Optical trapping core formation and general trapping mechanism in single-beam optical tweezers

Di Huang1, Pengcheng Wan1, Ling Zhou1, Haiqin Guo1, Ruihuang Zhao1, Jun Chen2,3, Jack Ng4,* and Junjie Du1,*

1 State Key Laboratory of Precision Spectroscopy, School of Physics and Electronic Science, East China Normal University, Shanghai 200062, People’s Republic of China
2 State Key Laboratory of Quantum Optics and Quantum Optics Devices, Institute of Theoretical Physics, Shanxi University, Taiyuan, Shanxi 030006, People’s Republic of China
3 Collaborative Innovation Center of Extreme Optics, Shanxi University, Taiyuan, Shanxi 030006, People’s Republic of China
4 Department of Physics, Southern University of Science and Technology, Shenzhen, Guangdong 518055, People’s Republic of China

* Authors to whom any correspondence should be addressed.
E-mail: wuzh3@sustech.edu.cn and phyjunjie@gmail.com

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Abstract

The working mechanism of single-beam optical tweezers is revisited using a recently established method. The optical force is split into conservative and nonconservative components, and these components are explicitly calculated for particles in the Rayleigh, Mie and geometrical optics regimes. The results indicate that optical trapping is attributable to the formation of an ‘optical trapping core’. Stable trapping is achieved when the conservative forces are larger than the nonconservative forces in the core region centered at the beam centers for all particle sizes. According to the conventional understanding, stability is a result of the conservative force overcoming the nonconservative force. In comparison, the concept of the optical trapping core more accurately illustrates the physical mechanism of optical trapping, for not only single-beam optical tweezers but also optical trapping settings.

1. Introduction

Optical forces represent an indispensable tool in many areas of science and technology [1–3]. In atomic physics, optical forces are the basis for laser cooling techniques [4], which have led to the realization of Bose–Einstein condensation systems [5, 6] and atomic lasers [7, 8]. When applied to colloidal particles, optical micromanipulation can realize all-optical sorting [9, 10], provides insight into Brownian motion [11, 12] and colloidal dynamics [13–15], as well as creates analogs of atomic and superconductive systems [16, 17]. Furthermore, in the domain of biological sciences, optical manipulation can allow the examination of biological processes at the single-molecule level or at the cellular and subcellular levels.

A milestone in optical micromanipulation is the stable optical trapping of nanoparticles by single-beam optical tweezers [18–23]. In general, the optical trapping of small Rayleigh particles [24–26] and large particles in the context of the geometrical optics limit [27] has been examined based on the decomposition of the optical force into two components, namely, conservative and nonconservative forces. These forces have different attributes and applications. Specifically, conservative and nonconservative forces can be applied to trap and to transport particles, respectively. Conservative forces $F_c$ are irrotational with $\nabla \times F_c = 0$, and the work done by them is path independent. This work can be derived from a scalar potential $U$ as $\int -\nabla U$, while nonconservative forces $F_{nc}$, which include scattering and absorption forces in general, is solenoidal with $\nabla \cdot F_{nc} = 0$. In the geometric optics and Rayleigh regimes, the analytical expressions of the conservative/nonconservative force can be derived by calculating the reflectance and transmittance representing the momentum transfer and by handling Rayleigh particles as a point dipole immersed in the light fields, respectively. In the Rayleigh regime, conservative forces are referred customarily to as the gradient force because they are proportional to $\nabla |E|^2$, while nonconservative forces...
for nanoparticles with negligible absorption, atoms and molecules are known as scattering forces. The conservative and nonconservative forces in the intermediate Mie regime can also be considered gradient and scattering forces when light absorption is negligible [28], respectively. However, the calculation of the conservative and nonconservative forces in the Mie regime is challenging. The difficulty in such calculations pertains to the comparable dimensions of the Mie particles and the wavelength, owing to which the Rayleigh and geometric approximations fail. In the absence of optical force decomposition techniques, we are not clear what is the difference between the magnitude of the conservative and nonconservative forces, as well as their respective spatial distribution. Consequently, experimental calibrations must be performed to estimate the nonconservative forces [29–33], which limits the physical understanding of the associated phenomena.

Recently, a numerical method based on the fast Fourier transform has been proposed for calculating the conservative and nonconservative forces in the Mie regime [34, 35]. Moreover, several analytical approaches have been established [36–38]. In general, the trapping of a particle by optical tweezers is considered to occur when the axial conservative force is larger than the axial nonconservative force. This rule holds for Rayleigh particles. However, Mie particles can be trapped by optical tweezers even when the maximum magnitude of the axial nonconservative forces is greater than that of the axial conservative forces, as the maxima of these forces need not coincide. The present study is focused on identifying the ‘optical trapping core’ near the beam center. Optical trapping can be interpreted within a unified theoretical framework when particle trapping is conceived to occur in this core. By examining the general mechanism, the spatial distribution of conservative and nonconservative forces can be considered to alleviate the requirement of the dominant conservative field.

2. Results and discussion

2.1. Optical trapping of Rayleigh particles

We use the decomposition technique presented in Refs. [36, 37] to calculate the optical conservative and nonconservative forces. Dielectric spherical particles with permittivity \( \varepsilon = 1.59^2 \) and permeability \( \mu = 1 \) are immersed in water (\( \varepsilon = 1.33^2 \) and \( \mu = 1 \)). In this paper, these particles are referred to as ‘low-index’ particles to distinguish them from silicon particles with \( \varepsilon = 12 \), discussed in subsequent sections. The incident beam is an \( x \)-polarized fundamental Gaussian beam propagating along the \( z \)-direction centered at the coordinate origin. The light wavelength is \( \lambda = 1.064 \ \mu \text{m} \), numerical aperture (NA) is 1.3, waist radius is approximately 260 nm and filling factor is 1. First, we investigate Rayleigh particles with radius \( r = 50 \ \text{nm} \).

Figures 1(a) and (b) show the profiles of the axial gradient and scattering forces, \( F_z^g \) and \( F_z^s \) in the \( y-z \) plane, respectively. All forces are presented in units of \( \varepsilon E_0^2 / k^2 \), where \( E_0 \) characterizes the amplitude of the optical field [36]. Each data point in the contour figures represents a gradient/scattering force when the sphere center is located at this position. The global maxima of \( F_z^g \) and \( F_z^s \) lie on the beam axis. To trap the particles, the gradient force, which functions as the restoring force, must be larger than the scattering force because the strongest gradient and scattering forces lie on the same line. Figure 1(c) shows the profiles of \( F_z^g \) and \( F_z^s \) along the \( z \)-axis. The gradient force is one order of magnitude larger than the scattering force, and thus, trapping can be realized in the axial direction. In practice, it is also necessary to overcome the Brownian motion if the trapping occurs in an aqueous environment, which is typically difficult for Rayleigh particles. In the transverse direction perpendicular to light beam axes, the gradient force is significantly larger than the scattering force. Consequently, the gradient force is dominant in all directions. In this scenario, the optical trapping of Rayleigh particles is a result of the competition between the gradient and scattering forces. The core region surrounded by the strongest gradient forces in various directions can be considered an optical trapping core. Thus, the optical trapping of Rayleigh particles can be interpreted from the concept of the optical trapping core.

2.2. Formation of optical trapping core for low-index dielectric Mie particles

Particles with radii comparable to or larger than the wavelength must be treated as Mie particles instead of Rayleigh particles. As shown in figures 1(d)–(f), a dielectric sphere with a radius of 2 \( \mu \text{m} \) and the same permittivity as that of the Rayleigh particle shown in figures 1(a)–(c) is used to investigate the trapping mechanisms of Mie particles. Similar to figures 1(a) and (b), figures 1(d) and (e) show the spatial profiles of the conservative and nonconservative forces along the \( z \)-direction on the \( y-z \) plane, \( F_z^g \) and \( F_z^nc \), respectively. \( F_z^g \) are analogous to the conservative force of Rayleigh particles; however, the nonconservative forces \( F_z^nc \) are considerably different. As shown in figure 1(b), the global maximum for \( F_z^nc \) for Rayleigh particles occurs at the beam center. In contrast, \( F_z^nc \) acting on the Mie particle is small near the beam center, and the maximum \( F_z^nc \) occurs far from the center. This difference is associated with the difference in the scattering characteristics for both types of particles. At the beam center, with the largest incident intensity, the light
scattering by Rayleigh particles reaches its strongest extent with the strongest dipole mode induced.
However, the light scattering by Mie particles is not strongest at the beam center. Figure 1(f) shows that
surprisingly $F_{z \text{nc}}$ is nearly zero at the beam center. The reason for this unexpected phenomenon is analyzed
in subsection D. Both $F_{z \text{c}}$ and $F_{z \text{nc}}$ in the central region are smaller than the maximum $F_{z \text{c}}$, which appears in
the region boundary. Moreover, $F_{z \text{c}}$ is larger than $F_{z \text{nc}}$ inside the region.

Subsequently, we consider the transverse optical force. The conservative and nonconservative forces
along the $y$ direction on the $y$–$z$ plane, $F_{y \text{c}}$ and $F_{y \text{nc}}$, respectively, are shown in figures 2(a) and (b) for
the dielectric Mie particle considered in figures 1(d)–(f). Similar to those for Rayleigh particles, the transverse
nonconservative force is approximately one order of magnitude weaker than the conservative force, and
thus, the particle can be trapped along the transverse directions. The transverse nonconservative force is
nearly zero at the beam center, and the conservative and nonconservative forces in the circular core region
near the beam center are smaller than the conservative force on the annulus, as shown in figure 2(a).

The axial and transverse conservative and nonconservative forces exhibit similar features on the $x$–$z$ and
$y$–$z$ planes. So far, we have been able to establish a three-dimensional profile of the complete optical force
field: in the core region near the trap center, the conservative forces are greater than the nonconservative
forces. However, both types of forces are smaller than the conservative forces in the boundary of the core
region, and outside the boundary, the nonconservative forces are larger than the conservative forces.
Figure 3. Axial conservative force $F_z^c$ (a) and axial nonconservative force $F_z^{nc}$ (b) on the $y$–$z$ plane for a spherical metallic Mie particle with radius $r = 1 \mu m$. (c) $F_z^c$ and $F_z^{nc}$ along the dashed line ($z$-axis) marked in (a) and (b). Axial conservative force $F_z^c$ (d) and axial nonconservative force $F_z^{nc}$ (e) on the $y$–$z$ plane for a high-index dielectric Mie particle with $\varepsilon = 12$ and $r = 1 \mu m$. (f) $F_z^c$ and $F_z^{nc}$ along the dashed line ($z$-axis) marked in (d) and (e).

Particles whose centers are inside this core region can be pulled toward the beam center by a large conservative force. Thus, the core region can be considered an optical trapping core for the particle, and the particle is optically trapped within this core. The maximum values of the nonconservative forces are larger than those of the conservative forces, as shown in figures 1(d) and (e). However, the comparison of the maximum values is meaningless because these values occur in different positions: in the boundary of and beyond the optical trapping core for the conservative and nonconservative forces, respectively. Hence, the explanation that the optical trapping of a particle depends on the competition between $F_c$ and $F_{nc}$ may be slightly vague, because the trapping success also depends on the spatial distribution of the forces. The trapping of low-index dielectric Mie particles is attributable to the formation of the optical trapping core. Notably, the strong nonconservative forces outside the optical trapping core prevent particles from entering the core region. Figure 1(e) highlights two characteristics of nonconservative forces: first, the magnitudes of these forces are considerably greater on the side of the beam than on the front and back. Second, the direction is consistent with the propagation direction of the beam. In practice, to trap a particle, the particle can be allowed to enter the optical trapping core along the beam axis. To ensure that a particle located before the beam waist enters this core, the particle must have a finite velocity along the beam propagation direction. In this case, the particle is subjected to conservative and nonconservative forces along the $z$-direction near the optical trapping core, and it can be easily trapped. Nevertheless, the particle may be accelerated by the optical forces. A particle located after the beam waist can enter the optical trapping core with an initial velocity in the direction opposite to the beam propagation direction. Specifically, the direction of the velocity is opposite to that of the nonconservative forces. Therefore, the particle velocity decreases, which is conducive to stable trapping.

2.3. Mechanism underlying the failed trapping of metallic or high-index dielectric Mie particles

We examine the profile of conservative and nonconservative optical forces for metallic and high-index dielectric Mie particles. In figures 3(a) and (b), profiles of the axial conservative and nonconservative forces $F_z^c$ and $F_z^{nc}$, respectively, are plotted on the $y$–$z$ plane for metallic Mie particles with $\varepsilon = -57.9 + 0.6i$ and $r = 1 \mu m$. As in the case of Rayleigh particles, the maximum values of $F_z^c$ and $F_z^{nc}$ simultaneously appear on the axis of the beam. However, $F_z^{nc}$ is larger than $F_z^c$ everywhere, as shown in figure 3(c), and thus, the optical trapping core is not generated. The core is not formed for high-index dielectric Mie particles either, as shown in figures 3(d)–(f), which illustrate the optical forces on a spherical silicon particle with $\varepsilon = 12$ and $r = 1 \mu m$. The observations based on figures 3(d) and (e) are strikingly different from those in figures 1(d) and (e). The optical trapping core is not formed in this case because the nonconservative force is considerably larger than the conservative force, as shown in figure 3(f). The absence of an optical
Figure 4. Axial conservative force $F_z^c$ (a) ((d)) and transverse conservative force $F_y^c$ (b) ((e)) on the $y$–$z$ plane; and axial nonconservative force $F_z^{nc}$ (c) ((f)) in the $x$–$y$ plane for a particle with a radius of $3 \, \mu$m ($6 \, \mu$m). (g) $F^c_z$ along the black dashed line marked in (a) and (d) for the two radii. (h) $F^c_y$ along the black dashed line marked in (b) and (e) for the two radii. (i) $F^{nc}_z$ along the black dashed line marked in (c) and (f) for the two radii. The peak positions of the forces are marked by the black dashed lines in (g), (h), and (i).

trap core explains why single-beam optical tweezers cannot be directly used to trap metallic or high-index dielectric Mie particles.

2.4. Properties of the optical trapping core
We investigate the correlation between the size of the optical trapping core and the particle size. Force components $F_z^c$, $F_y^c$ and $F_z^{nc}$ are sufficient for investigating the three-dimensional profile of the optical force fields, as indicated in figures 1 and 2, because components $F_x^{nc}$ and $F_y^{nc}$ are negligible, and $F_z^c$ is comparable to $F_y^c$. Therefore, we present the axial and transverse conservative forces on the $y$–$z$ plane ($F_z^c$ and $F_y^c$, respectively) in figures 4(a) and (b) for a particle with a radius of $3 \, \mu$m and in figures 4(d) and (e) for a particle with a radius of $6 \, \mu$m. The axial and transverse conservative forces shown in figure 4 are similar to those shown in figures 1(d) and 2(a), respectively. The axial nonconservative force $F_z^{nc}$ of the two differently sized particles on the $y$–$z$ plane is similar to that shown in figure 1(e). To characterize the optical trapping core, figures 4(c) and (f) show the $F_z^{nc}$ values of the two particles on the $x$–$y$ plane instead of the $y$–$z$ plane. The large $F_z^{nc}$ is distributed on a circle, indicating that the optical trapping core is approximately spherical.

Figures 4(g)–(i) show the change in the force components $F_z^c$, $F_y^c$ and $F_z^{nc}$, respectively, represented as black dashed lines. The distances from the beam center to the peaks of the force components represent the radius of the spherical optical trapping core. Because the conservative forces are larger than the nonconservative forces within the region, the particle can be trapped. All the peaks lie approximately $3 \, \mu$m from the beam center for a particle with a radius of $3 \, \mu$m. In other words, the radius of the optical trapping core is nearly equal to the radius of the particle. A similar observation can be made for the particle with a radius of $6 \, \mu$m. These findings demonstrate that the radius of the optical trapping core is related to the particle size and is approximately equal to the radius of spherical particles.

To quantitatively examine the size of the optical trapping core, we evaluate the distances between the beam center and peaks of $F_z^c$, $F_y^c$ and $F_z^{nc}$ for Mie particles with radii ranging from $1 \, \mu$m to $8 \, \mu$m, expressed as $R_z^c$, $R_y^c$ and $R_z^{nc}$, respectively. The ratios of $R_z^c$, $R_y^c$, and $R_z^{nc}$ to the particle radius $r$ are plotted as a function of $r$ in figures 5(a)–(c), respectively. The ratios are nearly unity for all force components. Therefore, the optical trapping core can be considered to be nearly spherical, with radii approximately equal to those of trapped particles.
We attempt to clarify the mechanism of formation of the optical trapping core. For a low-index dielectric spherical particle with a size comparable to or larger than the wavelength, the geometrical optics approximation is applicable. When the particle center coincides with the center of an aplanatic beam, the light ray is incident normally on the spherical surface of the particle. Notably, the reflection coefficient for normal incidence is small for low-index dielectric particles in water (i.e., 1.57/1.33), and thus, most of the ray simply passes through without transferring momentum to the particle. Therefore, the optical force intensity is low when the particle is located in the beam center. As the particle moves away from the beam center, several rays are incident at an oblique angle, corresponding to an increase in the force. Furthermore, this system is scalable, for example, the size of the optical trapping core for a particle with a radius of 6 μm is approximately double that of a particle with a radius of 3 μm, because the geometrical optics theory is valid. In contrast, when high-index or metallic particles are located in the beam center, the optical waves are strongly scattered and optical trapping core is not generated. Therefore, the formation of the optical trapping core allows the trapping of low-index Mie and geometric particles. The failure of formation of an optical trapping core is the reason why a single beam cannot trap high-index and metallic particles of the same size.

3. Conclusions

This study clarifies the physical mechanism of an ‘optical trapping core’ to understand optical trapping in single-beam optical tweezers. This mechanism, which holds for the Rayleigh, Mie and geometrical optics regimes, is generalized for optical trapping applications. In the case of Rayleigh particles, the region surrounded by the gradient forces can be considered the optical trapping core because the scattering forces are smaller than the gradient forces at all locations. In the case of low-index dielectric Mie particles, the most intense parts of nonconservative force fields lie far from the beam centers. In the core region, conservative forces are larger than nonconservative one. The core region thus functions as an ‘optical trapping core’ to trap particles. Accordingly, high-index dielectric and metallic Mie particles cannot be trapped because ‘optical trapping core’ is not formed. Therefore, optical trapping in single beam optical tweezers can be generally explained by the concept of ‘optical trapping core’. The picture of ‘optical trapping core’ offered in this paper should be useful in the precise control of particles.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.
ORCID iDs

Junjie Du https://orcid.org/0000-0003-4311-1707

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