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SIMULATION ON POWER SPECTRUM DENSITY (PSD) OF AN OPTICALLY TRAPPED PARTICLE

Sugeng Riyanto[1], Shahrul Kadri Ayop[2] and Wan Nor Suhaila Wan Aziz[3]

Department of Physics, Faculty Science and Mathematics,
Universiti Pendidikan Sultan Idris, MALAYSIA

Abstract

Microrheology studies are based on Brownian motion (BM) of particles. The main causes of BM are thermal fluctuation and viscosity of medium. One of the microrheological methods is single probe study using Optical Tweezers (OT) to extract information about the material characteristics. The OT uses single particle, which undergoes BM. For analysis of the BM, we need Power Spectrum Density (PSD). Therefore, this paper discuss on the simulation of the PSD calculation of single particle in liquid. We generate random number, which represent the displacement of the particle for on allocated period of time. The PSD is calculated using Origin Pro 9.1. The resulted PSD is useful for further investigations, for example in characterization of storage and loss modulus of a material.

Keywords: Microrheology, Brownian motion (BM), Power Spectrum Density (PSD).

INTRODUCTION

Microrheology is the field of exploring rheological properties of materials at the micro-sized scale. Microrheology technique has been widely used in the analysis of complex fluid or viscoelastic materials in micro-sized, such as emulsions, suspensions and polymer solutions. [1]. Microrheology theory was established earlier by Einstein-Stokes and later revised by Mason and co-workers. [2] The theory approximated the behaviour of the Brownian motion (BM) of particles using the second Newton's law of motion. One of the microrheology techniques is the utilization of Optical Tweezers (OT). OT acts as a probe in the materials under the investigations to trap a single particle that undergoing BM. The motion of the probe in one axis of freedom represented by particle displacement, *x*, subject to stochastic force, F_s, on the probe due to thermal fluctuation is described by the following relation:

$$m\ddot{x} + \gamma\dot{x} + kx = F_s(t) \qquad (1)$$

Where *m* is the mass of the probe [kg], γ is the drag coefficient [kg/s] and k is the stiffness of the optical trap [N/s]. The solution of Equation (1) via power spectrum is given by

$$\left\langle |\tilde{x}(\omega)|^2 \right\rangle = \frac{\left\langle |F_s(\omega)|^2 \right\rangle}{(m\omega^2 - k)^2 + \gamma^2\omega^2} = \frac{4\gamma k_B T}{(m\omega^2 - k)^2 + \gamma^2\omega^2} \qquad (2)$$

where k_B is Boltzmann constant [J/K] and *T* is the absolute temperature [K]. [3]

Equation (2) describes the Brownian motion due to only thermal driven force. We can deduce that at low frequency region, the denominator of the equation resulted in constant value. Meanwhile, the value significantly decreases at high frequency region. However, this behavior is only valid in the solution where a mechanical property does not change greatly in the wide range of frequency response. In the materials where viscosity and elasticity are significant the values also change accordingly giving the information about the physical structure of the material at microscopic level [4].

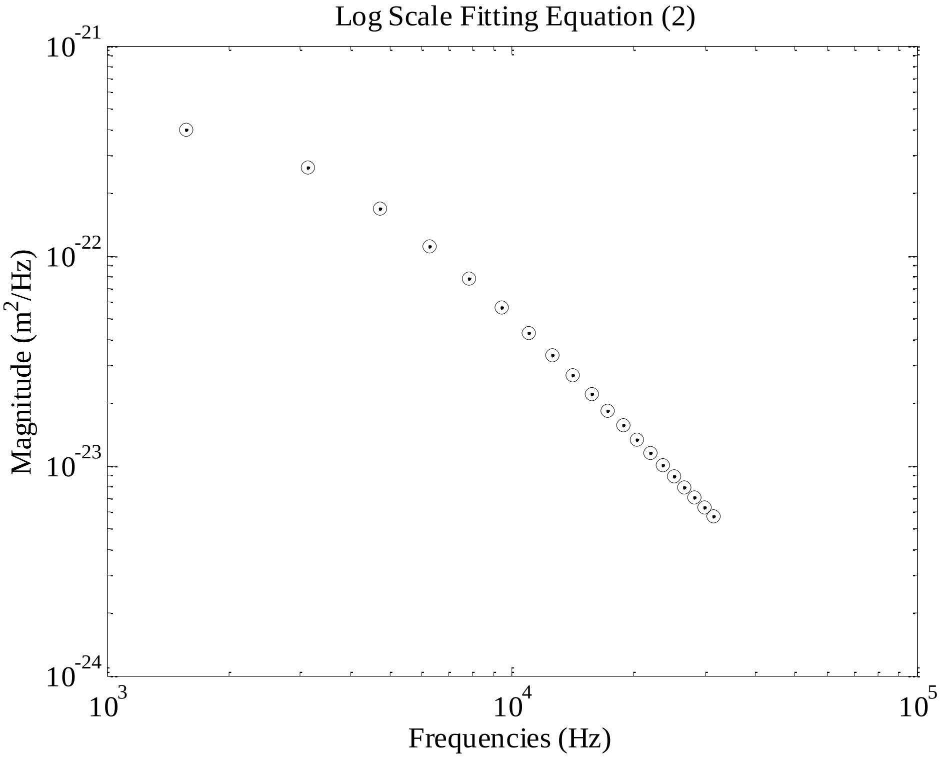


Figure 1. Pattern of the Equation (2) for the varying frequencies.

Figure 1 shows the graph from Equation (2) with the following parameters: k = 10^{-2} N/m; $\gamma = 2.9\times10^{6}$ kg/s; Rate sampling, f_s =2.5 MHz; Number of data, N = 10^4. The magnitude of power spectrum was flat at low frequencies and it decreases a high frequencies. It has mean the power spectrum at low frequencies contributed by temperature and stiffness constant of particle. At high frequencies, the power spectrum will be informed how the response of particle to the drive frequencies.

Many studies have reported on the finding resulted from Equation (2) [3,4,5]. However, less detail has been shown to demonstrate clearly how calculation was done. This becomes the problem for novice researchers to understand and analyze their data to get the meaningful result. Therefore, in this paper we explain the detail calculation of the BM resulting in Power Spectrum Density (PSD). We simulate the motion of a single particle, as a probe in OT or any microrheology technique. The simulation is expected to provide benefit researchers in microrheology study in order to understand how the equation of motion leads to physical interpretation of BM.

DISCUSSION

In order to simulate the PSD calculation, we generate raw data using random function in Microsoft Excel. The data represents the random displacement of a trapped particle from its equilibrium point in an optical trap due to the thermal fluctuations. We describe step by step how we do the simulation.

Random Number Generation

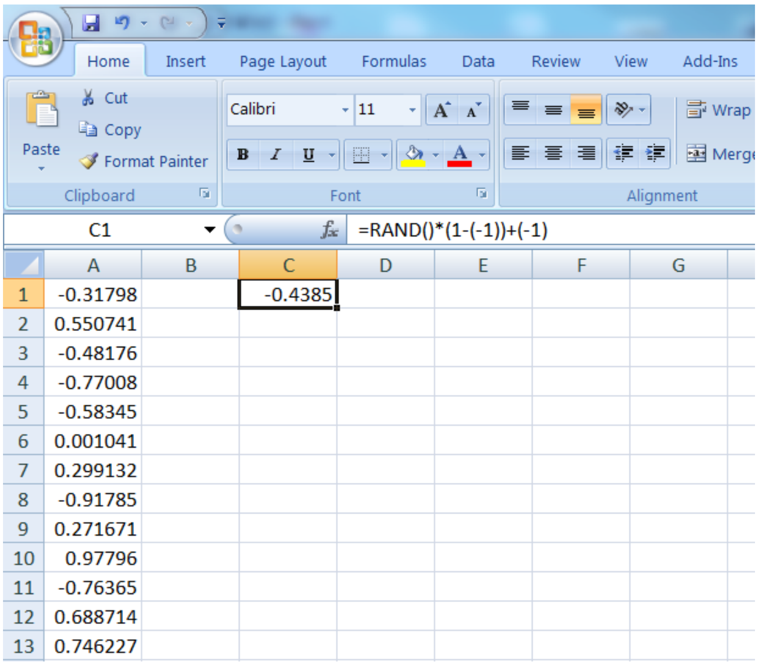
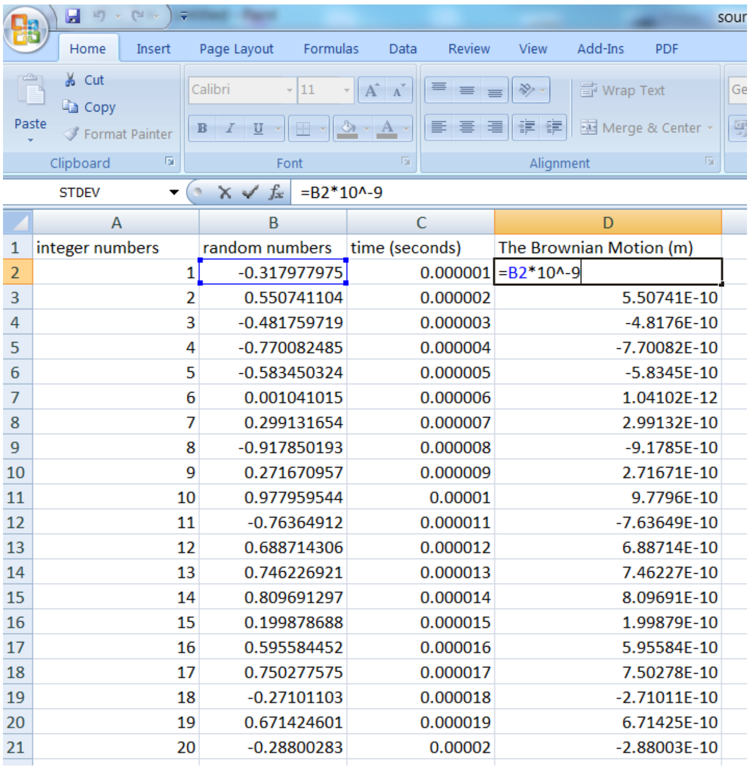


Figure 2. The syntax is to generate random number using Microsoft Excel TM.

One of the simplest technique to generate series of random number is using easily available Microsoft Excel TM software. The syntax command is RAND()*(*b*-*a*)+*a*, where *a* is the low value and *b* is the high values. We generate a series of 10,000 random numbers of lower and upper limits of -1 to 1. The sign of the generated number represents the displacement direction from equilibrium point, to the right or left in one dimension. Figure 2 shows the syntax is written in the formula field of cell. Once, the formula is inserted for first cell, further numbers are generating by simply dragging down the bottom left side of the first cell until 10,000 numbers are generated.

Dimension Assignment

The generated numbers are dimensionless. Therefore, we assign the unit and logical factor to simulate the actual particle motion. We multiplied the data number cell by the factor of 10^{-6} s for time of measurement and multiplied it by the factor of 10^{-9} m for particle displacement. Figure 3 shows how we did the multiplication. These two columns represent the particle displacement in the function of time.



STDEV =B2*10^-9

	A	B	C	D
1	integer numbers	random numbers	time (seconds)	The Brownian Motion (m)
2	1	-0.317977975	0.000001	=B2*10^-9
3	2	0.550741104	0.000002	5.50741E-10
4	3	-0.481759719	0.000003	-4.8176E-10
5	4	-0.770082485	0.000004	-7.70082E-10
6	5	-0.583450324	0.000005	-5.8345E-10
7	6	0.001041015	0.000006	1.04102E-12
8	7	0.299131654	0.000007	2.99132E-10
9	8	-0.917850193	0.000008	-9.1785E-10
10	9	0.271670957	0.000009	2.71671E-10
11	10	0.977959544	0.00001	9.7796E-10
12	11	-0.76364912	0.000011	-7.63649E-10
13	12	0.688714306	0.000012	6.88714E-10
14	13	0.746226921	0.000013	7.46227E-10
15	14	0.809691297	0.000014	8.09691E-10
16	15	0.199878688	0.000015	1.99879E-10
17	16	0.595584452	0.000016	5.95584E-10
18	17	0.750277575	0.000017	7.50278E-10
19	18	-0.27101103	0.000018	-2.71011E-10
20	19	0.671424601	0.000019	6.71425E-10
21	20	-0.28800283	0.00002	-2.88003E-10

Figure 3. Data generation is BM of a trapped particle.

PSD Calculation

The BM was in time domain, now it can be transformed into frequency domain in the form of PSD. For that purpose we used Origin Pro 9.1 ™ software. We have chosen Sum Squared Amplitude (SSA) on the menu option to represent the peak magnitude for each frequency in the length of data sequence or data recorded. We display one sided spectrum or frequencies to compute the Power Spectrum Density (PSD).

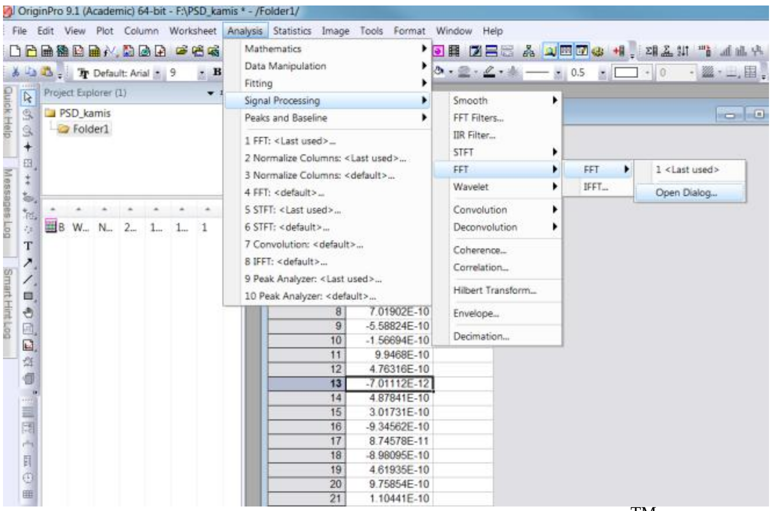


Figure 4. Menu PSD is chosen in Origin Pro 9.1 ™.

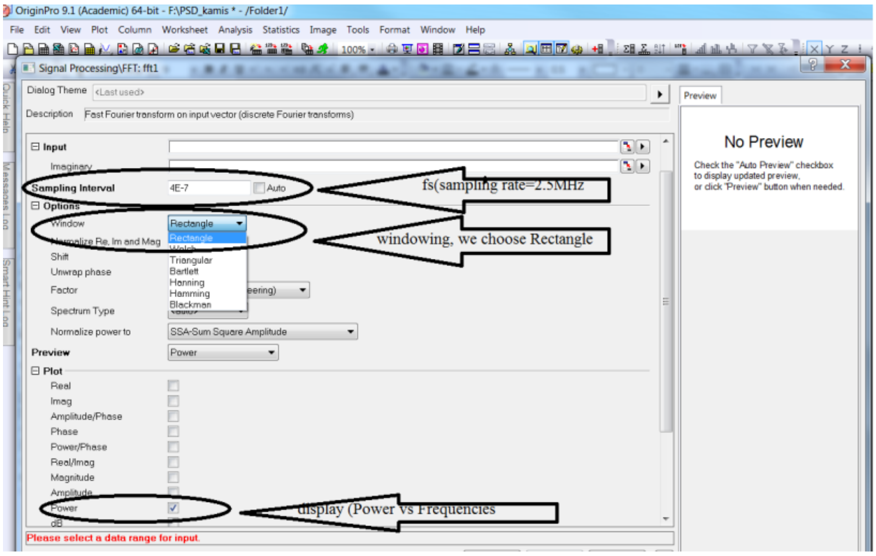


Figure 5. Setting in the signal processing window. We have chosen sampling rate to be 4×10^{-7} seconds and the windowing type to be rectangular.

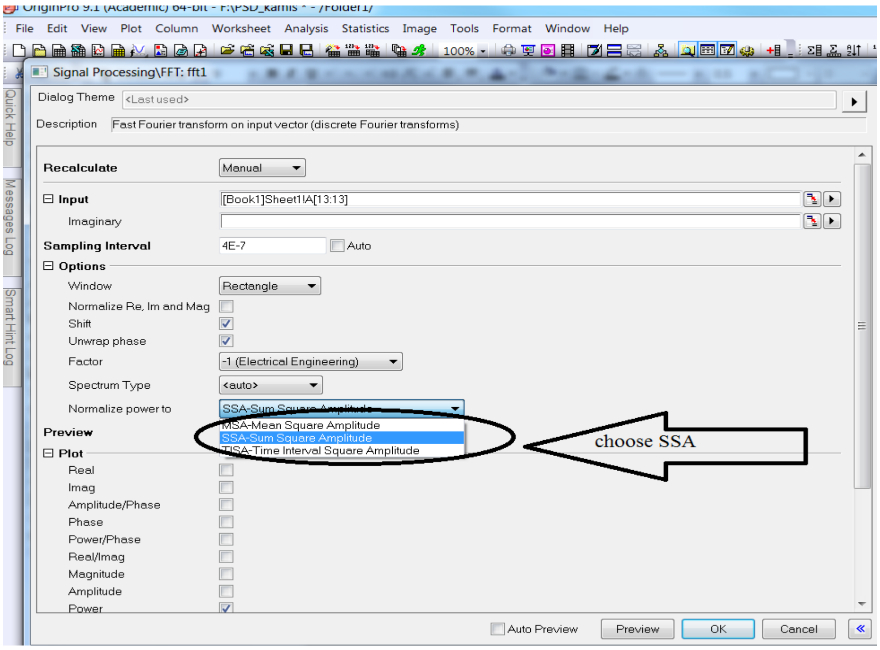


Figure 6. There are three options to normalize power. Since we want to understand the peak of energies distribution, we choose Sum Squared Amplitude (SSA).

We have generated a series of random number, which represent the displacement of the particle for on allocated period of time. The motion of a trapped particle depicted in Figure 7.

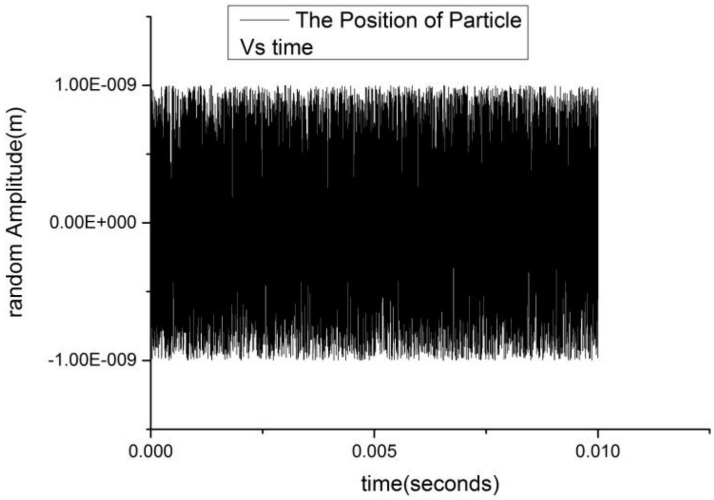


Figure 7. Simulation is the motion of a trapped particle.

The random nature of the motion is clearly simulated. The displacement fluctuation contains physical characteristics of the surrounding medium. The analysis of BM was done using Power Spectrum Density (PSD). FFT calculation resulted in a series data of frequencies domain, also known as spectrum frequencies. In the real-world, the spectrum frequencies are displayed in positive half. The spectrum is symmetrical around at DC component, so the negative frequency information is redundant. Another important quantity is the magnitude of power spectrum. The power spectrum is the sum squared amplitude for every frequency while no phase information. The phase information yield is the phase relative to begin of the signal at time domain.

The power spectrum computed using following

$$\text{Power Spectrum } PS_A(\omega) = \frac{FFT(\omega) \bullet FFT^*(\omega)}{N^2} \tag{3}$$

where FFT*(ω) is the complex conjugate of FFT (ω).

To calculate the PSD, the OriginLab Pro 9.1 ™ following relation

$$PSD(\omega) = \frac{PS_A(\omega)}{(\Delta f)(NPB\_of\_window)} \tag{4}$$

where Δf is the resolution of frequency, the *NPB_window* is the window of noise bandwitdh which is preselected by user. [4]

Δf is chosen based on the Nyquist criteria as follow

$$\Delta f = \frac{f_s}{N} = \frac{1}{N\Delta t}, \tag{5}$$

with Δt is time interavel [s] and f_s is the rate sampling (Hz)
Based on the guidelines above, the simulated BM is transformed using the following parameters: the *NPB_window* is rectangular, N = 10,000 and f_s = 2.5 MHz. The result is shown in Figure 8.

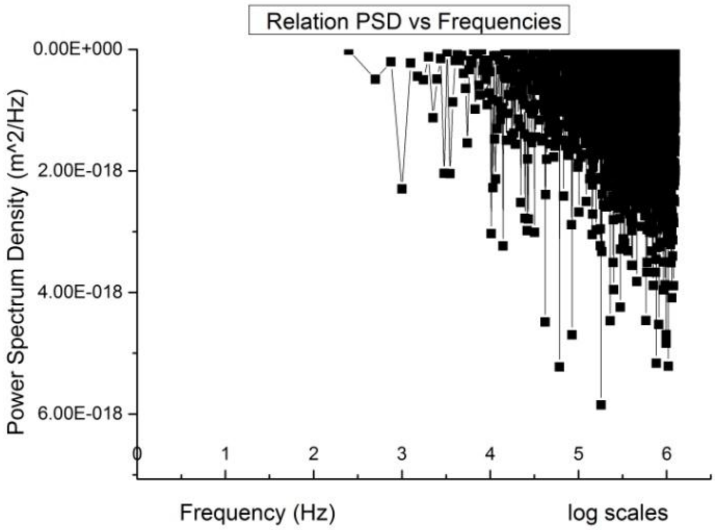


Figure 8. The PSD is result from the data Figure 7.

The Figure 8 gives information the resolution of frequencies; it is following Equation (5). The resolution of frequency is 250 Hz. We can increase the resolution frequencies of the PSD by appending number of data in the time domain. However, this procedure requires more time and computer memory to calculate it. The other alternatif is by maintaining data number and reducing time interval.

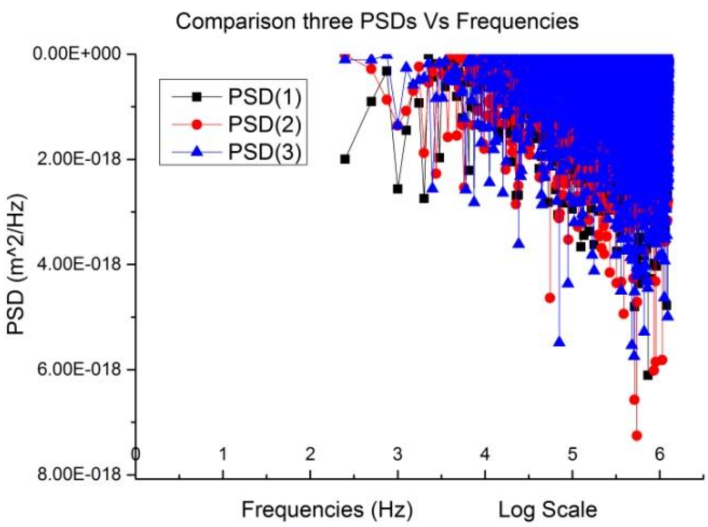


Figure 9. PSD for 3 separately generated BM data.

We generated another 2 sets of BM data. The PSD of these data is put together with prior set of data in Figure 9. The randomness of these data shows the same pattern. The PSD represent the real BM within OT. The collisions between particles in a medium become more frequent as the surrounding temperature increases. By using the PSD, we can calculate the contribution of the BM to explore the mechanical properties of particles. One of the mechanical properties is complex shear modulus [7]. The complex shear modulus can be obtained from the response of particle under stress. The particle will give response unique to change environment.

CONCLUSION

We have calculated the BM using PSD with modes are Sum Squared Amplitude (SSA) and rectangular window. These modes have function to displays peaks of distribution energies and to decrease the leakage signal of the BM. The distributions of energy in the BM can be included within the analysis behavior of particle under constant stress.

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