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Dynamics of a Kerr Nanoparticle in a Single Beam Optical Trap

Romeric Pobre¹ and Caesar Saloma²

¹Physics Department, CENSER, College of Science, De La Salle University-Manila

²National Institute of Physics, University of the Philippines-Diliman
Philippines

1. Introduction

Single beam optical traps also known as optical tweezers, are versatile optical tools for controlling precisely the movement of optically-small particles. Single-beam trapping was first demonstrated with visible light (514 nm) in 1986 to capture and guide individual neutral (nonabsorbing) particles of various sizes (Ashkin *et. al.*, 1986). Optical traps were later used to orient and manipulate irregularly shaped microscopic objects such as viruses, cells, algae, organelles, and cytoplasmic filaments without apparent damage using an infrared light (1060 nm) beam (Ashkin, 1990). They were later deployed in a number of exciting investigations in microbiological systems such as chromosome manipulation (Liang *et.al.*, 1993), sperm guidance in all optical *in vitro* fertilization (Clement-Sengewald *et.al.*, 1996) and force measurements in molecular motors such single kinesin molecules (Svoboda and Block, 1994) and nucleic acid motor enzymes (Yim *et.al.*, 1995). More recently, optical tweezer has been used in single molecule diagnostics for DNA related experiments (Koch *et.al.*, 2002). By impaling the beads onto the microscope slide and increasing the laser power, it was tested that the bead could be "spot-welded" to the slide, leaving the DNA in a stretched state- a technique was used in preparing long strands of DNA for examination via optical microscopy.

Researchers continue to search for ways to the capability of optical traps to carry out multi-dimensional manipulation of particles of various geometrical shapes and optical sizes (Grier, 2003; Neuman & Block, 2004). Efforts in optical beam engineering were pursued to generate trapping beams with intensity distributions other than the diffraction-limited beam spot e.g. doughnut beam (He *et.al.*, 1995; Kuga *et.al.*, 1997), helical beam (Friesen *et.al.*, 1998), Bessel beam (MacDonald *et.al.*, 2002). Multiple beam traps and other complex forms of optical landscapes were produced from a single primary beam using computer generated holograms (Liesener *et.al.*, 2000; Curtis *et.al.*, 2002; Curtis *et.al.*, 2003) and programmable spatial light modulators (Rodrigo *et.al.*, 2005; Rodrigo *et.al.*, 2005).

Knowing the relationship between characteristics of the optical trapping force and the magnitude of optical nonlinearity is an interesting subject matter that has only been lightly investigated. A theory that accurately explains the influence of nonlinearity on the behavior of nonlinear particles in an optical trap would significantly broaden the applications of optical traps since most materials including many proteins and organic molecules, exhibit

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considerable degrees of optical nonlinearity under appropriate excitation conditions (Lasky, 1997; Clays *et.al.*, 1993; Chemla & Zyss, 1987; Prasad & Williams, 1991; Nalwa & Miyata, 1997). One possible reason for the apparent scarcity of published studies on the matter is the difficulty in finding a suitable strategy for computing the intensity-dependent refractive index of the particle under illumination by a focused optical beam.

We have previously studied the dynamics of a particle in an optical trap that is produced by a single tightly focused continuous-wave (CW) Gaussian beam in the case when the refractive index n_2 of the particle is dependent on the intensity I (Kerr effect) of the interacting linearly polarized beam according to: $n_2 = n_2^{(0)} + n_2^{(1)}E^*E$, where $n_2^{(0)}$ and $n_2^{(1)}$ are the linear and nonlinear components of n_2 , respectively. We have calculated the (time-averaged) optical trapping force that is exerted by a focused TEM₀₀ beam of optical wavelength λ on a non-absorbing mechanically-rigid Kerr particle of radius a in three different value ranges of the size parameter α : (1) $\alpha = 2\pi a/\lambda \gg 100$ geometric optics (Pobre & Saloma, 1997), (2) $\alpha \approx 100$ Mie scattering (Pobre & Saloma, 2002), and (3) $\alpha \ll 100$ Rayleigh scattering regime (Pobre & Saloma, 2006; Pobre & Saloma, 2008).

Here we continue our effort to understand the characteristics of the (time-averaged) optical trapping force F_{trap} that is exerted on a Kerr particle by a focused CW TEM₀₀ beam in the case when $a \leq 50\lambda/\pi$. A nanometer-sized Kerr particle (bead) exhibits Brownian motion as a result of random collisions with the molecules in the surrounding liquid. The Brownian motion is no longer negligible and has to be into account in the trapping force analysis. The characteristics of the trapping force are determined as a function of particle position in the propagating focused beam, beam power and focus spot size, ω_0 , a , and relative refractive index between the nanoparticle and its surrounding medium. The behavior of the optical trapping force is compared with that of a similarly-sized linear particle under the same illumination conditions.

The incident focused beam polarizes the non-magnetic Kerr nanoparticle ($a \ll \lambda$) and the electromagnetic (EM) field exerts a Lorentz force on each charge of the induced electric dipole (Kerker, 1969). We derive an expression for F_{trap} in terms of the intensity distribution and the nanoparticle polarizability $\alpha = \alpha(n_1, n_2)$, where n_2 and n_1 are the refractive index of the Kerr nanoparticle and surrounding medium, respectively. Optical trapping force (F_{trap}) has two components, one that accounts for the contribution of the field gradient and the other from the light that is scattered by the particle. The two-component approach for computing the magnitude and direction of F_{trap} was previously used on linear dielectric nanoparticles in arbitrary electromagnetic fields (Rohrbach & Steltzer, 2001). We also mention that the calculation of the intensity distributions near Gaussian beam focus is corrected up to the fifth order (Barton & Alexander, 1989).

In the next section, we will show the equation of the motion of a Kerr nanoparticle near the focus of a single beam optical trap in a Brownian environment. Simulation results will be presented and discussed in detail for other sections.

2. Theoretical framework

A linearly polarized Gaussian beam (TEM₀₀ mode) of wavelength λ , is focused via an objective lens of numerical aperture NA and allowed to propagate along the optical z -axis in a linear medium of refractive index n_1 (see Fig 1). The beam radius ω_0 at the geometrical focus ($x = y = z = 0$) is: $\omega_0 = \lambda/(2NA)$.

Fig. 1. Nonlinear nanoparticle of radius a and refractive index n_2 is located near the focal volume of a tightly-focused Gaussian beam of wavelength $\lambda \gg a$ and beam focus radius ω_0 . Gaussian beam propagates in a linear medium of index n_1 . Nanoparticle center is located at $\mathbf{r}(x, y, z)$ from the geometrical focus at $\mathbf{r}(0, 0, 0)$. Enlarged figure in the focal volume shows Kerr nanoparticle undergoing Brownian motion near the focus.

The focused beam interacts with a Kerr particle of radius $a \leq 50\lambda/\pi$. The refractive index $n_2(\mathbf{r})$ of the Kerr particle is given by: $n_2(\mathbf{r}) = n_2^{(0)} + n_2^{(1)} I(\mathbf{r})$, where $I(\mathbf{r}) = \mathbf{E}^*(\mathbf{r})\mathbf{E}(\mathbf{r})$ is the beam intensity at particle center position $\mathbf{r} = \mathbf{r}(x, y, z)$ from the geometrical focus at $\mathbf{r} = 0$ which also serves as the origin of the Cartesian coordinate system. Throughout this paper, vector quantities represented in bold letters.

The thermal fluctuations in the surrounding medium (assumed to be water in the present case) become relevant when the particle size approaches the nanometer range. We consider a Kerr nanoparticle that is located at $\mathbf{r}$ above the reference focal point in the center of the beam waist ω_0 that is generated with a high NA oil-immersed objective lens of an inverted microscope – the focused beam propagates in the upward vertical direction (see inset **Fig. 1**). The dynamics of the Kerr nanoparticle as it undergoes thermal diffusion can be analyzed in the presence of three major forces: (1) Drag force, $\mathbf{F}_{\text{drag}}(d\mathbf{r}/dt) = \mathbf{F}_{\text{drag}}$, that is experienced when the particle is in motion, (2) Trapping force $\mathbf{F}_{\text{trap}}(\mathbf{r})$, which was derived in (Pobre & Saloma, 2006), and (3) time-dependent Brownian force $\mathbf{F}_{\text{fluct}}(t) = \mathbf{F}_{\text{fluct}}$, that arise from thermal motion of the molecules in the liquid. The Kerr nanoparticle experiences a net force $\mathbf{F}_{\text{net}}(\mathbf{r}, t) = \mathbf{F}_{\text{net}}$, that can be expressed in terms of the Langevin equation as:

$$\begin{aligned} \mathbf{F}_{\text{net}}(\mathbf{r}, t) &= \mathbf{F}_{\text{drag}}(\dot{\mathbf{r}}) + \mathbf{F}_{\text{trap}}(\mathbf{r}) + \mathbf{F}_{\text{fluct}}(t) \\ m\ddot{\mathbf{r}} &= -\gamma\dot{\mathbf{r}} + \mathbf{F}_{\text{trap}}(\mathbf{r}) + \mathbf{F}_{\text{fluct}}(t) \end{aligned} \quad (1)$$

where: $\mathbf{F}_{\text{drag}} = -\gamma d\mathbf{r}/dt$, and γ is the drag coefficient of the surrounding liquid. According to Stokes law, $\gamma = 6\pi\eta a$, where η is the liquid viscosity. While the optical trapping force or optical trapping force, $\mathbf{F}_{\text{trap}}(\mathbf{r})$, on the Kerr nanoparticle was shown to be (Pobre & Saloma, 2006):

$$\mathbf{F}_{trap}(\mathbf{r}) = \left(\frac{2\pi n_1 a^3}{c} \right) \frac{\left(\frac{\left\{ \frac{n_2^{(0)} + n_2^{(0)} I(r)}{n_1} \right\}^2}{\left\{ \frac{n_2^{(0)} + n_2^{(0)} I(r)}{n_1} \right\}^2} - 1 \right)^2}{+2} \nabla I(r) + \left(\frac{8\pi n_1}{3c} \right) (|\mathbf{k}| a)^4 a^2 \frac{\left(\frac{\left\{ \frac{n_2^{(0)} + n_2^{(0)} I(r)}{n_1} \right\}^2}{\left\{ \frac{n_2^{(0)} + n_2^{(0)} I(r)}{n_1} \right\}^2} - 1 \right)^2}{+2} I(r) \quad (2)$$

Equation (2) reveals that $\mathbf{F}_{trap}$ consists of two components. The first component represents the gradient force and depends on the gradient of $I(r)$ and it is directed towards regions of increasing intensity values. The second component represents the contribution of the scattered light to $\mathbf{F}_{trap}$. The scattering force varies with $I(r)$ and it is in the direction of the scattered field. Hence, the relative contribution of the scattering force to $\mathbf{F}_{trap}$ is weak for a particle that scatters light in an isotropic manner.

The Gaussian beam has a total beam power of P (Siegman, 1986) and its intensity distribution $I(\mathbf{r})$ near the beam focus is calculated with corrections introduced up to the fifth-order (Barton & Alexander, 1989). Focusing with a high NA objective produces a relatively high beam intensity at $z = 0$, which decreases rapidly with increasing $|z|$ values. On the other hand, low NA objectives produce a slowly varying intensity distribution from $z=0$.

The molecules of the surrounding fluid affect significantly on the mobility of the Kerr nanoparticle since their sizes are comparable. As a result, the Kerr nanoparticle moves in a random manner between the molecules and exhibits the characteristics of a Brownian motion. The associated force can be generated via a white-noise simulation since it mimics the behavior of the naturally occurring thermal fluctuations of a fluid. The assumption holds when both the liquid and the Kerr nanoparticle are non-resonant with λ . Localized (non-uniform) heating of the liquid is also minimized by keeping the average power of the focused beam low for example with a femtosecond laser source that is operated at high peak powers and relatively low repetition rate.

3. Optical trapping potential

As previously discussed, the Kerr nanoparticle of mass m and $2\pi a/\lambda \leq 100$ and $a \ll \lambda$, exhibits random (Brownian) motion in the liquid (Rohrbach & Steltzer, 2002; Singer *et.al.*, 2000). The thermal fluctuation probability increases with the temperature T of the liquid. To determine the dynamics of a Kerr nanoparticle near the focus of a single beam optical trap, we first determine the potential energy $V(\mathbf{r})$ of the optical trap near the beam focus, which can be characterized in terms of $\mathbf{F}_{trap}$. The potential $V(\mathbf{r})$ as a function of the optical trapping force from all axes (in this case along the x , y , and z axes) is given by:

$$\begin{aligned} V(r) &= - \int_{r_0}^{r_f} \mathbf{F}_{trap}(\mathbf{r}) d\mathbf{r} \\ &= - \int_{x_0}^{x_f} \mathbf{F}_{trap,x}(\mathbf{r}) dx - \int_{y_0}^{y_f} \mathbf{F}_{trap,y}(\mathbf{r}) dy - \int_{z_0}^{z_f} \mathbf{F}_{trap,z}(\mathbf{r}) dz \end{aligned} \quad (3)$$

where: $F_{\text{trap},x}$, $F_{\text{trap},y}$ and $F_{\text{trap},z}$ are the Cartesian components of F_{trap} , and $\mathbf{r}_0(x_0, y_0, z_0; t_0) = \mathbf{r}_0(t_0)$ and $\mathbf{r}_f(x_f, y_f, z_f; t_f) = \mathbf{r}_f(t_f)$ are the initial and final positions of the nanoparticle. For a nanoparticle in the focal volume of a Gaussian beam, $V(\mathbf{r})$ can be approximated as a harmonic potential since the magnitude of F_{drag} is several orders larger than that of the inertial force. Equation (1) then describes an over-damped harmonic motion that is driven by time-dependent thermal fluctuations.

A nanoparticle at location $\mathbf{r}(t)$ in the optical trap has a potential energy $V(\mathbf{r})$ and a kinetic energy $m|\mathbf{v}|^2/2$ where $\mathbf{v} = \mathbf{v}(t)$ is the nanoparticle velocity. The probability that the Kerr nanoparticle is found at position $\mathbf{r}(t)$, is described by a probability density function $\Pi(\mathbf{r}) = \Pi_0 \exp[-V(\mathbf{r})/k_B T]$, where Π_0 is the initial probability density, T is the temperature of the surrounding medium, and k_B is the Boltzmann constant.

Figure 2 plots the potential energy (2a) of the optical trap and the corresponding time-dependent displacement trajectory (2b) of the Kerr nanoparticle (initial z position = $0.4 \mu\text{m}$) along the optical z -axis assuming a zero initial velocity and a room temperature condition of $3.1 k_B T$ background energy of the surrounding medium. The trajectory (in blue trace) can be ascribed as overdamped oscillations of the Kerr nanoparticle that arise from the complex interplay of three forces indicated in the Langevin's differential equation. The oscillations

Fig. 2. **(a)** Potential energy and probability density function along the z -axis with trapping input parameters: $z_0=0$, $p=100\text{mW}$, $a=30\text{nm}$, $N.A.=1.2$, $\lambda=1.064\mu\text{m}$, $n_1=1.33$, $n_2^{(0)}=1.4$, and $n_2^{(1)}=1.8 \times 10^{-12}\text{m}^2/\text{W}$. **(b)** Thermal diffusion of the Kerr nanoparticle along the z -axis with zero initial velocity at $0.4 \mu\text{m}$ with a $3.1 k_B T$ ambient energy ($T=300K$) of the surrounding water (in red dashed line).

are caused by random collisions between the Kerr nanoparticle and the relatively-large molecules. The narrower confinement of the Kerr nanoparticle indicates a stiffer potential trap that is contributed by the effects of the nonlinear interaction between the Kerr nanoparticle and the tightly focused Gaussian beam.

Figure 3 presents the three-dimensional (3D) plots of the trapping potential that is created by a focused beam ($NA = 1.2$) in the presence of a linear and a Kerr particle. The potential wells are steeper along the x -axis than along the z -axis since a high NA objective lens produces a focal volume that is relatively longer along the z -axis. The potential well associated with a Kerr nanoparticle is deeper than that of a linear nanospshere.

Fig. 3. Three-dimensional plot of the trapping potential energy along the transverse plane for both linear and nonlinear nanosphere as the focused laser beam propagates from left to right of the z -axis with the following trapping parameters: $z_0=0$, $p=100\text{mW}$, $a=30\text{nm}$, $N.A.=1.2$, $\lambda = 1.064\mu\text{m}$, $n_1=1.33$, $n_2^{(0)}=1.4$, and $n_2^{(1)}=1.8 \times 10^{-12}\text{m}^2/\text{W}$.

Under the same illumination conditions, a Kerr nanoparticle is captured more easily and held more stably in a single beam optical trap than a linear nanoparticle of the same size. A Kerr nanoparticle that is exhibiting Brownian motion is also confined within a much smaller volume of space around the beam focus as illustrated in 3D probability density of **figure 4**. The significant enhancement that is introduced by the Kerr nonlinearity could make the simpler single-beam optical trap into a viable alternative to multiple beam traps which are costly, less flexible and more difficult to operate.

Fig. 4. Probability density distributions of linear and nonlinear (Kerr) nanospheres in a single-beam optical trap at $T = 300\text{K}$ where $t = 100,000$ iterations, $P = 100\text{mW}$, $a = 5\text{ nm}$, $NA = 1.2$, $\lambda = 1.064\text{ }\mu\text{m}$, and $n_1 = 1.33$: a) Location probability distribution of linear ($n_2 = n_2^{(0)}$) and b) Kerr nanoparticle ($n_2^{(0)} = 1.4$, $n_2^{(1)} = 1.8 \times 10^{-12}\text{ m}^2/\text{W}$). Initially ($t = 0$), the nanoparticle is at rest at $z = 0.5\text{ }\mu\text{m}$.

4. Parametric analysis of the optical trapping force between linear and nonlinear (Kerr) nanoparticle

To better understand the underlying mechanism on how Kerr nonlinearity affects the trapping potential, let us perform a parametric analysis on how optical trapping force changes with typical trapping parameters on both linear and nonlinear (Kerr) nanoparticle. The optical trapping force $\mathbf{F}_{\text{trap}}(\mathbf{r})$ that is described by Eq (2) was calculated using *Mathematica* Version 5.1 application program. **Figure 5a** presents the contour and 3D plots of $\mathbf{F}_{\text{trap}}(\mathbf{r})$ at different locations of the linear nanoparticle ($n_2 = 1.4$, $a = 5\text{ nm}$, $\lambda = 1.062\text{ }\mu\text{m}$, $NA = 1.2$) while **Figure 5b** shows the contour and 3D plots of $\mathbf{F}_{\text{trap}}(\mathbf{r})$ at different locations of the Kerr nanoparticle ($n_2^{(0)} = 1.4$, $n_2^{(1)} = 1.8 \times 10^{-11}\text{ m}^2/\text{W}$, $a = 5\text{ nm}$, $\lambda = 1.062\text{ }\mu\text{m}$, $NA = 1.2$). The $n_2^{(1)}$ value is taken from published measurements done with photopolymers which are materials that exhibit one of the strongest electro-optic Kerr effects (Nalwa & Miyata, 1997). Also shown is the contour plot of $\mathbf{F}_{\text{trap}}(\mathbf{r})$ for the case of a linear nanoparticle ($n_2^{(0)} = 1.4$, $a = 5\text{ nm}$) of the same size.

For values of $z > 0$, $\mathbf{F}_{\text{trap}}$ is labeled negative (positive) when it pulls (pushes) the nanoparticle towards (away from) $\mathbf{r} = 0$. For $z \leq 0$ the force is positive (negative) when it pushes (pulls) the nanoparticle towards (away from) the beam focus at $\mathbf{r} = 0$. For both linear and nonlinear nanoparticles, the force characteristics are symmetric about the optical z -axis but asymmetric about the $z = 0$ plane. The asymmetry of the force is revealed only after the fifth-order correction is applied on the intensity distribution of the tightly focused Gaussian beam. The strongest force magnitude happens on the z -axis and it is 30% stronger in the case of the Kerr nanoparticle.

The stiffness of the optical trap may be determined by taking derivative of $\mathbf{F}_{\text{trap}}(\mathbf{r})$ with respect to $\mathbf{r}$. **Figure 6b** plots the stiffness at different locations of the Kerr nanoparticle. The stiffness distribution features a pair of minima at $r = (x^2 + y^2)^{1/2} \approx 0.1\text{ micron}$ with a value of $-25 \times 10^{-12}\text{ N/m}$. Also presented in **Fig 6a** is the force stiffness distribution for the case of a

Fig. 5. Optical trapping force at different locations of both linear and Kerr nanoparticle ($n_2^{(0)} = 1.4$, $n_2^{(1)} = 1.8 \times 10^{-11} \text{ m}^2/\text{W}$) where $r = (x^2 + y^2)^{1/2}$. Parameter values common to both nanoparticles: $P = 100 \text{ mW}$, $a = 5 \text{ nm}$, $NA = 1.2$, $\lambda = 1.064 \text{ microns}$, and $n_1 = 1.33$. The focused beam propagates from left to right direction. In all cases, $F_{\text{trap}} = 0$ at $r(x, y, z) = 0$.

linear nanoparticle exhibits a similar profile but a lower minimum value of $-18 \times 10^{-12} \text{ N/m}$ at $r \approx 0.1 \text{ micron}$. The Kerr nanoparticle that is moving towards $r = 0$, experiences a trapping force that increases more rapidly than the one experienced by a linear nanoparticle of the same size. Once settled at $r = 0$, the Kerr nanoparticle is also more difficult to dislodge than its linear counterpart.

Figure 7a plots the behavior of F_{trap} at different axial locations of a linear nanoparticle ($n_2 = 1.4$) with $a(\text{nm}) = 50, 70, 80, 90$ and 100 . In larger Kerr nanoparticles ($a > 50 \text{ nm}$), the scattering force contribution becomes significant and the location of $F_{\text{trap}}(\mathbf{r}) = 0$ shifts away from $z = 0$ and towards $z > 0$. Our results are consistent with those previously reported with linear dielectric nanoparticles (Rohrback and Steltzer, 2001; Wright *et.al.*, 1994).

Figure 7b plots the behavior of $F_{\text{trap}}(\mathbf{r})$ at different axial locations of a bigger Kerr nanoparticle with $a(\text{nm}) = 50, 70, 80, 90$ and 100 . The maximum strength of $F_{\text{trap}}(\mathbf{r})$ increases with a . For $a < 50 \text{ nm}$, $F_{\text{trap}}(\mathbf{r}) = 0$ at $z = 0$ since $F_{\text{trap}}(\mathbf{r})$ is contributed primarily by the gradient force. For larger Kerr nanoparticles, the relative contribution of the scattering force becomes more significant and the location where $F_{\text{trap}}(\mathbf{r}) = 0$ is shifted away from $z = 0$ and towards the direction of beam propagation.

Figure 8a plots the behavior of $F_{\text{trap}}(\mathbf{r})$ as a function of the objective NA ($0.4 \leq NA \leq 1.4$) for a Kerr nanoparticle [$n_2^{(0)} = 1.4$, $n_2^{(1)} = 1.8 \times 10^{-11} \text{ m}^2/\text{W}$, $P = 100 \text{ mW}$, $a = 5 \text{ nm}$] that is located at $r(0, 0, 0.5 \text{ micron})$. Also plotted is the behavior of $F_{\text{trap}}(\mathbf{r})$ with NA for a linear nanoparticle of the same size and initial beam location. Both the Kerr and the linear nanoparticle

Fig. 6. Optical trapping force stiffness of optical trap at different locations of both linear ($n_2^{(0)} = 1.4$) and Kerr nanoparticle ($n_2^{(0)} = 1.4$, $n_2^{(1)} = 1.8 \times 10^{-12} \text{ m}^2/\text{W}$) where $r = (x^2 + y^2)^{1/2}$. Common parameter values: $P = 100 \text{ mW}$, $a = 5 \text{ nm}$, $NA = 1.2$, $\lambda = 1.064 \text{ microns}$, and $n_1 = 1.33$.

Fig. 7. Optical trapping force at different axial locations of: a) linear ($n_2 = n_2^{(0)} = 1.4$), and b) Kerr ($n_2^{(0)} = 1.4$, $n_2^{(1)} = 1.8 \times 10^{-12} \text{ m}^2/\text{W}$) nanoparticle of radius $a(\text{nm}) = 50, 70, 80, 90$ and 100 . Common parameter values: $P = 100 \text{ mW}$, $NA = 1.2$, $\lambda = 1.064 \text{ microns}$, and $n_1 = 1.33$.

experience a trapping force that pulls them towards $r = 0$. The effect of the Kerr nonlinearity which is to increase the strength of $\mathbf{F}_{\text{trap}}(\mathbf{r})$, becomes more significant at $NA > 1$. At $NA = 1.4$, the force magnitude on the Kerr nanoparticle approximately twenty percent stronger than that experienced by the linear nanoparticle. The nonlinear effect is negligible in low NA focusing objectives ($NA < 0.6$). For the Kerr nanoparticle, the dependence of the force strength with NA is accurately described by a fourth order polynomial.

Fig. 8. (a) Optical trapping force on Kerr nanoparticle (solid line; $n_2^{(0)} = 1.4$, $n_2^{(1)} = 1.8 \times 10^{-12}$ m^2/W) as a function of objective NA . Also plotted is the corresponding force (dotted line) on a linear nanoparticle with $n_2 = n_2^{(0)} = 1.4$. Common parameter values: $z = 0.5$ micron, $P = 100$ mW, $a = 5$ nm, $\lambda = 1.064$ microns, and $n_1 = 1.33$. For the Kerr nanoparticle the curve is accurately described by: $\mathbf{F}_{\text{trap}} = 1311.65(NA)^4 - 3959.965(NA)^3 + 3656.265(NA)^2 - 1388.114NA + 188.105$. (b) Optical trapping force on non-absorbing Kerr (solid line; $n_2^{(1)} = 1.8 \times 10^{-12}$ m^2/W) and linear ($n_2 = n_2^{(0)} = 1.4$) nanoparticle versus $n_2^{(0)}$, at $\lambda = 1.064$ microns. Also plotted (circles) is force difference ($F_{nl} - F_l$) as a function of $n_2^{(0)}$.

Figure 8b shows the behavior of $\mathbf{F}_{\text{trap}}(\mathbf{r})$ as a function of $n_2^{(0)}$ for a Kerr nanoparticle that is located at $\mathbf{r}(0, 0, 0.5 \text{ micron})$ in a surrounding medium with index $n_1 = 1.33$. Also plotted is the behavior of $\mathbf{F}_{\text{trap}}(\mathbf{r})$ with $n_2^{(0)}$ for a linear nanoparticle ($n_2 = n_2^{(0)}$) of the same size and initial beam location. The $\mathbf{F}_{\text{trap}}(\mathbf{r})$ profiles are similar for both the Kerr and linear nanoparticles. At $n_2^{(0)} > 1.1$, the Kerr nanoparticle experiences a negative (trapping) force that pulls it towards from $r = 0$. The trapping threshold is less than $n_2^{(0)} = 1.33$ because of the additional contribution of the nonlinear (Kerr) term $n_2^{(1)} I(r)$. For the linear nanoparticle, trapping is possible at a higher value of $n_2^{(0)} > 1.33$. Also plotted is the difference between the forces that are experienced by the two nanoparticles. The difference between the two trapping forces is highest near $n_2^{(0)} = 1$. The difference decreases with increasing $n_2^{(0)}$ value since the contribution of the Kerr term which has been held constant, becomes relatively small.

Figure 9 shows the dependence of $\mathbf{F}_{\text{trap}}(\mathbf{r})$ with λ for a non-resonant Kerr nanoparticle at $\mathbf{r}(0, 0, 0.5 \text{ micron})$ in the range: $400 \leq \lambda(\text{nm}) \leq 1000$. Also presented is the behavior of $\mathbf{F}_{\text{trap}}(\mathbf{r})$ for a linear nanoparticle of the same size and initial beam location. For a given P and NA value, the magnitude of $\mathbf{F}_{\text{trap}}(\mathbf{r})$ increases nonlinearly with decreasing λ for both nanoparticles. However, the increase in the trapping force strength with λ is more rapid for the Kerr

nanoparticle. In practice, λ is selected to avoid absorption by the nanoparticle and the surrounding liquid. Absorption could significantly heat up the nanoparticle and change its optical and mechanical properties. It can also lead to rapid evaporation of the surrounding liquid. In both cases, absorption reduces the efficiency of the optical trap.

Fig. 9. Optical trapping force on non-absorbing Kerr nanoparticle (solid line, $n_2^{(0)} = 1.4$, $n_2^{(1)} = 1.8 \times 10^{-12} \text{ m}^2/\text{W}$) as a function of wavelength λ . Also plotted (dotted line) is the force on a linear nanoparticle ($n_2 = n_2^{(0)} = 1.4$). Other parameter values: $P = 100 \text{ mW}$, $a = 5 \text{ nm}$, $NA = 1.2$, $z = 0.5 \text{ micron}$, and $n_1 = 1.33$.

Figure 10a plots the dependence of $\mathbf{F}_{\text{trap}}(\mathbf{r})$ with beam power P for a Kerr nanoparticle at $\mathbf{r}(0, 0, 0.5 \text{ micron})$. Also presented is the behavior of $\mathbf{F}_{\text{trap}}(\mathbf{r})$ for a linear nanoparticle of the same size and initial beam location. For the linear nanoparticle, the trapping force strength is directly proportional to P . For the Kerr nanoparticle, the trapping force strength increases more quickly (quadratically) with P for the Kerr nanoparticle. Figure 8b reveals that the force strength increases at a faster rate as the Kerr nanoparticle gets bigger.

Fig. 10. (a) Optical trapping force on Kerr (filled circles; $a = 5 \text{ nm}$) and linear nanoparticle (circles; $a = 5 \text{ nm}$) as a function of beam power P , and (b) Force versus P for different radii of Kerr nanoparticle. Common parameter values: $NA = 1.2$, $z = 0.5 \text{ micron}$, $n_2 = n_2^{(0)} = 1.4$, $n_2^{(1)} = 1.8 \times 10^{-12} \text{ m}^2/\text{W}$, and $n_1 = 1.33$. In (a) the force $\mathbf{F}_{\text{trap}}$ acting on the Kerr nanoparticle is accurately described by: $\mathbf{F}_{\text{trap}} = 0.006P^2 - 2.742P + 0.052$.

Figure 11, plots the trapping potential $V(\mathbf{r})$ at different axial locations of a nanoparticle ($a = 5$ nm, $\lambda = 1.064$ microns, $P = 100$ mW) in the absence ($n_2 = n_2^{(0)}$) and presence ($n_2^{(1)} = 1.8 \times 10^{-11}$ m²/W) of Kerr nonlinearity. Compared to its linear counterpart, the Kerr nanoparticle is subjected to a $V(\mathbf{r})$ that is significantly deeper and narrower. From the previous plots, **Figure 5a** and **5b** plot the movement of a linear and Kerr nanoparticle respectively, when they exhibit Brownian motion in the single beam optical trap. The Kerr nanoparticle is released from rest at $\mathbf{r}(0, 0, 0.5 \mu\text{m})$ and it is pulled towards $\mathbf{r} = 0$ and confined to move within a region of about $0.2 \mu\text{m}$ radius, that is centered at $\mathbf{r} = 0$ (Fig 5b). A linear nanoparticle that is released at $\mathbf{r}(0, 0, 0.5 \mu\text{m})$ is constrained to move within a larger region of about $0.5 \mu\text{m}$ radius (Fig 5a).

Fig. 11. Optical trapping potential in a single-beam optical trap at $T = 300\text{K}$ where $t = 100,000$ iterations, $P = 100\text{mW}$, $a = 5$ nm, $NA = 1.2$, $\lambda = 1.064 \mu\text{m}$, and $n_1 = 1.33$: Kerr nanoparticle ($n_2^{(0)} = 1.4$, $n_2^{(1)} = 1.8 \times 10^{-12}$ m²/W). Initially ($t = 0$), the nanoparticle is at rest at $z = 0.5 \mu\text{m}$.

Fig. 12. Optical trapping potential at different axial locations of: a) linear ($n_2 = n_2^{(0)} = 1.4$), and b) Kerr ($n_2^{(0)} = 1.4$, $n_2^{(1)} = 1.8 \times 10^{-12}$ m²/W) nanoparticle of radius $a(\text{nm}) = 50, 70, 80, 90$ and 100 . Common parameter values: $P = 100$ mW, $NA = 1.2$, $\lambda = 1.064$ microns, and $n_1 = 1.33$.

Figure 12a presents the $V(z)$ profile at different z -locations of a linear nanoparticle with $a(\text{nm}) = 50, 70, 80, 90$ and 100 . For comparison, **Figure 12b** shows the behavior of $V(\mathbf{r})$ at

different z -locations of a Kerr nanoparticle ($\lambda = 1.064$ microns, $P = 100$ mW, $n_2^{(1)} = 1.8 \times 10^{-11}$ m²/W) with radius a (nm) = 50, 70, 80, 90 and 100. With respect to $z = 0$, the $V(z)$ profile becomes asymmetric with increasing a for $a > 50$ nm. The distortion is caused by the increasing contribution of the scattering force to the net force $F_{\text{trap}}(\mathbf{r})$. It shifts the location of potential minimum away from $z = 0$, as well as lowers the escape threshold of a trapped Kerr nanoparticle in the direction of beam propagation. Optical trapping potential trends are similar except for differences in strengths, the $V(z)$ profiles evolve in a similar manner with increasing nanoparticle size for both linear and nonlinear case.

5. Enhancement of single-beam optical trap due to Kerr nonlinearity

Our simulation results indicate that the performance of the single-beam optical trap is enhanced by the Kerr effect. For the same focused beam, a Kerr nanoparticle ($n_2^{(0)} = 1.4$, $n_2^{(1)} = 1.8 \times 10^{-11}$ m²/W, $P = 100$ mW, $NA = 1.2$, $\lambda = 1.064$ microns, $n_1 = 1.33$) is subjected to a stronger trapping force than a linear nanoparticle ($n_2 = 1.4$), of the same size (see Figs 7 - 10). The force magnitude increases rapidly as the nanoparticle approaches geometrical focus at $\mathbf{r} = 0$ (Fig 8) especially along the optical z -axis. At the minimum of the trapping potential $V(\mathbf{r})$, a Kerr nanoparticle encounters a higher escape threshold and therefore needs a greater amount of kinetic energy to escape from the optical trap (see Fig 11). Under the same illumination conditions, a Kerr nanoparticle that is exhibiting Brownian motion, is confined to move to within a much smaller region around $\mathbf{r} = 0$, than a linear nanoparticle of the same size (see Fig 5).

The optical trapping force F_{trap} that is exerted on a Kerr nanoparticle with $a \leq 50$ nm = $\lambda/21.3$, is contributed primarily by the gradient force component. In such cases, $F_{\text{trap}} = 0$ at $z = 0$ (see Figs 8) and $V(z)$ is symmetric about $z = 0$ (Figs 12 - 13). At $a = 5$ nm, we found that the maximum strength of the gradient force is about three orders of magnitude larger than that of the scattering force. The axial location where $F_{\text{trap}} = 0$ is shifted away from $z = 0$ and towards the general direction of the beam propagation, when the contribution of the scattering force component becomes comparable (see Fig 11). The corresponding $V(z)$ profile becomes asymmetric with a lower escape barrier along the direction of beam propagation (see Fig 13). Such instances occur with larger Kerr nanoparticles ($a > \lambda/21.3$).

Except for differences in their relative magnitudes, the axial profiles of F_{trap} exhibit the similar characteristics with increasing nanoparticle size for the both the nonlinear and linear case. Our results indicate that the index increase that is introduced by the Kerr effect, does not affect the ability of a small Kerr nanoparticle ($a \leq \lambda/21.3$) to scatter light in an isotropic manner - the increase in n_2 is uniform distributed in the nanoparticle. The gradient force contribution to F_{trap} becomes significant when the non-absorbing nanoparticle scatters light in an anisotropic manner.

Figure 8a illustrates that the enhancement that is gained from the Kerr effect in trapping a non-resonant nanoparticle, is realized only with high NA focusing objectives ($NA > 0.6$). The strength of F_{trap} becomes stronger at shorter λ values (see Fig.10). The increase is faster for the Kerr nanoparticle due to the dependence of its refractive index with $I(\mathbf{r})$ - the force strength increases quadratically with λ . We note that the strong dependence of F_{trap} with λ is not observed in larger Kerr nanoparticles especially in the regime of $a > 100$ and $a \gg \lambda$) (Pobre & Saloma, 1997; Pobre & Saloma, 2002).

The optical trapping force increases rapidly with beam power P for the same NA and λ values (see Fig 10a). For a linear nanoparticle, the force strength is directly proportional to P .

For a Kerr nanoparticle, the relationship of the force strength with P is nonlinear - the Kerr effect permits the use of low power light sources that tend to be less costly to acquire and maintain. Trapping at low beam powers also minimizes the optical heating of the surrounding medium and even the nanoparticle itself. Reductions in unwanted thermal effects are vital in the manipulation and guidance of biological samples.

6. Summary and future prospects

We have analyzed the optical trapping force F_{trap} that is exerted on a Kerr nanoparticle by a focused Gaussian beam when $2\pi a/\lambda \leq 100$ and $a \ll \lambda$. The optical trapping mechanism consists of two dominant optical forces representing the contribution of the field gradient and that of the EM field that is scattered by the nanoparticle. The contributions of the two force components become comparable for nanoparticles with $a > \lambda/21.3$. The gradient force contribution is more dominant with smaller non-absorbing nanoparticles such that $F_{\text{trap}} = 0$ at the beam focus $\mathbf{r} = 0$. The Brownian motion of the Kerr nanoparticle has an over-damped harmonic motion enveloped by white noise function due to thermal fluctuations generated by moving molecules defined by the background energy of $3.1 k_b T$ of the surrounding fluid. Confinement of the Kerr nanoparticle depends on the nonlinear refractive index of the nanoparticle as shown in the widths of the probability density of the Kerr nanoparticle.

Under the same illumination conditions, a Kerr nanoparticle is captured more easily and held more stably in a single beam optical trap than a linear nanoparticle of the same size. A Kerr nanoparticle that is exhibiting Brownian motion is also confined within a much smaller volume of space around the beam focus. The significant enhancement that is introduced by the Kerr nonlinearity could make the simpler single-beam optical trap into a viable alternative to multiple beam traps which are costly, less flexible and more difficult to operate.

Kerr nonlinearity enhances the performance of a single beam trap by increasing the magnitude of the trapping force. It permits the trapping of nonlinear nanoparticles with $n_2^{(0)}$ values that are less than the index n_1 of the surrounding liquid and at lower NA values and optical beam powers. Low NA focusing objectives and low power laser sources are relatively inexpensive and are less likely to cause irreversible thermal damage on the sample and the surrounding medium.

Localized (non-uniform) heating of the liquid is also minimized if the average power of the focused beam is kept low using a femtosecond laser source with high peak powers and relatively low repetition rate.

Kerr nanoparticle can be an alternative probe handler when applied to photonic force microscope configuration for the imaging of hollow microbiological structures.

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Recent Optical and Photonic Technologies

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Research and development in modern optical and photonic technologies have witnessed quite fast growing advancements in various fundamental and application areas due to availability of novel fabrication and measurement techniques, advanced numerical simulation tools and methods, as well as due to the increasing practical demands. The recent advancements have also been accompanied by the appearance of various interdisciplinary topics. The book attempts to put together state-of-the-art research and development in optical and photonic technologies. It consists of 21 chapters that focus on interesting four topics of photonic crystals (first 5 chapters), THz techniques and applications (next 7 chapters), nanoscale optical techniques and applications (next 5 chapters), and optical trapping and manipulation (last 4 chapters), in which a fundamental theory, numerical simulation techniques, measurement techniques and methods, and various application examples are considered. This book deals with recent and advanced research results and comprehensive reviews on optical and photonic technologies covering the aforementioned topics. I believe that the advanced techniques and research described here may also be applicable to other contemporary research areas in optical and photonic technologies. Thus, I hope the readers will be inspired to start or to improve further their own research and technologies and to expand potential applications. I would like to express my sincere gratitude to all the authors for their outstanding contributions to this book.

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University Campus STeP Ri
Slavka Krautzeka 83/A
51000 Rijeka, Croatia
Phone: +385 (51) 770 447
Fax: +385 (51) 686 166

InTech China

Unit 405, Office Block, Hotel Equatorial Shanghai
No.65, Yan An Road (West), Shanghai, 200040, China
中国上海市延安西路65号上海国际贵都大饭店办公楼405单元
Phone: +86-21-62489820
Fax: +86-21-62489821

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