A New Type of Motion: Active Materials

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The study of Soft and Living Matter is relatively new in comparison to more well established fields, such as Particle or Nuclear physics. The goal of my project was to explore the dynamics of active nematic liquid crystals, including the motion of defects in this system. Specifically I aimed at understanding the types of dynamics of active materials and the difference between the dynamics of active and passive particles. To characterize the dynamics, we calculated the mean-squared displacement (MSD) of active particles and of active nematic defects, and compared it to the MSD of passive Brownian particles and to ballistic motion which have both been previously well-characterized.

I. INTRODUCTION

Active matter does not rely on external force to propel. Active materials are composed of particles that consume energy and use that energy to self-propel. This is in contrast to most physical systems that require external forces to be set into motion. All biological systems are active, and therefore studying the dynamics of synthetic active particles and of active nematics will advance our understanding of the complex dynamical structures observed in biology.

With this goal in mind, I have investigated and quantified the dynamics of active Janus particles and of defects in active nematics and compared their dynamics to Brownian and ballistic motion.

The goal was to analyze the microscopic dynamics of particles in a fluid to understand the difference between the dynamics of Brownian and active particles.

FIG. 1. FFT and Threshold Processed Image of Experimental Brownian Particles.

II. BROWNIAN AND BALLISTIC MOTION

Particles immersed in a medium at finite temperature undergo incessant motion due to constant collisions with the particles of the medium. This motion is known as Brownian motion from the name of Robert Brown who first observed it in the 1800's while looking at pollen grains in water under a microscope. It is very close to random motion, and therefore cannot be predicted. Particles that are moving through Brownian motion have no net motion, on average. Figure:1 shows an image of Brownian particles obtained using brightfield microscopy. The brightfield microscopy technique is when a light shines on the beads for better visualization while the images are being captured with a camera connected to the microscope.

A random walk is a simple model for Brownian motion. A random walk is the particle randomly taking N steps. Each step is equally likely to be in any direction on a set lattice. These steps form a trajectory which resembles Brownian motion.

I have implemented a simulation of a random walk in both one and two dimensions using Python. In two dimensions, the program was designed to randomly select a coordinate direction from a step of the random walker from the array of elements $([1,0],[-1,0],[0,1],[0,-1])$ and to create a trajectory by iterating this procedure over N steps This procedure is then repeated to create a new trajectory, and each trajectory is saved. Figure 2 shows a histogram of the positions for a simulated random walk. The particle's positions are isotropically distributed around the starting point - here the origin and form a cloud around the origin. This figure shows that the probability of finding the particle decreases as the distance from the origin increases. After N steps the most likely position of the particle will be the origin. Therefore, the average displacement of a Brownian particle is zero. This can also be seen by plotting the trajectories

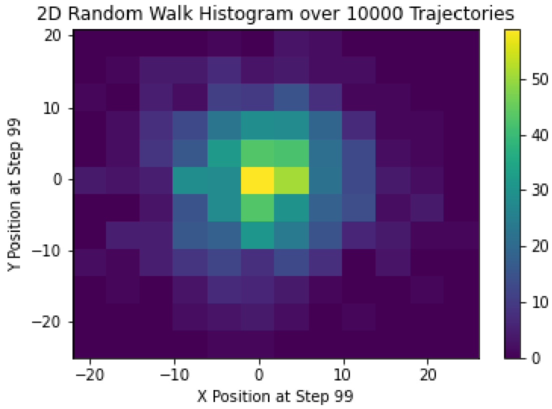

FIG. 2. Histogram of random walker positions at step 99 for 10000 trajectories.

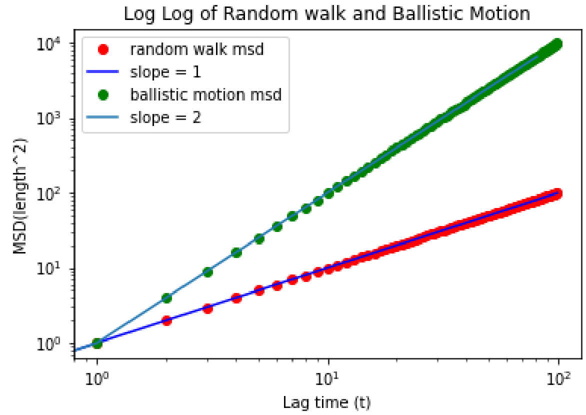

FIG. 3. Slope of Simulated Random Walk vs. Ballistic Motion

as a function of time.

The random nature of the dynamics requires a statistical way to quantify it. To do this I calculated the mean-squared displacement (MSD) that measures the particle displacement from its origin in time time (or its diffusion rate) and is given by

$$MSD(t) = < [x(t + t_0) - x(t_0)]^2 > \quad (1)$$

where the brackets denote an average over trajectories, corresponding to an average over many particles. The MSD of a random walker grows in time as

$$MSD(t) = 2dDt\ , \quad (2)$$

where d is the dimensionality of the system and D the diffusion constant. For Brownian particles driven by thermal noise the diffusion constant is given by $D = \mu k_B T$, with μ the particle mobility, which is determined by the particle size and shape.

Figure 3 shows the MSD of a simulated random walk (red points) on a log-log plot versus lag time. The blue line through the points is a fit to a straight line of slope 1.

It is useful to compare the dynamics of a Brownian particle to that of a particle moving at constant velocity v. In this case, the displacement grows linearly in time $x(t+t_0) - x(t_0) = vt$. The motion is not random, as the particle travels along a straight line. This type of motion is known as ballistic. The square of the displacement is given by

$$[x(t + t_0) - x(t_0)]^2 = v^2 t^2 \quad (3)$$

and grows like t^2. Figure 3 compares the MSD of a Brownian particle to the square displacement of a ballistic particle. If $MSD(t) \sim t^\alpha$, then $\log[MSD] \sim \alpha \log t$. By making a log-log plot we can then immediately extract the exponent α that governs the growth in time of the MSD as the slope of the straight line. It is clear that for a Brownian particle $\alpha = 1$, while ballistic motion corresponds to $\alpha = 2$. The MSD can therefore be used to characterize different types of dynamics.

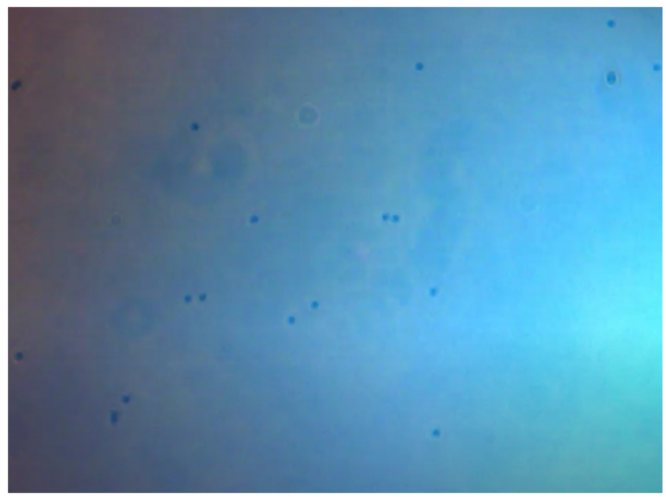

FIG. 4. Active Janus Particles

III. ANALYSIS OF EXPERIMENTAL DATA

I analyzed the dynamics of three types of particles: polysterene beads in water, self-propelled Janus particles, and nematic defects in microtubule-kinetic suspensions. The defects are strong distortion of microtubule alignment, and they move and behave like particles. The dynamics was analyzed by extracting the particles' trajectories from images taken with optical microscopes and using a Python code to calculate mean square displacements from the trajectorie

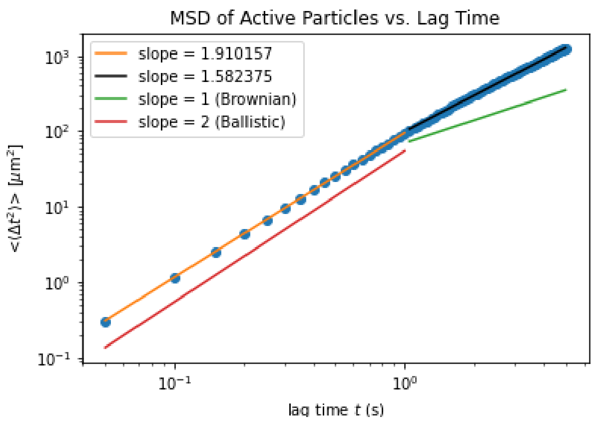

FIG. 5. MSD Active Particles Exhibiting Brownian and Ballistic Motion on a Log Scaled Graph

A. Brownian Particles

The experimental Brownian particles were polystyrene beads in a water solvent. This particles are in equilibrium and undergo random walks driven by random kicks from the solvent molecules. Their MSD was found to be diffusive with $\alpha = 1$.

B. Self-Propelled Janus Particles

Janus particles are synthetic beads with a radius of $0.13 \pm 0.02 \mu m$. We analyzed experimental images that we obtained from collaborator Jeremie Palacci, then at UC San Diego. The particles are placed in a water solvent. Light is used to activate catalytic reactions that endow the particles with self-propulsion. I analyzed the images that were taken in the lab using the microscope to capture the particle's position every second for 15 minutes.

To track the particles over the entire image sequence, I used a python program which utilizes trackpy. In order for trackpy to read the image sequence, it had to be filtered through the image processing platform, ImageJ. In ImageJ we adjusted the FFT and Threshold to reduce the noise in the data and to enhance the outlines of the particles to track their trajectories based on their radius.

The MSD of the active spherical particles shows two different slopes, as shown in Fig. 7. At short times, the particles move ballistically with a fixed self-propulsion speed and direction, and the MSD has slope $\alpha = 2$. At longer times they begin to change their direction, resulting in a Brownian-like motion. Figure 7 shows the beginning of a crossover of the MSD to a smaller exponent. I expect that at even longer times one would find a purely diffusive dynamics with $\alpha = 1$.

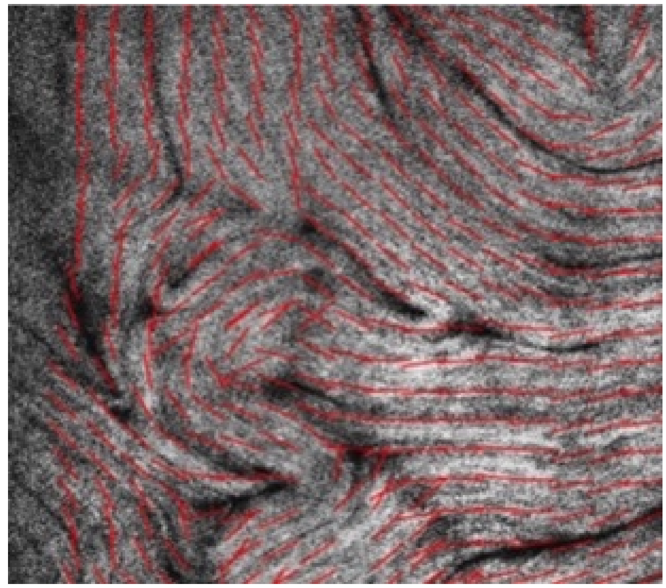

FIG. 6. Snapshot of the nematic liquid crystal of microtubule bundles with nematic order shown by the red lines.

C. Defects in active nematics

The experimental system studied in the Dogic lab is a suspension of bundles of microtubules cross-linked by kinesin motor proteins. Microtubules are long filamentary biopolymers composed of stacked tubulin dimers. They are polar, in the sense that the two ends, referred to as $+$ and $-$ ends, have different properties. Each microtubule has a diameter of 25 nanometers and length that varies based on the amount of tubulin dimers that are stacked. The microtubules in the active nematics were one to five microns long. A depletant is added to the salty water solution so that the microtubules will clump together into bundles. Bundles of microtubules appear as white streaks in Figure 6. Microtubules within a bundle are linked by a motor protein called kinesin. Kinesin uses the energy from the hydrolysis of ATP to walk along microtubules towards their $+$ end. Within a bundle one can find a group of kinesin motors linking microtubules with $+$ ends in opposite direction. In this case the stepping motion of kinesin can result in the sliding of the microtubules relative to each other, extending the bundle and exerting forces on its surrounding. These forces, known as active stresses, result in sustained flows of the whole suspensions and strong distortion of microtubule alignment known as topological defects. The defects can be tracked to examine their dynamics. I have analyzed video of the motion of defects obtained in the Dogic lab.

Unlike active Janus particles, I was able to track defects only on short timescales. Therefore, I was only able to see their ballistic motion. The MSD of both positive one-half and the negative one-half defects have a slope that approaches two, as is shown in Figure 7.

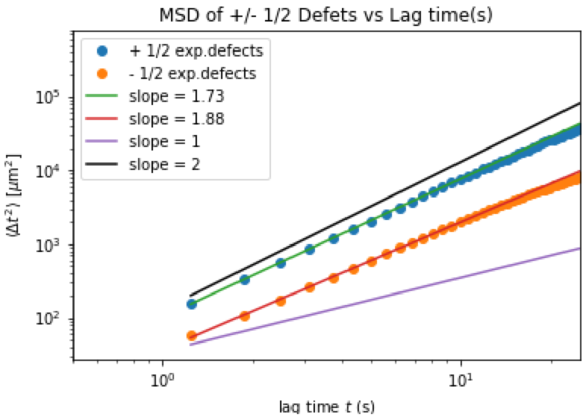

FIG. 7. MSD Positive 1/2 and Negative 1/2 Defects Exhibiting Brownian and Ballistic Motion on a Log Scale Graph

IV. CONCLUSIONS

The MSD for passive Brownian motion has a slope of one. This behavior can be attributed to the lack of any directed motion of the passive particles. In comparison, the MSD of directed ballistic motion has a slope of two. Active particles are moving in a ballistic-like motion at short timescales, and as time increases their motion is more similar to random Brownian-like motion with a large step size. Defects in active nematics can be thought of as point like active particles. On short time scales, the positive one-half and negative one-half defects exhibited ballistic motion. For extended time scales, they should mainly exhibit characteristics from both Brownian. However, due to experimental limitations, we were not able to track defects in active nematic liquid crystal to verify this assumption. Exploring this regime would be useful for further characterization of active materials.

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