacements \( d \) can more or less disturb this condition.

### 4. SINUSOIDALLY MODULATED OBJECT

In this section we will consider an object with sinusoidally modulated radius along \( z \) axis that forms a sinusoidal chain as depicted in Fig. 1-B. The amplitude of this modulation is denoted \( A \) and other parameters are the same as for the spherically modulated object. The axial optical force acting upon the object coat is calculated using Eq. (2) and can be expressed as

\[
F^\sin_{z \text{coat}} = F_0 (T_1 + T_2) \sin(2kZ),
\]
Figure 4. Amplitude of the axial optical force $F_{z}^{\text{optical}}$ as a function of the distance $D$ between the centres of neighbouring overlapping spheres and the sphere radius $R$ for optimized displacements of bases $d = \lambda/8$ (upper graph) and $d = -\lambda/8$ (lower graph) resulting in extreme forces. Number of units $N = 4$ is the same for both graphs. Refractive index of the environment $n_2 = 1.33$, refractive index of the object $n_1 = 1.35$, and $F_0$ is normalized to 1 pN. The marked points indicate local extremes of the force calculated numerically.

where the dimensionless terms $T_1$ and $T_2$ are equal to

\begin{align}
T_1 &= (kA)^2 \frac{\tilde{D} \cos(kL) \sin(2kd/\tilde{D}) - \sin(kL) \cos(2kd/\tilde{D})}{(\tilde{D} + 1)(\tilde{D} - 1)}, \\
T_2 &= (kA)(kR - kA) \frac{2\tilde{D} \cos(kL) \sin(kd/\tilde{D}) - \sin(kL) \cos(kd/\tilde{D})}{(\tilde{D} + 1/2)(\tilde{D} - 1/2)},
\end{align}

with modulation period in wavelength units $\tilde{D} \equiv D/\lambda$. The sum of both terms $T_1 + T_2$ is a nontrivial function of the dimensionless parameter $\tilde{D}$ with many local extremes. However, there are always two dominant extremes at singular points $\tilde{D}_1 = 1$ and $\tilde{D}_2 = 1/2$. This property enables to express the extreme total optical forces analytically.

Following our previous results expressed by Eq. (5) the force on the object bases takes analogous form

\begin{equation}
F_{z}^{\text{bases}} = -2F_0 (kB)^2 \sin(kL) \sin(2kZ),
\end{equation}

where the bases radii are denoted by $B \equiv r(z_A) = r(z_B)$.

The total axial optical force is done as

\begin{equation}
F_{z}^{\text{total}} = F_{z}^{\text{coat}} + F_{z}^{\text{bases}} = -F_0 [2(kB)^2 \sin(kL) - T_1 - T_2] \sin(2kZ).
\end{equation}

Due to the mirror symmetry of this object the position term $\sin(2kZ)$ can be again separated and the position independent amplitude of the total force can be expressed analytically. Extreme value of the total force in
Figure 5. Amplitude of the axial optical force $F_{z}^{Naph}$ (see Eq. (19)) as a function of the distance $D$ between the centres of neighbouring overlapping spheres and the sphere radius $R$ for the bases displacements $d = 0$ (upper graph) and $d = R$ (lower graph). Number of units $N = 4$ is the same for both graphs. Refractive index of the environment $n_2 = 1.33$, refractive index of the object $n_1 = 1.35$, and $F_0 = 1 \text{pN}$. The marked points indicate local extremes of the force calculated numerically.

Eq. (25) at extreme points $D_1$ and $D_2$ is reached for $d = (2Q + 1)\lambda/8$, where $Q$ is an integer. Because of restrictive conditions on bases displacement $d$ given by Eq. (17) only one solution $d = \lambda/8$ is allowed and the extreme amplitude of the total force has the following forms for the two cases $D_1 = \lambda$, $D_2 = \lambda/2$:

$$F_{z_1}^{\text{max total}} = F_0(kR)^2 \left\{ \left[ \frac{2}{3} \sqrt{2} - \frac{3}{4} + (3 - 4N) \frac{\pi}{16} \right] v^2 + \left[ 2 - \frac{4}{3} \sqrt{2} v - 2 \right] \right\},$$

$$F_{z_2}^{\text{max total}} = (-1)^N F_0(kR)^2 \left\{ \left[ \frac{5}{16} - (2N - 1) \frac{\pi}{4} \right] v^2 + \left[ (2N - 1) \frac{\pi}{2} - 2 \right] v + 2 \right\},$$

where we used the dimensionless coefficient $v \equiv 2A/R \in (0; 1)$ expressing deviation of the object shape from a cylinder ($v = 0$). We see that the amplitudes of both forces in Eq. (26) and Eq. (27) grow with the area of the widest profile ($\pi R^2$) and number of units $N$ if the parameter $v$ is fixed. However, only the force amplitude in Eq. (27) changes its sign with consequent numbers of $N$. If $N = 1$, both forces amplitudes reach extreme value at $v = 0$ and they are equal; it gives the shape of a cylinder of length $L = \lambda/4$. If $N \geq 2$, the force amplitude of Eq. (27) is extreme for

$$v = 1 - \frac{2}{3\pi(2N - 1) - 10},$$

which is always larger than the extreme force amplitude from Eq. (26) occurring at $v = 1$. Both extreme values of the forces occur for $v$ close to 1. Interestingly, if the parameter $v$ grows from 0 to 1 and the force amplitude increases, the volume of the object decreases

$$V_2 = R^2 \frac{\lambda}{8} \left[ 2v(2 - v) + \pi(2N - 1) \left( 2 - 2v + \frac{3}{4} v^2 \right) \right].$$
Figure 6. Amplitude of the total axial optical force $F_{z, \text{total}}$ (done by Eq. (25)) acting upon the sinusoidal chain as a function of modulation period $D$ and coefficient $v = 2A/R$ with fixed $R = 0.6\lambda$ (upper graph) or radius $R$ with fixed $v = 0.5$ (lower graph) for the same displacements of bases $d = \lambda/8$, number of units $N = 4$, and $F_0 = 1\, \text{pN}$.

Figure 6 demonstrates how the amplitude of the total axial optical force acting upon sinusoidal chain varies with $D$, $R$, and $v$. They illustratively demonstrate the analytical conclusions in Eqs. (26,27,28) presented above, too.

5. CALCULATION BY COUPLED DIPOLE METHOD

The analytical results of the previous sections enable us to study the problem of optimized shape in a great detail. Even though the results are limited by the assumption of small relative refractive index between studied objects and medium there could a possibility to generalize the behaviour also to systems where the scattering from the studied objects plays substantial role. In order to prove this assumption, a more rigorous method must be used to express the optical forces using proper light scattering theory. We used our numerical code based on coupled dipole method (CDM) which was previously successfully employed in the calculation of the scattered light and subsequently the optical forces acting upon several objects of various sizes.\textsuperscript{25–27} In CDM the shape of the object is approximated by induced elementary dipoles spread in a cubic lattice. We used the cubic lattice parameter of the order of 0.01$\lambda$ to have quite smooth surface of the object. This distance between dipoles amply satisfies the upper limit $\lambda/20$ given by CDM.\textsuperscript{28}

Figure 7 compares the axial optical force acting upon five overlapping spheres calculated analytically and by CDM. Two different object refractive indices were considered $n_1 = 1.35$ and $n_3 = 1.41$ (e.g. silica). Figure 7 demonstrates that the resulting force amplitudes obtained from CDM are in very good agreement with the analytical ones if the object refractive index is very close to the host medium refractive index ($n_2 = 1.33$; $m \equiv n_1/n_2 = 1.015$). It also shows significant deviations for the object made of silica.

The influence of the refractive index of several overlapping spheres on the optical force is shown in Fig. 8 in more details. It again reveals very good coincidence between analytical approximation and numerical computation by CDM for low refractive indices but significant deviations for higher refractive indices of the object.
Figure 7. Comparison of the amplitudes of the axial optical forces acting upon five overlapping spheres made of refractive indices $n_1 = 1.35$ and $n_1 = 1.41$ (silica). The forces are calculated analytically (dashed line) and numerically by CDM (solid line) as a function of sphere diameter $2R$. The following parameters were used: refractive index of the host medium $n_2 = 1.33$, number of units $N = 5$, sphere period $D = 0.7\lambda$, bases displacement $d = 0$, and $F_0 = 1$ pN.

Figure 8. Comparison of the axial optical force amplitudes as a function of period $D$ of overlapping spheres (Fig. 1-A) and object refractive index $n_1$. Lower graph shows analytical results from Eq. (19) and middle graph shows results by numerical CDM, both for the sphere radius $R = 0.6\lambda$, bases displacement $d = 0$, refractive index of the host medium $n_2 = 1.33$, and $F_0 = 1$ pN. Number of units $N = 4$ is the same for all graphs. The profiles of the force amplitudes at $n_1 = 1.35$ are in a very good agreement (see upper graph). However with increasing the object refractive index $n_1$ locations of the axial force extremes with respect to $D$ and force magnitudes change. This is because of the optical field scattered by the object that cannot be neglected anymore and that modifies the incident (standing wave) field.

We can immediately see that the value of $D$ giving extreme force amplitude decreases uniformly with the object refractive index. The optimized shape of the object again ensures extreme force which increases with number of units $N$. By proper design of the object composed of several units one can reach the optical force several times stronger comparing to the single unit.
6. CONCLUSION

Up to now mainly optical forces acting upon spherical or cylindrical objects have been studied. Obtained optical forces are generally very weak and any method is very useful which increases them keeping the same incident laser power. This study shows a novel way that combines two possible optical methods how to address such a force increase - utilization of structured light illumination of the trapping beam combined with the spatially structured shape of the object. We considered a prolate object with radially modulated shape placed into a spatially periodic light pattern (optical standing wave). First we assumed that the refractive index of the object is close to the refractive index of the surrounding medium. It allowed us to express the optical forces analytically for objects composed of several units in the form of overlapping spheres or sinusoidal chain. We found analytical conditions giving maximal amplitude of the optical force. This force amplitude increases linearly with the number of units and with the squared radius of the bases. Proper distance between the centres of the units ensures rapid increase of the force. To extend our study to objects of higher refractive index we used coupled dipole methods to calculate numerically the optical forces. We obtained very good coincidence with the analytical results for low refractive indices. The expected significant deviations from the analytical results were obtained for higher refractive indices. Especially, the distance $D$ between the units (axial periodicity of the object), providing the extreme force amplitude, decreases with increasing refractive index of the object. However, if this condition is fulfilled, obtained optical force can be many times stronger.

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