Trapping double negative particles in the ray optics regime using optical tweezers with focused beams

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Abstract: The capabilities of optical tweezers to trap DNG (double negative) spherical particles, with both negative permittivity and permeability, are explored in detail by analyzing some interesting theoretical features not seeing in conventional DPS (double positive) particles possessing positive refractive index. The ray optics regime is adopted and, although this regime is quite simple and limited, its validity is already known and tested for DPS particles such as biological cells and molecules trapped by highly focused beams. Simulation results confirm that even for ray optics, DNG particles present unusual and interesting trapping characteristics.

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1. Introduction

In 1970, A. Ashkin [1,2] performed the first experiments on optical trapping by the forces of radiation pressure, opening a new and exciting research area in the physical sciences. Although the existence of the radiation pressure was proved at the beginning of the twentieth century, it took about seventy years so that this radiation could be used in manipulating dielectric particles and individual atoms by either two-beam traps or levitation traps [3].

Since three-dimensional trapping of dielectric particles was demonstrated for a single, highly focused beam [4], optical tweezers has found interesting applications in manipulating biological cells, such as trapping of viruses and bacteria [5], induced cell fusion [6], studies of chromosome movement [7] and cellular microscopy [8].

Another interesting research area began in 1968 with Veselago [9] and his first considerations on materials possessing both theoretical negative permittivity and permeability. But his theoretical hypothesis had to wait about 30 years when the first experiments, based on periodic array of interspaced conducting nonmagnetic split ring resonators and continuous wires, showed double negative (DNG) behaviors in the microwave regime [10]. Since then, diverse applications appear, such as perfect lens and subwavelength focusing [11], antennas, couplers and resonators, etc. (see, for example, [12,13]).

In this work, we make some considerations about what would happen if one places an optical tweezers in a (so far) hypothetical DNG sphere of the order of one micron. In the ray optics regime, a conventional – DPS - material with refractive index higher (less) than the medium would experience a force toward (away from) regions of high intensity of the beam. As we shall see, this is not necessarily the case when we deal with a DNG sphere.

2. Theoretical analysis

Consider a sphere possessing either a positive or a negative refractive index and suppose that two distinct rays impinge it at different angles like shown in Figs. 1(a) and 1(b). Part of the ray is reflected, and part is transmitted into the particle, according to Snell’s law and energy considerations. If we assume negative refractive index, the rays deviate inversely (“negative” angle [9]) when it enters the particle, which can be represented by dashed lines. The point \( f \) is the focus of the beam, where all incident rays would converge in the absence of the sphere.

In both cases, the expected path followed by the rays in a conventional medium results in repulsive forces \( F_1 \) and \( F_2 \) for \( n_1 > n_2 \) and the particle is directed away from their axis; for \( n_1 < n_2 \), these forces become attractive, and the particle tends to be aligned with the optical axis.

However, the situation becomes more complicated for a DNG particle, where simple rays, depending on their incidence angle, could cause an attractive or a repulsive force for \( n_1 > |n_2| \). This could be explained in terms of geometrical considerations using Fig. 1(a), or by recalling the change of momentum as directly related to the produced force, using vector notation. In any case, the new force \( F_1' \) is directed along the bisector of the triangle formed by ray 1 and its transmitted rays. To explain this result mathematically, we can calculate these forces just as they were calculated for a conventional particle based on Fig. 1(c) where an incident ray with power \( P \) hits the particle with an angle \( \theta_i \) to the normal of its surface. The difference from past considerations lies on the distinct paths for the infinite series of transmitted and reflected rays when that particle has a negative refractive index [14].

Consider the gradient force \( F_x \) to be the \( x \)-component of the vector force that points in a direction perpendicular to the axis of the ray, and the scattering force \( F_s \) to be the component along this axis. As a result of the negative refractive angle, we find

\[
F_s = \frac{n_i P}{c} \left( R \sin 2\theta_i \frac{T^2 \left[ \sin (2\theta_i + 2\theta_t) + R \sin 2\theta_t \right]}{1 + R^2 + 2R \cos 2\theta_t} \right)
\]  
(1)
2 \cos \theta_i \cos \theta_t \right] \right] \right], \quad (2)

where \( c \) is the speed of light in vacuum, \( R \) and \( T \) are the Fresnel coefficients of reflection and transmission, respectively. Due to the difference of \( 2 \theta_i \) for the first transmitted ray, in Eqs. (1) and (2) there is a change in sign in the argument of both cosine and sine of \((2 \theta_i + 2 \theta_t)\) when compared to conventional particles, resulting in different forces [14]. To illustrate this situation, consider Fig. 2, where \( F_g \) and \( F_s \) are plotted as functions of \( \theta_i \), supposing a highly focused beam with a numerical aperture of 66°, typical of the microscopes used in experimental setups. A circularly polarized beam has been assumed, and we have imposed \( n_1 = 1.33 \) for the medium, \(|n_2| = 1.62 \) (Figs. 2(a) and 2(b)) or \(|n_2| = 1.21 \) (Figs. 2(c) and 2(d)).

Fig. 1. Geometric optics when (a) the medium possesses an refractive index \( n_i \) higher than the modulus of the refractive index of the sphere, \(|n_2|\), and (b) the inverse case. In (a), transmitted angles are greater than the incident ones, whereas for (b) those angles are smaller. Stronger forces act on the particle when it is DNG, due to a more intense variation of the momentum of the ray. In (c), a series of infinite rays appears when the incident ray, with power \( P \), hits the DNG particle (\( n_1 > |n_2| \) or vice-versa).

For Figs. 2(a) and 2(c) the particle has positive refractive index and \( F_g \) (solid lines) is directed toward the ray axis - tending to bring it closer to the ray itself – for \( n_2 > n_1 \), or away from this axis – repulsive force – for \( n_2 < n_1 \). The scattering force (dashed lines) is always positive, growing in magnitude for higher angles of incidence, as expected.

As for Figs. 2(b) and 2(d), however, the scattering force is highest for intermediate incidence angles, whereas attractive gradient force occurs only for low angles, with a peak at \( \theta_i \approx 25^\circ \). One important characteristic of DNG particles is that, at least in the ray optics regime, gradient forces do not change sign if we change from \(|n_2| < n_1\) to \(|n_2| > n_1\).

If we explore the case \(|n_2| < n_1\), one can conclude by looking at Figs. 2(c) and 2(d) that, as the beam has its maximum intensity along its optical axis, the forces exerted in the particle will be repulsive when its index \( n_2 \) is positive and, for a metamaterial, although the scattering force is attractive, the gradient component of the total force for a ray will be either attractive or repulsive, depending on the angle of incidence.

2.1 Total forces as functions of the angle \( \gamma \)

Next, we sum Eqs. (1) and (2) over all incident rays that composes the beam. So, we are interested in obtaining the surface integral of all individual forces, i.e., the total force \( \mathbf{F} \) when the converging cone of the beam is restricted within \( 0 \leq \theta \leq \theta_{\text{max}} = 66^\circ \) being the numerical aperture of the lens. We must, however, adopt the new coordinate system shown in Fig. 3(a) because now the \( z \) axis is not along one single ray, but represents the optical axis of the beam as a whole. For this situation, \( \mathbf{F} = \mathbf{F}_g \hat{\mathbf{x}} + \mathbf{F}_s \hat{\mathbf{z}}. \)

In Fig. 3(a), \( \gamma \) is defined as the angle between the \( z \) axis and the distance vector \( \mathbf{r} = r \hat{\mathbf{r}} \). We may regard the \(-z\) axis as the optical axis of the – focused – Gaussian beam, whose focus
is the same as those in Figs. 1(a) and 1(b). A tridimensional perspective is given in Fig. 3(b), including the converging cone of the beam. Note that the apex angle is equivalent to $2\theta_{\text{max}}$, i.e., all incident rays are interior to or at the surface of this cone. Due to the symmetry of the Gaussian beam, the problem can be reduced to two dimensions or, explicitly, the $x$-$z$ plane (as mentioned before, the beam is circularly polarized and shifting the particle along $x$ or $y$ makes no difference on the intensity of the total force $F$, although its direction changes, as expected).

In practice, the direction of $F$ depends upon the vector $r$, which is intimately related to $\gamma$, so that good theoretical predictions of experimental setups can be achieved by plotting $F$ versus $\gamma$. By considering displacements only along the $x$-$z$ plane and summing up all incident rays, $F$ is found by numerically evaluating the integral

$$F = \iint_A \vec{F} \, dA / \iint_A dA,$$  (3)

Fig. 2. Normalized (over $n_1 P / c$) values of $F_g$ (solid) and $F_S$ (dashed), for both conventional case ((a) and (c)) and DNG case ((b) and (d)) with $n_1 = 1.33$. The refractive indexes are: (a) $n_2 = 1.62$; (b) $n_2 = -1.62$; (c) $n_2 = 1.21$ and (d) $n_2 = -1.21$.

Fig. 3. (a). The total scattering and gradient forces for a focused collimated beam will depend on the angle $\gamma$ between the $z$-axis and the distance vector $r$, directed from the focus $f$ of the beam to the centre $O$ of the sphere of radius $a$. (b). A tridimensional view of the problem. The incident cone and the sphere were cut for clearness.

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where \( \mathbf{F}' = F'_x \mathbf{x} + F'_z \mathbf{z} \) is the vector force of every incident ray in this new coordinate system and \( A \) is the area of the sphere delimited by its intersection with the converging cone of the beam which is equivalent to consider one ray as being a differential \( d\theta d\phi \) (inside the region \( 0 \leq \theta \leq \theta_{\text{max}} \)), and whose power is proportional to the lens’ surface area. The differential of this area is, using Abbe sine condition, proportional to \( \sin \theta \cos \theta d\theta d\phi \), \( \theta \) and \( \phi \) associated with the usual spherical angles of a spherical coordinate system centered at the focus \( f \) of the beam.

Gradient and scattering forces in Eqs. (1) and (2) for individual rays must be spatially oriented according to Fig. 3(a), and \( \theta_i \) must be written as a function of \( \gamma \) in order to evaluate Eq. (3). This can be accomplished by using the following relations, which can be deduced from Fig. 3(a) and simple geometrical considerations:

\[
\begin{align*}
\mathbf{r} &= (r \sin \gamma, 0, r \cos \gamma) \\
\mathbf{d} &= r \left[ \sin \theta \cos \phi \sin \gamma + \cos \theta \cos \gamma \right] + \\
& \sqrt{a^2 \left( 1 - \frac{r}{a} \right)^2 + r^2 \left( \sin \theta \cos \phi \sin \gamma + \cos \theta \cos \gamma \right)^2} \\
\theta_i &= \cos^{-1} \left[ \frac{a}{2d} \left( 1 + \frac{a}{d} \right)^2 - \left( \frac{r}{a} \right)^2 \right]
\end{align*}
\]

After this insight, let us vary the angle \( \gamma \) for \( |r| = 0.5a \) and the same refractive index used before, still normalizing the forces over \( n_1 P/c \), and perform the surface integral in Eq. (3) by making use of Eq. (4). The results for a conventional dielectric particle with \( n_2 = 1.62 \) is shown in Fig. 4(a), while the DNG case can be appreciated in Fig. 4(b). Physical interpretations for the first case are found elsewhere [14].

Fig. 4. Scattering (dashed) and gradient (solid) total forces as functions of the angle \( \gamma \) for \( n_1 = 1.33 \). (a) \( n_2 = 1.62 \); (b) \( n_2 = -1.62 \); (c) \( n_2 = 1.21 \) and (d) \( n_2 = -1.21 \).

Compared to the conventional case, the situation for a DNG particle is almost the same. But we can see from Fig. 4(b) that, considering the behavior of the scattering total force, points of stable equilibrium would appear only about \( \gamma = 135^\circ \) and \( 235^\circ \), and the range of repulsive scattering force is found for \( 90^\circ < \gamma < 135^\circ \) and \( 235^\circ < \gamma < 270^\circ \). Besides that, now the maximum values for the gradient force does not happen at \( \gamma = 90^\circ \) and \( 270^\circ \), as in the
conventional case, but for $\gamma \approx 120^\circ$ and $240^\circ$ instead. Finally, note the difference in magnitude for both plots, showing a more effective trapping for DNG particles or, in other words, that the same trapping effectiveness could be achieved for a DNG particle using less incident power.

The situation becomes more interesting when we consider that the particle has a refractive index lower (in modulus) than that of the external medium. For conventional particles, this would result in an inversion of the forces relative to the $x$ and $z$-axis (see Fig. 4(c)), thus proving that particles where $n_2 > n_1$ are shifted toward regions of high intensity of the beam whereas, for $n_2 < n_1$, towards regions of nulls of intensity, i.e., far away from the optical axis and the focus.

When a DNG particle has a refractive index $|n_2| < n_1$, the total forces does not change sign, as shown in Fig. 4(d). Thus, and at least in theory, optical trapping for this kind of particle is unaffected when the relative refractive index changes from $n = |n_2|/n_1 > 1$ to $n' = 1/n < 1$.

2.2 Total forces as functions of $r = |r|$

Let us change the distance $r$ between the beam focus and the centre of the sphere for three different angles $\gamma = 0^\circ$, $\gamma = 90^\circ$ and $\gamma = 180^\circ$. Fig. 5 shows the forces for DNG particles.

An important detail is that, in Fig. 2(a) the scattering force is positive, or repulsive, because it is oriented in the same direction of the incident ray. As for Fig. 4(a), due to the system of coordinates chosen - see Fig. 3, in which the $z$-axis is oppositely directed along the optical axis of the beam (against its direction of propagation), repulsiveness is represented by negative forces. Other characteristics can be found elsewhere (see [1-5] and [14]).

As seen in Figs. 5(a)–5(c), optical trapping for metamaterial particles can present certain particular features not observable until now. Let us pose one feature by one.

As expected, the gradient total force is zero for $\gamma = 0^\circ$. In this case, the scattering force is negative (scattering total forces will never be zero for $r = 0$), giving the vertical displacement of the particle towards the focus, located just below its center. We can see that this force diminishes not for $r/a \approx 1$, but instead for $r/a > 0.78$, revealing a trapping efficiency diminishement. Yet, comparing the diminishement in magnitude with the conventional case, the total force is still much higher than that of a conventional particle. Therefore, in general, even in this case for $0.78 < r/a < 1$, the efficiency in trapping is higher when the particle presents...
negative refractive index (a better look in Fig. 4 could have already given this conclusion, as total gradient and scattering forces are higher in cases (b) and (d) than in (a) and (c), respectively).

Now, let us go back to Fig. 5(b). Again, the scattering force decreases when $r/a \to 1$; however, this force is always negative, meaning that the particle will not have a point of stable equilibrium in the same horizontal plane of the focus; rather, this position will be slightly down. The gradient force reaches a maximum peak of $\approx -0.9$ arbitrary units (a.u.), more than twice that for a conventional particle when $r/a \to 1$. A curious fact is the inversion of the gradient force when $r/a > 0.88$. This means that, for distances above $r/a = 0.88$, forces acting on this particle become repulsive, and no trapping is achieved.

Maybe more surprising is the point of zero total force in Fig. 5(c). This point – close to $r/a = 0.73$ – is, indeed, an unstable point. If we were capable of placing a metamaterial particle under $\gamma = 180^\circ$ and $r/a > 0.73$, the total force would be repulsive. For shorter distances between focus and centre of the sphere, it would become more attractive. It must be emphasized that this situation is quite hypothetical and, experimentally, placing a DNG particle in this unstable point is practically unrealizable.

So, the trapping characteristics for a DNG particle are very different from those observed until now for a positive index particle for a focused Gaussian beam, even when, in modulus, they have the same refractive index and with values higher than that of the external environment. But once trapping of a DNG particle is achieved, this shall be much stronger, since the restoring forces are stronger.

The same comments that were made, concerning the inversion of the direction of scattering and gradient forces relative to the chosen coordinates are applicable: a conventional particle tends to regions of high intensities of the beam when the relative index of refraction is $n = n_2/n_1 > 1$ and, to $n' = 1/n < 1$, to regions of lower intensities, i.e., the particle is repelled; for DNG particles, the trapping characteristics are conserved when we go from $n = n_2/n_1 > 1$ to $n' = 1/n < 1$ (Figs. 5(d)-5(f)).

Distinct behaviors of a DNG particle in an optical tweezers can occur. The scattering and gradient forces for a single ray have been calculated, and they show completely different characteristics from the conventional case - positive refractive index. In our simulations, we have shown that a DNG particle may tend to regions of high intensity of a Gaussian beam even if its refractive index is (in modulus) lower than that of the medium.

When the total scattering and gradient forces are simulated, some characteristics that had not been observed for conventional particles were shown. We have not found, so far, any contribution of this kind in the literature, relating the capabilities of optical tweezers to trap DNG particles in the ray optics regime.

Although micro-spheres made of both negative permeability and permittivity are not experimentally available yet, their feasibility is just a matter of time. We believe that the manipulation of such particles can be useful in biological applications. Further studies may confirm this possibility.

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