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A THREE-ANGLE LIGHT SCATTERING DETECTION SCHEME FOR PROBING ORIENTATIONAL DYNAMICS OF OPTICALLY TRAPPED MICROSPHERE DIMERS

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Abstract

Obtaining Static Light Scattering profiles from optically trapped entities poses considerable engineering challenge due to space constraints in a typical Optical Trap setup. We propose here a three-angle light scattering technique that can not only help characterize the structure but also be useful in understanding the dynamics of microscopic objects that are trapped optically. In this work, we demonstrate the use of such a measurement scheme in determining the optimal angles for light scattering measurements and probing the orientational dynamics of a microsphere dimer.

1 Introduction

Since their invention in the late 1980's by Arthur Ashkin [1], Optical Tweezers have found application in experiments ranging from single-molecule Biophysics [2] to those that test fundamental assumptions of Quantum Mechanics [3]. Perhaps the most common use of the Optical Tweezer is in force transduction and sensing [4]. While Raman Scattering is used to characterize the trapped particles [5], this technique cannot shed light on the dynamics of the trapped microparticles. In contrast, light scattering can be used to both characterize the trapped micro-structure and also obtain information on dynamics. However, adapting Light Scattering measurements in an Optical Tweezer Setup, typically involving an inverted microscope arrangement, is a significant engineering challenge as the oil-immersion objective used for trapping makes physical contact with the coverslip of the sample holder and thus rules out the possibility of introducing a second scattering wavelength from the bottom of the sample holder. A further complexity is the collection of scattered light at precise angles with a reasonably small angular range. Both these concerns were addressed by Saffran and co-workers [6] where they measured light scattering from a trapped microbead using an optical fibre placed precisely at 75-degree with respect to the direction of incidence of the scattering light which was also the trapping light. Since they collect scattered light at one angle only, they were reliant on autocorrelation estimates for characterizing the trapped bead.

We propose a three-angle light scattering detection scheme and explore its suitability to characterize trapped microstructures. We further discuss the usefulness of this scheme in inverting the light scattering problem to determine the orientation of the microsphere dimer from a light scattering measurement at only 3 angles.

We hope to extend this technique to study the orientations and dynamics of more complex shapes trapped in an optical tweezer in a subsequent full-length paper.

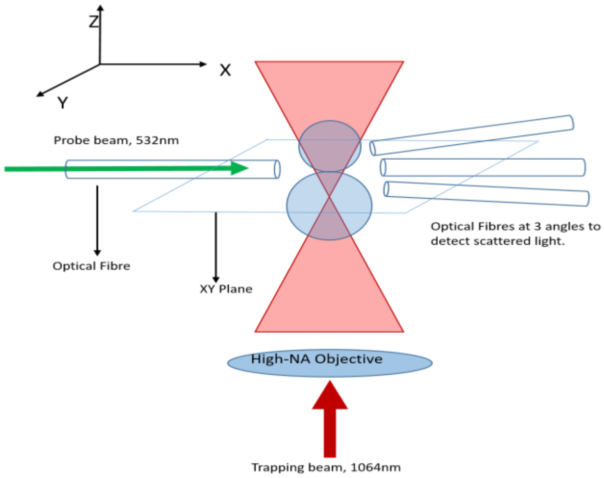

Figure 1: Schematic of Light scattering detection from an optically trapped asymmetric microsphere doublet. The optical fibre carrying the probe beam and the 3 fibres used to detect scattered light are all in the XY plane. The reference frame is assumed to be coincident with the trap-centre and the z-axis is assumed to be along the propagation direction of the trapping beam

2 Methodology

2.1 Optimization Protocols for solving the Inverse light scattering problem

In this section, we formulate a method to determine the optimal angles at which one may collect scattered light in order to deduce the orientation of the pair of particles. The orientation of the particles is labelled by the unit vector $\hat{n}$ which points from the centre of particle 1 to the centre of particle 2 (Fig 1) and its components along X, Y, and Z directions are indicated as nx, ny, and nz respectively. Shining a plane wave on these particles will produce a scattering pattern $I(\theta, \hat{n})$ which will depend on the orientation $\hat{n}$. The angle dependent scattering from the particles is calculated at several different orientations $\hat{n}$

using the T-Matrix based, package MSTM v3.0 [7] which is capable of computing scattered light from microsphere clusters.

The intensity of scattered light can vary by orders of magnitude at different angles. Instead of using these measurements directly, the values are scaled so that the response y_k at each angle k is normalized as

$$y_k(\hat{n}) = \frac{I(\theta_k,\hat{n}) - \langle I(\theta_k)\rangle}{\langle I^2(\theta_k)\rangle - \langle I(\theta_k)\rangle^2}$$

Where $\langle I(\theta_k)\rangle = \int d\hat{n} I(\theta_k,\hat{n})$ and $\langle I^2(\theta_k)\rangle = \int d\hat{n} I^2(\theta_k,\hat{n})$ The intensity of the scattered light is only collected at three angles θ_1, θ_2, and θ_3. When the particle is in orientation $\hat{n}$, we denote the measurement as the three dimensional vector $\bar{y}_q(\hat{n})$; the subscript q denotes the particular choice of angles at which the measurements were performed (i.e., the specific values θ_1, θ_2, and θ_3), and different sets of angles correspond to different values of q.

The Scattering simulations give us the expected measurement values $\bar{y}_q(\hat{n})$ when the particles are at a particular orientation $\hat{n}$. In practice, there are uncertainties associated with a measurement. We assume that these are Gaussian, with a standard deviation σ. The scattering simulations give us the conditional probabilities $p(y|\hat{n})$, which is the probability that a particle in orientation $\hat{n}$ will yield a light-scattering measurement y as:

$$p_q(y|\hat{n}) = (2\pi\sigma^2)^{-d/2} e^{-|y-\overline{y_q(\hat{n})}|^2/2\sigma^2} \quad (2)$$

We are interested in determining the orientation of the particle given a light scattering measurement. This can be formulated as the conditional probability $p_q(\hat{n}|y)$, the probability that the particles are in orientation $\hat{n}$ given the measurement y. This probability can be determined from Bayes' theorem

$$p_q(\hat{n}|y) = \frac{p_q(y|\hat{n})p(\hat{n})}{p_q(y)} \quad (3)$$

Where $p(\hat{n})$ is the prior estimate that the particles are in orientation $\hat{n}$ and $p_q(y)$ is the prior probability that a measurement y will be obtained $p_q(y) = \int d\hat{n} p(\hat{n}) p_q(y|\hat{n})$. Without any prior evidence, we assume that the orientation of the particles is distributed as $p(\hat{n})$, which can be uniformly oriented or oriented with respect to some Boltzmann distribution. Knowledge from previous measurements (e.g., immediately before the current measurement) can also be used to inform the estimate for $p(\hat{n})$.This gives us an estimate of the orientation of the particle, given a particular value of the measurement. In principle, this solves the inversion problem; however, if the probability distribution $p_q(\hat{n}|y)$ is broad or has multiple peaks, then we will have a poor estimate of the particles' orientation. A probability distribution with more than one peak points at the fact that there are multiple sets of orientations possible for a given scattering measurement. This problem can then be mitigated by changing the angles at which we perform the measurements. Such a choice of measurement angles can help optimize $p_q(\hat{n}|y)$.

(1) From the probabilities, it may be possible to write down the information content 'H' as $H = -\int d\hat{n} p(\hat{n}) \ln p(\hat{n})$ while the information content for a prior measurement may be written as $H_q(y) = -\int d\hat{n} p_q(\hat{n}|y) \ln p_q(\hat{n}|y)$ which is $H_q = -\int dy H_q(y) p_q(y)$. The expected information gain from obtaining measurements is $H_q - H$.

$$H_q - H = \frac{1}{2} + \frac{3}{2}\ln(2\pi\sigma^2) + \int dy p_q(y) \ln p_q(y) \quad (4)$$

A maximization of the parameter above should help determine the best possible choice of 3 angles at which to measure the light scattering, given the dynamics of the dimers and also the noise expected in a typical photodetector based measurement.

2.2 Orientational Brownian Motion simulation for (2) dimers

To test the ability of the method to invert the light scattering measurements and determine the particle orientation, we simulate the Brownian motion of a dimer of rigidly connected polystyrene spheres in water at 25°C that is optically trapped. The stochastic dynamics of the trapped dimer was simulated using the software package in [7] which outputs positions of the centre-of-mass of the dimer and it's orientation along the 3 axes of a laboratory-frame centred on the trap-centre. The diffusion coefficient for the dimer was adopted from [9].

In Fig [2], we show a typical time evolution of the orientation of microsphere dimers made of polystyrene spheres of radii 1 micron and 0.5 micron in (a), 1 micron and 0.2 micron in (b), and 1-micron each in (c). The orientations along the three axes of a reference frame centred on the trap-centre with the z-axis pointing along the propagation direction of the trapping laser are indicated as nx, ny, and nz.

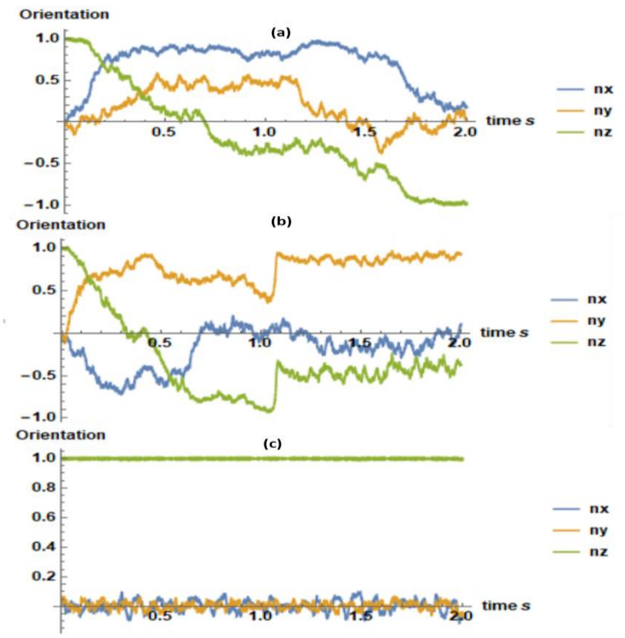

Figure 2 *Time evolution of orientation of dimers of radii (a)1:0.5-micron (b) 1:0.2-micron and (c) 1:1-micron. Dimers are suspended in water at 25°C and are being trapped in an Optical Trap of NA 1.2.*

The dimers are suspended in water at a temperature of 25°C and are trapped in an Optical Trap generated using an objective of numerical aperture 1.2 and with 1064nm laser light whose power was assumed to be 5mW. The scattering laser is assumed to be a plane wave, linearly polarized along x-axis, and propagating along the x-direction as shown in Figure (1).

In Figure (3) we show the time evolution of the position of the centre of mass of the three dimers.

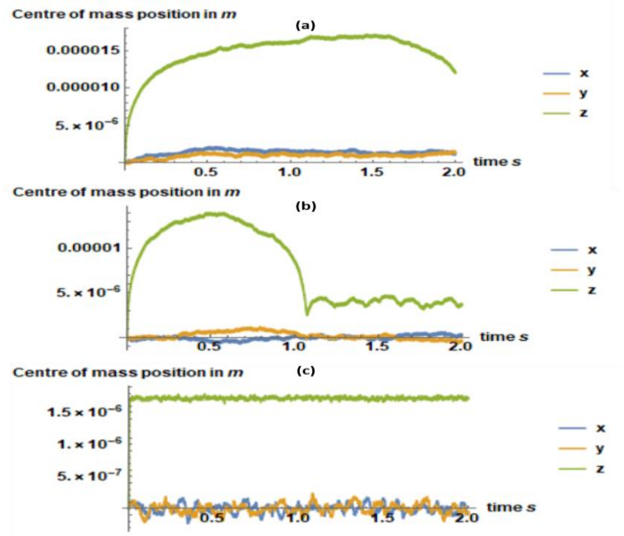

Figure 3 *Time evolution of the position of the centre of mass of dimers of radii (a)1:0.5-micron (b) 1:0.2-micron and (c) 1:1-micron. These positions are being reported with respect to the centre of the laser-trap*

As seen in Figures (2) and (3), the dynamics of the dimers are dependent sensitively on size and one may expect the proposed light scattering detection scheme to detect signatures of the dimers' orientation and position.

Our computer programs are presently capable of generating light scattering for each position and orientation of the dimers and we are working towards implementing the inverse light-scattering protocols. We expect to benchmark these protocols against light scattering signals obtained from dimers of known size in an actual experiment and also from MSTM based calculations so that they may be useful in characterizing trapped dimers of unknown size ratios. This, we hope will open up the possibilities of extending this technique to characterize more complex shapes.

3 Conclusions and future work

We assess the feasibility of characterizing trapped entities in an optical trap by use of a 3-angle light scattering detection technique and propose a protocol to optimize the detection angles therein. We have setup Brownian motion and light scattering computations and are presently working on the computations aimed at optimizing the choice of measurement angles given a realistic estimate for measurement noise.

We hope to write up these results in a subsequent full-length paper.

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