Temperature Measurements in Optical Tweezer Experiments

Mathias Höld, BSc.

2016

1 Introduction

2 Motivation

3 The experiment

The starting point of this thesis is an experiment conducted by Gieseler et al [5]. It is an optical tweezer experiment, where the motion of a glass nanoparticle in a laser trap was used to investigate the fluctuation theorem[3].

3.1 Experimental setup

In the experiment, a silica nano particle with a radius of about 75 nm and mass of about 3×10^{-18}kg is trapped in a laser beam within a vacuum chamber. The trapping of the silica nano particle (which will be referred to as *glass particle*) is achieved by a gradient force of the laser beam acting on the particle. The experimental setup is depicted in fig. 1.
The particle fluctuates within the trap in all three spatial directions. These fluctuations can be approximated such that they are decoupled, which means that they can be described by a 1-dimensional Langevin equation:

$$\ddot{x} + \Gamma_0 \dot{x} + \Omega_0^2 x = \frac{1}{m} \left(F_{\text{fluct}} + F_{\text{ext}} \right) \tag{1}$$

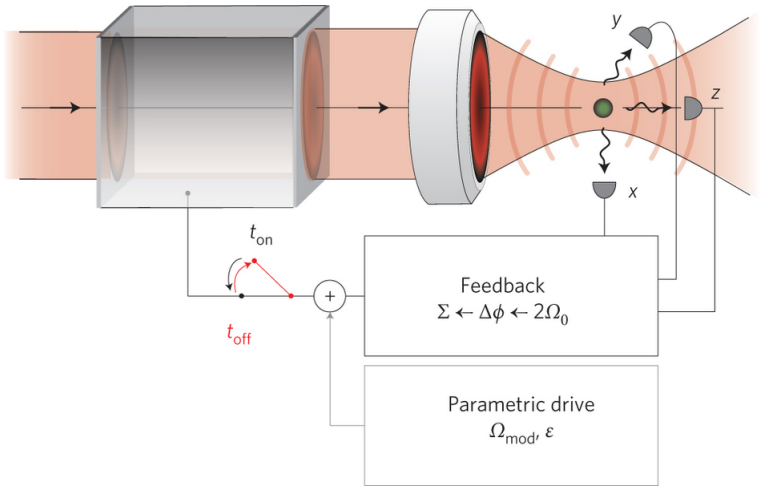


Figure 1: Experimental setup of the optical tweezer experiment. A silica nano particle is trapped in a laser beam via gradient force in a vacuum. The feedback is used to cool down the particle and create a non-equilibrium steady state. In the first part of the experiment, the feedback is turned off and the motion of the particle towards an equilibrated state is observed. In the second part of the experiment, the steady state of the particle is modified by a parametric drive. Both the parametric drive and the feedback are turned off and – as in the first part – the motion of the particle towards an equilibrated state is observerd.

On the left hand side we have the friction coefficient Γ_0 and the angular frequency that describes the fluctuation along the chosen axis. On the right hand side, there are two forces. The first one is F_{fluct}, which describes a stochastic force caused by interactions with the gas in the vacuum chamber. This force is given by

$$F_{\text{fluct}} = \sqrt{2m\Gamma_0 k_B T_0}\ \xi\left(t\right) \tag{2}$$

where T_0 is the temperature of the heat bath (i.e. the surrounding gas in the vacuum chamber), k_B is the Boltzmann constant and $\xi(t)$ is white noise, which obeys the equations $\langle\xi(t)\rangle = 0$ and $\langle\xi(t)\xi(t')\rangle = \delta(t-t')$, which means that it is a random force. The term Γ_0 appears in the formulat due to the fluctuation-dissipation theorem, which links the damping rate to the stochastic force.
The external force F_{ext} is part of the experimental setup, where the frequency of the fluctuation along an axis, Ω_0, is measured and used to suppress the motion along said axis. This causes a decrease in the particle fluctuations and thus acts as a cooling mechanism for the particle in the trap. This process creates a non-equilibrium steady state $\rho_{ss}(u,\alpha)$, which is not known analytically. This state is the starting point of this thesis.

4 Simulation

The problem at hand can be studied on an atomic level with the use of computer simulation. There is a variety of methods for computer simulations that are widely used, one of which being Molecular Dynamics (MD) simulations. The following section will give a brief overview of the concepts of this method, which is followed by the application to the simulation of the experiment.

4.1 Molecular Dynamics

Molecular Dynamics[4] simulations is a technique for simulating, as the name suggests, the dynamics of a classical many-body system. In this case, classical means, that the trajectories of the individual particles are calculated using classical mechanics rather then quantum mechanics. For relatively big atoms/molecules this is a very good approximation, whereas for systems consisting of hydrogen or helium the effects of quantum mechanics cannot be neglected and other methods (such as ab-initio simulation) has to be used.
The dynamics of the system are obtained by solving Newton's equations of motion for every particle.

4.2 The Glass Particle

The glass particle from the experiment will be modeled as a system of particles interacting via a Lennard-Jones pair potential,

$$U(r) = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \tag{3}$$

where ε is the depth of the potential well (and thus its unit is energy) and σ is the distance at which the potential is zero. The form of the potential and the relation to the parameters is depicted in Fig. 2. Since ε and σ are crucial parameters for the simulation and do (usually) not change over time, it is practical to use them to define the dimensions of the system. This means that the unit of distance is σ, the unit of energy is ε and the unit of mass is the mass of the simulated particle. The so called *reduced units* can be constructed from these three parameters and put into relation to the original units. Here are some examples:

- distance: $r^* = r/\sigma$
- potential energy: $U^* = U/\varepsilon$
- temperature: $T^* = k_B T/\varepsilon$

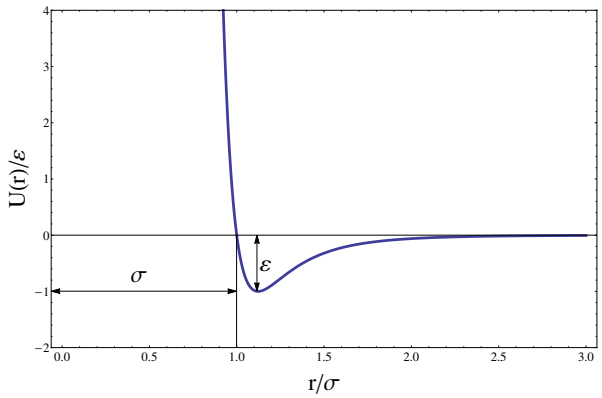


Figure 2: The Lennard-Jones 12-6 potential from (3). The x-axis is the particle distance divided by σ and the y-axis is the potential divided by the depth of the potential well.

- time: $t^* = t\sqrt{\varepsilon/(m\sigma^2)}$
- pressure: $P^* = P\sigma^3/\varepsilon$
- density: $\rho^* = \rho\sigma^3$

One very popular choice for the simulated atoms is Argon because it is an inert gas and the atoms behave approximately like hard spheres which attract each other with weak van der Waals forces, which justifies the use of the Lennard-Jones potential. Argon has a mass of m $= 6.69 \times 10^{-26}$ kg, $\sigma = 3.4 \times 10^{-10}$m and $\varepsilon = 1.65 \times 10^{-21}$J.
With the above introduced reduced units, the Lennard-Jones potential can be written as

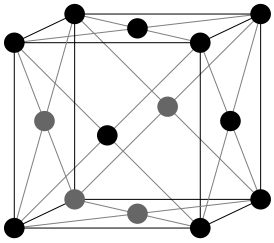
$$U(r^*) = 4\left[r^{*-12} - r^{*-6}\right]. \tag{4}$$

Since the reduced units will be used throughout the rest of this thesis, i will drop the asterisk henceforth.
From the Lennard-Jones potential the corresponding force can be calculated by taking the derivative with respect to the direction of interest:

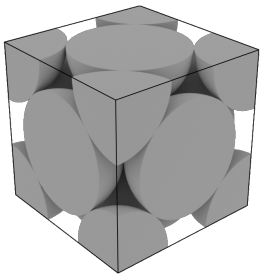
$$\begin{aligned} F_x &= -\frac{\partial}{\partial x}U(r) \\ &= -\frac{\partial}{\partial x}4\left[r^{-12} - r^{-6}\right] \\ &= -4\left[(-12)r^{-13} - (-6)r^{-7}\right]\frac{\partial r}{\partial x} \\ &= 48\left[r^{-13} - 0.5\ r^{-7}\right]\frac{x}{r} \\ &= 48\left[r^{-14} - 0.5\ r^{-8}\right]x \end{aligned} \tag{5}$$

The force in the y and z direction can be calculated analogously.
The initial configuration of the particles is a face centered cubic (FCC) lattice. A schematic of the FCC lattice is depicted in fig. 3a. With the choice of FCC as initial configuration, there are optimal numbers for the numbers of the particles in the system. Since once FCC cell (as depicted) shares its atoms with its next neighbours, the number of atom per unit cell is 4, as depicted in fig. **??**. The whole system of atoms is then created by repeating this cell structure. One convenient way is to arrange the unit cells in a cubic system, so if there are M FCC unit cells on one edge, the whole system consists of M^3 cells. Since there are 4 particles per cell, there are ideal or so called *magic numbers* for atoms for which this setup works perfectly: $N = 4M^3 = 4, 32, 108, 256, 500, 864, \ldots$.

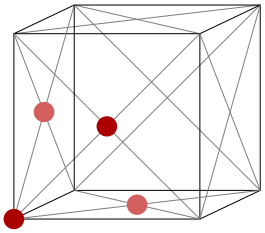
There are several ways to achieve this initial configuration and the one used in



(a) Schematic figure of a face centered cubic (FCC) lattice



(b) Schematic of the number of particles contained in one FCC unit cell. The atoms on the edges are shared by 8 cells and the ones on the faces by 2 cells[1]



(c) Setup for successively building a FCC lattice

this thesis [2] was to create a kind of unit cell consisting of four atoms, as shown in fig. 3c, which can be described by a set of points

$$\begin{aligned} p_1 &= \{0, 0, 0\} \\ p_2 &= \{0.5, 0.5, 0\} \\ p_3 &= \{0.5, 0, 0.5\} \\ p_4 &= \{0, 0.5, 0.5\} \end{aligned}$$

From the particle number N and the number of FCC unit cells per edge M the lattice constant a can be calculated

$$a = \frac{L}{M} \tag{6}$$

where L is the side length of the cube that is the whole system and it is calculated via the density of the system

$$L = \sqrt[3]{\frac{N}{\rho}} \tag{7}$$

With the lattice constant and the 4 points of the FCC cell, all the particles can be put into place.

4.3 The Velocity-Verlet Algorithm

When we look at the system from a thermodynamical standpoint, we see that it follows some kind of path in the phase space as time progresses. Every point in this space corresponds to a set of positions and momenta and the connection between two points corresponds to the evolution of the system from one state to another. As mentioned above, this evolution (the dynamics of the system) is a crucial element to Molecular Dynamics. Since the equations of motion cannot be solved analytically in general, we need to approximate the solution.
The method used here is called finite difference approach. The trajectory of the system in the phase space is cut into finite pieces of length Δt and the equations of motion are solved for every segment separately (see fig. 4).

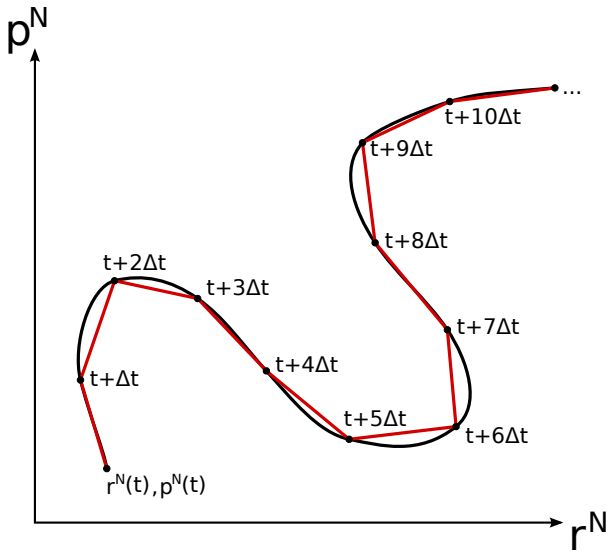


Figure 4: Simplified graphical schematic of the finite difference approach. The evolution of the system from a point $(r^N(t), p^N(t))$ in the phase space is approximated by slicing it up into pieces of length Δt. On every stop after the starting point ($t + \Delta t$, $t + 2\Delta t$, $t + 3\Delta t$,...) the equations of motion can be solved numerically.

5 Results

6 Conclusion

References

[1] Image taken from `https://upload.wikimedia.org/wikipedia/commons/2/27/Elementarzelle_einer_kubisch_raumzentrierten_Elementarzelle.png`.

[2] Idea taken from the Molecular Dynamics part of this lecture: `http://www.physics.buffalo.edu/phy411-506/`.

[3] Gavin E. Crooks. Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences. *Phys. Rev. E*, 60:2721–2726, Sep 1999.

[4] D. Frenkel and B. Smit. *Understanding Molecular Simulation: From Algorithms to Applications*. Computational science series. Elsevier Science, 2001.

[5] Jan Gieseler, Romain Quidant, Christoph Dellago, and Lukas Novotny. Dynamic relaxation of a levitated nanoparticle from a non-equilibrium steady state. *Nat Nano*, 9(5):358–364, May 2014.