Optical tweezers modelling - basics and references

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1 What optical tweezers are

The name "optical tweezers" is fitting - they are literally tweezers made of light. Using them one can catch and move micro-, or even nano-, scale objects. The object which is held must be made of dielectric material, because optical tweezers use a specific interaction between light and dielectric, which causes the small dielectric object to move towards the peak of the light's intensity.

Therefore, if one creates a light pattern with high gradient of intensity, then it becomes possible to repulse or drag objects, which at given point x behave like feeling the potential $V(x)$ proportional to minus intensity of light $V(x) \propto -I(x)$. So, if the intensity $I(x)$ has the shape of some "mould", the potential is some hole and it traps chosen object. Such shape of light intensity can be relatively easily generated using laser. When one moves the position of the light speck, the minimum of potential $V(x)$ moves along it, and it drags the object.

The usefulness of optical tweezers is clear - they allow for precise manipulation of very small objects. They allow for moving and sorting of single cells, or even molecules, for stretching and squashing necessary for measuring hardness of small structures. Moreover, the movements of bead depend not only on the laser, but also on the medium, because it interacts with it continuously. Because of this, optical tweezers allow for measurements of properties of biological liquids, various suspensions, and others.

2 How is data collected

There are two main ways to collect data about the motion of object held by optical tweezers: illumination from below and observation of the shadow on the photo-sensible plate, or recording using CCD camera. Both methods have its advantages and disadvantages, generally observation of shadow is very precise, but limited, whereas CCD camera recording is less precise, but much more flexible, allowing e.g. for simultaneous observation of many object. We will consider the latter. The image of the held object is projected on small CCD matrix using precise lenses, which results in data having form of series of matrices containing pixels' intensities, which can be shown as a movie. The main property of interest is the position of the object $X(t)$, which is obtained simply as a **center of the mass** of the visible shape.

3 How are optical tweezers modelled

The main model of the particle trapped in the optical tweezers is deceptively simple; it is classical Newton equation for the particle's position X.

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}X = F_0 + F_f + F_T.$$

The three forces present are F_0-optical force caused by tweezers, F_f - force of friction caused by movement within liquid, and F_T - the so-called "thermal force" present due to random collisions with the particle of the medium.

We have experimental control over the force F_O, the preferable situation is when it is harmonic $F_O(x) = -\kappa x$; it is worthy to check from the data if this assumption is reliable. The form of F_f and F_T depends on the medium and shape of held object. The most popular type of held objects are balls of various sizes, and the calibration of optical tweezers is usually performed in the water environment. In such conditions good assumptions are $F_f(x) = -\beta\frac{\mathrm{d}}{\mathrm{d}t}x$ (classical linear friction) and F_T being the so-called **white noise** $F_T(t) = \xi(t)$, which is the derivative of the motion of a free particle, the **Brownian motion**. The process $\xi(t)$ is random and it causes also $X(t)$ to be random and unpredictable.

4 About statistical analysis

Because the position of the bead $X(t)$ is random, one needs statistical methods to analyse its properties, mainly **time series analysis**, in particular methods related to **ARMA models**. The three main aspects, which are worth considering, are:

- analysis of the state - what distribution $X(t)$ has and how it depends on the trapping potential and different phenomena, e.g. moments (**mean, variation**, etc.), probability density, characteristic function and so on
- analysis of the memory - how position at one time depends on the position in the past, it shows how the process "remembers" its history, this include **autocorrelation function** and similar measures
- Fourier analysis - we go into Fourier space and look how the process looks considered as a mixture of sinusoids, e.g using **periodogram**.

The analysis of this three aspects would be hard enough, but at the same time we must remember that the data that we have can be distorted in various ways. Our equipment has finite precision and it can even introduce new effects, which would be not present in the original phenomena. For example, the pixels in the CCD camera add some noise to any image that it records, therefore we do not observe the pure position $X(t)$, but the distorted $\tilde{X}(t) = X(t) + N(t)$, where $N(t)$ is the added noise.

One should not only try to extract the needed properties from the data, but also include the influences of the noise and different types of disturbances. In order to achieve that it is necessary to derive precisely the properties of the tweezers' model and explain all observed deviations proposing the form of distortions.

5 Why we do that

Thorough understanding of the optical tweezers' data gives many profits:

- it allows for precise calibration of the tweezers - we can measure and therefore control how much force we want to use and when,
- we can study the properties of the environment, in which the held object is embedded, if we can explain the behaviour of the tweezers acting in the water, we can look for differences when acting in the different and more complex type of medium,
- we can remove sources of distortions, e.g. tweak the used CCD camera, lightning, laser set-up and so on, it would be impossible if we do not know what is wrong.

It is worth to add, that the data collected from the tweezers can be considered typical in the sense that very similar models are used in different branches of physics or even seemingly unrelated topics, like econometrics and financial mathematics. The most simple model of the trajectory $X(t)$ is called **Ornstein-Uhlenbeck process** is one of the most useful models for random data available.

6 Useful tools

To analyse optical tweezers' data and model their behaviour one needs proper programming environment and statistical tools. The most suitable are:

- **Matlab** - whole programming environment and language, it has advanced matrix operations, basic statistical tools and very nice plotting options; unfortunately it is expensive and rarely used outside of academia, free alternative suitable for most of the purposes is **Octave**,
- **Python** - programming language, which together with some libraries (**numpy, pandas, matplotlib**) is an environement which is free and has similar capabilities as Matlab; at the same time Python is much more flexible than Matlab language,
- **R language** - it is less efficient than Matlab or Pyhon, but is free and has an advantage of having enormous library of statistical packages available; some methods available in R are hard to find anywhere else and would be very tiresome to implement by itself.

Actually it is possible to use nearly any programming language to analyse data such as considered and perform simulations. The fastest would be C or Fortran, but most of the needed computations will probably not be very demanding in terms of efficiency, so it is sensible to use tools in which the modelling is the simplest.

7 Useful literature

Statistics:

- **Introduction of Time Series and Forecasting**, P. Brockwell, R. Davies - very clear and accessible book which explains both basics and advanced methods of dealing with time-series data,
- **Time Series Analysis, Forecasting and Control**, G. Box, G. Jenkins, G. Reinsel - more advanced book, they are less examples and more detailed explanations and proofs about concepts related to time series, it is worth to look into this book if we need additional information and more strict approach.

Physical models:

- **An Introduction to Stochastic Process in Physics**, D. Lemons - gentle introduction into topic of stochastic processes and their applications, it contains information about models that will be needed - Langevin equation, Brownian motion and Ornstein-Uhlenbeck process, they are even methods of simulation described there,
- **Handbook of Stochastic Methods** C. Gardiner - more advanced book, it contains a lot of material, one can find there precise explanation of stochastic integration and differential equations together with more mathematical details about the considered models.

Programming and simulation:

- **Python for Data Analysis**, W. McKinney - it gives information about most important Python libraries about data analysis and their usage, mainly numpy and pandas,
- **Introductory time series with R**, P. Coperwait, A. Metcalfe - libraries, models, simulation and lot of examples for dealing with data in R.

Some publications about modelling of optical tweezers:

- **Power spectral analysis of optical trap stiffness calibration from high-speed camera position detection with limited bandwith**, A. van der Horst, N. Forde, in *Optic Express* vol 18 - it describes a model of motion in the frequency space and the effect of the main distortions and noises, publication is quite technical, but one can see how the typical plots in the frequency space look,
- **Optimized holographic optical traps** M. Polin, K. Ladavac, Sang-Hyuk Lee, Y. Roichman, D. Grier, in *Optic Express* vol. 13 - contains general information about tweezers, motion detection, and, in the second half, specific and long formulas which may be useful during the statistical analysis,
- **Power spectrum analysis for optical tweezers** K. Berg-Sørensen, H. Flyvbjerg, in *Review of Scientific Instruments* vol. 75 - different approach to fitting Fourier spectra, once again technical paper, but they are some useful techniques described and the plots are fairy typical.