particle i at time t. We furthermore show in Fig. 6 the MSD as a function of time t for subsets defined based on the particles' squared displacements $(\mathbf{r}_i(t_0+t)-\mathbf{r}_i(t_0))^2$:

- the fastest 10% of all particles (red full line),
- the fastest 20% of small particles (red dashed-dotted line),
- the slowest 10% of all particles (blue full line),
- the slowest 20% of small particles (blue dashed-dotted line)

and compare them to the corresponding quantities for all particles.

We find, in accordance with Fig. 13 of [10], a vast difference between fast and slow particles. While the 10% fastest particles move a distance several times the radius r_1 of the small particles, the slowest 10% of particles barely move. The restriction to small particles does not significantly change this observation. The drastic differences of particle mobility give us an idea of the strength of the dynamical heterogeneity.

The full distribution of displacements in the x-direction, $\Delta x(t)=[x_i(t_0+t)-x_i(t_0)]$ at a fixed time difference t is shown in Fig. 7(a) for various packing fractions and in Fig. 7(b) for several times t. For a fluid far from dynamical arrest, the particles are expected to perform a simple random walk, and the displacement distributions are expected to have a Gaussian form $P_g(\Delta x,t)=\left(1/\sqrt{4\pi Dt}\right)\exp[-(\Delta x)^2/(4Dt)]$, where D is the diffusion coefficient. Gaussian fits to the data, with D used as a fitting parameter, are shown with dotted-dashed lines in Fig. 7. We observe that the distributions deviate strongly from the Gaussian fit for all packing fractions and times. The tails of the distributions follow approximately exponential behavior, $P_e(\Delta x,t)\propto\exp(-|(\Delta x)/x_0(t)|)$, shown as solid lines. Also, the tails become wider both for increased packing fraction and for longer times. Exponential tails have been studied also in non-dissipative glassy systems [20–22] and have been established as an indirect signature of spatial dynamical heterogeneity [22].

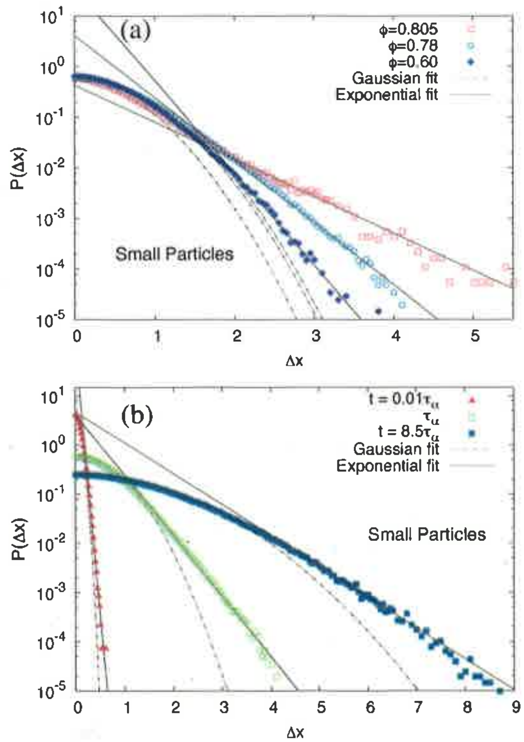

FIG. 7: (Color online) (a) Distribution of small particle displacements for different packing fractions $\phi=0.805$, 0.78, and 0.60 (from right to left) at time τ_α. (b) Distribution of small particle displacements for $\phi=0.78$ at different times $t=0.01\tau_\alpha$, $t=\tau_\alpha$ and $t=8.5\tau_\alpha$ (from left to right). The tails of the distributions are better described by an exponential fit (solid lines) than by a gaussian fit (dotted-dashed lines).

Another expected consequence of the presence of heterogeneous dynamics is that supercooled liquids near the glass transition in 3D violate both the Stokes-Einstein relation $D\eta/T=const$ [1, 2] connecting the diffusion coefficient D with the viscosity η, and the related condition $D\tau_\alpha/T=const'$ connecting D with the α-relaxation time τ_α. Both ratios, $D\eta/T$ and $D\tau_\alpha/T$, show strong increases as the liquid approaches dynamical arrest. In two dimensional thermal systems, a slightly different phenomenology has been found [23]: both ratios behave as power laws as functions of temperature, even far from dynamical arrest, but the exponents for the power laws show significant changes as the liquid goes from the normal regime to the supercooled regime.

In our case, we focus on the relation between D and τ_α. We obtain the values of D by fitting the long time limit of the MSD (see Eq. (8)) with the form $\Delta(t)=4Dt$. This is known to be problematic in 2D, because long time tails of the velocity autocorrelation threaten the existence of hydrodynamics [10]. However, these tails are strongly suppressed in the vicinity of the glass transition, so that the above naive definition of D is presumably only weakly – if at all – affected.

Fig. 8 is a plot of D as a function of τ_α, for all values of ϕ. For packing fractions not too close to dynamical arrest, a power law behavior $D\propto{\tau_\alpha}^{-\theta}$ is found, with $\theta\approx1.47$. For higher packing fractions, one observes a crossover to a power law with a different exponent, $\theta'\approx0.91$. These results are similar to the above mentioned results of Ref. [23] for 2D non-dissipative glass forming systems.

C. Clusters of slow and fast particles

In this section we investigate *directly* the *spatial* distribution of dynamical heterogeneities. We look at the whole system as one unit, instead of dividing it into sub-boxes.

To visually observe dynamical heterogeneity in our system we color–code particles according to their mobility. As in Sec. III A, we define *slow particles* as those that for a given time interval t have a displacement smaller than the cutoff a. Additionally, we define *fast particles* as those that in the same time interval have a displacement larger than $3a$. The spatial distribution of slow and fast particles is shown in Fig. 9, for

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Simulating Active Particles Driven by Shot Noise to Find Velocity Distributions

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We study active particles which convert an internal energy source into motion to propel themselves. We introduce a model for these active particles to study their motion in a viscous medium. In particular, we consider a model in which the self-propelling kicks occur randomly according to a Poisson process and are modeled as white shot noise of constant size. Using an event driven simulation, we determine the velocity distributions for particles of this kind and classify it as anomalous, meaning non-Maxwell-Boltzmann, with exponential tails.

I. INTRODUCTION

There has been interest in understanding the behavior of systems of what is known as active matter, meaning a particle propelled by an internal energy supply. The study of these active particles is particularly relevant to biological systems such as proteins and bacteria. Particles undergoing Brownian motion will have Maxwell-Boltzmann velocity distributions. It is the introduction of a self propelling force that leads to an anomalous velocity distribution. Stationary probability distributions for various models of self-propelling forces have been been known for some time [1], and with growing interest in active matter in recent years, the study of anomalous velocity distributions has progressed. Recently further studies on the dynamics of these active particle systems have used theoretical and experimental methods. Experimental data taken from multiple cell types was used in Ref. [2] to study the characteristics of the velocity distributions of the these cells and analysis revealed exponential distributions and work in Ref. [3] has resulted in a deeper understanding of the underlying mechanisms.

Simulations of these particles moving through granular fluids have also provided many insights including one study which examined the behavior of these particles through simulating the dynamics of an intruder particle in a three-dimensional granular fluid [4]. In a simulation with a similar physical model and simulation algorithm, velocity distributions for these active particles were found numerically and compared to a theoretical model [5]. This simulation agreed with the proposed theory and revealed a dependence in the velocity distributions only on the damping constant of the medium and the frequency of the random kicks. These two simulations introduce shot noise as the models for the self-propelling kicks of the active matter as we do in our active particle model.

The model introduced in this paper follows a similar physical model introduced in the above mentioned simulations [4, 5]. We investigate particles moving in one-dimension with periodic boundary conditions. The random kicks are modeled as white shot noise of constant size. Using an event driven simulation, we find and characterize the velocity distribution of this system.

II. MODEL

In this project we explore the velocity distributions of active particles in one-dimension with periodic boundary conditions. The motion of the ith particle is governed by the stochastic differential equation

$$m\frac{d^2 v_i}{dt^2} = f(x_i, v_i) + g(x_i, v_i)\xi. \tag{1}$$

The random variable ξ represents the self-propelling force of the particles. We consider the motion of these particles in a viscous material with damping constant γ which yields a simplified equation of motion:

$$m\frac{d^2 v_i}{dt^2} = -\gamma v_i + \xi. \tag{2}$$

This is known as the Langevin equation and is often used to model Brownian motion [6].

This equation is derived straight from Newton's second law. $-\gamma v$ is a damping force from the viscous medium and ξ is a random variable representing the self-propelling force of the active particles. ξ can be modeled as a number of different random processes. When modeling Brownian motion, ξ is taken to be a process of Gaussian white noise, which is often used to represent thermal fluctuations. This model would result in an equilibrium system for which we would expect to find the Maxwell-Boltzmann velocity distribution [6].

Other random processes can be used for ξ to model non-equilibrium systems such as that of active particles. To model the random kicks of the active particles, we use shot noise given by

$$\xi_S = \sum_i h(t - t_i), \tag{3}$$

where h is a function describing the kick and t_i is the time of the ith kick. The times inbetween successive kicks are drawn from a Poissonian exponential waiting time distribution

$$P(t) = \lambda e^{-\lambda t}, \tag{4}$$

where λ is the kick rate. We specifically consider white shot noise in which the function h is proportional to a Dirac δ function. We consider these δ function peaks to be of constant size so that the effect of every kick is of the same size. Taking these kicks to be δ functions, their effects on the particles are instantaneous and result in an immediate change in velocity.

Since we use white shot noise, between kicks and collisions the Langevin equation simplifies to the following solvable ordinary differential equation

$$m\dot{v}_i = -\gamma v_i. \tag{5}$$

Solving Eq. 5 yields an expression for the velocity of particle i at any given time t following an event at time t_0:

$$v_i(t) = v_i(t_0)e^{-\gamma(t-t_0)}. \tag{6}$$

Integrating Eq. 6 we find the position of each particle i at any given time t following an event at time t_0:

$$x_i(t) = x_i(t_0) + v_i(t_0)\frac{1-e^{-\gamma(t-t_0)}}{\gamma} \tag{7}$$

Eq.'s 6 and 7 give the velocities and position of each particle for any time t, respectively and are valid until another kick or collision occurs.

Since the equation of motion can be solved analytically for time intervals without a kick or collision event, the collisions can be handled independently. The particles move in only one-dimension with periodic boundary conditions, so we need only consider collisions between adjacent particles. Using Eq. 7 we solve for the time of the next collision for any two adjacent particles to be

$$t = t_0 - \frac{1}{\gamma}\ln\left(1 - \frac{\gamma(x_2(t_0) - x_1(t_0))}{v_1(t_0) - v_2(t_0)}\right), \tag{8}$$

where t_0 is the time of the last kick or collision.

Using Eq. 8 along with the random kick times drawn from the Poissonian distribution, we implement an event-driven simulation based on the algorithm used in Ref. [4], where the key events are the random kicks and collisions between any two adjacent particles. According to this algorithm, we find the time of the next event and jump forward to that point and appropriately handle the interaction. In the case of a kick, we adjust the velocity based on the constant size of the Dirac δ functions. We treat the collisions as elastic and use a minimum image approach to account for the periodic boundary conditions ultimately resulting in a swap of velocities for the two colliding particles.

III. RESULTS

We use the event driven model outlined above to simulate the interactions of 500 active particles with a damping rate $\gamma = 1$. The waiting times inbetween the random kicks for each particle are drawn from the Poissonian distribution of Eq. 4, where the kick rate was chosen to be $\lambda = 1$. We consider the random kicks of the self-propelling active particles to be of constant size, meaning we take the random variable ξ, which represents these random kicks, to equal 1 at the times of the kicks and 0 at all other times. The 500 particles began in an initial state evenly distributed across a one dimensional line with velocities drawn from a Maxwell-Boltzmann distribution with $\sigma = 1$. The simulation ran until $t = 100.0$ and the distribution of velocities compiled from 500 runs of 500 particles is shown in Fig. 1.

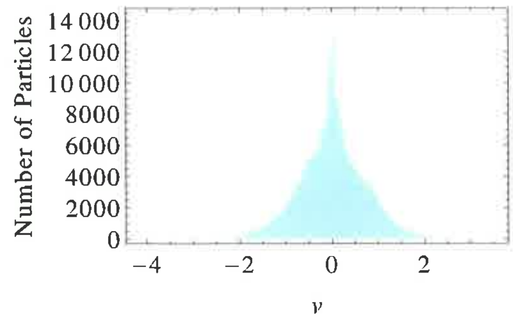

FIG. 1: Velocity distribution of 500 runs with 500 particles each

Normalizing this distribution we fit a Gaussian of the form:

$$P(v) = Ae^{-(v-v_0)^2/\sigma^2} \tag{9}$$

in an attempt to characterize the velocity distribution. Fig. 2 shows the raw probability density data with the Gaussian fit (solid curve in Fig.2). Fig. 3 shows a plot of $\ln(P(v))$ vs. v with a parabolic fit (solid curve in Fig. 3). From these two plots we conclude our system does not finish in equilibrium. We find a higher probability of

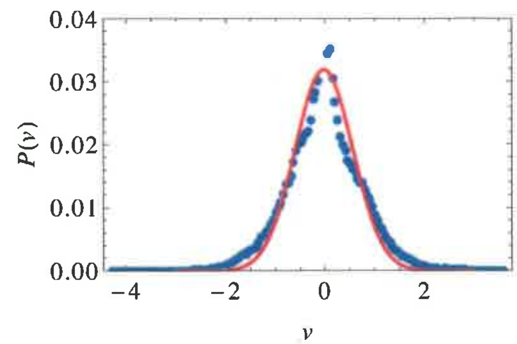

FIG. 2: Normalized velocity distribution (blue dots) with a Gaussian distribution fit (solid red curve).

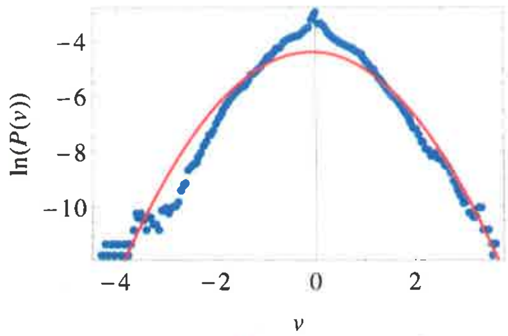

FIG. 3: Normalized velocity distribution on logarithmic scale (blue dots) with parabolic fit (solid red curve).

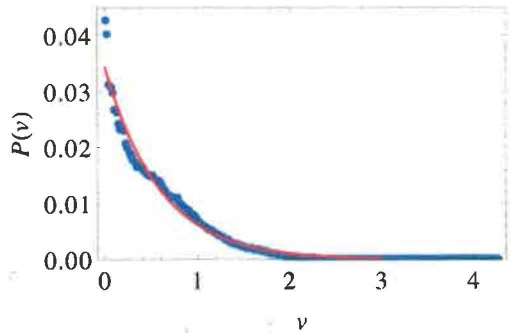

FIG. 4: Distribution of velocity magnitudes (blue dots) with exponential decay fit (solid red curve).

particles having a large velocity in magnitude than we would see in an equilibrium system. These higher probabilities correspond to particles that have just undergone a random kick. We also see more particles with small velocities close to zero. This is a result of the damping force in our systems so particles having not experienced a kick or collision for a long time will have small velocities.

To further characterize the behavior of the system, we show in Fig. 4 the distribution of the magnitudes of the velocities. We find good agreement with an exponential decay fit (solid curve in Fig. 4) to this distribution. To further analyze the distribution, we plot $\ln(P(v))$ vs. v in Fig 5 and find a clearly linear region in the tails of the distribution (solid line in Fig. 5). We are unable to characterize the peak or the distribution as a whole due to the complicated dynamics of including random kicks, collisions, and damping.

IV. CONCLUSION

We've discussed a physical model for studying of the behavior of active matter. We considered these active particles to have an internal energy supply which allows the particles to self-propel through a viscous medium. We modeled the internal kicks as white shot noise and of constant size and include elastic collisions on a one-dimensional line with periodic boundary conditions. Using an event driven simulation, we studied the dynamics of these particles and concluded they follow an anomalous velocity distribution with exponential tails. Future work could include systems with white shot noise kicks of varying size, or systems with random kicks modeled by colored shot noise.

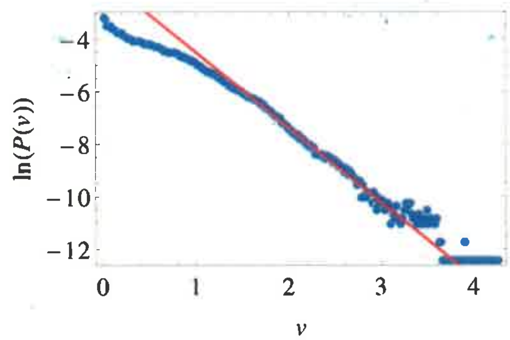

FIG. 5: Distribution of velocity magnitudes on logarithmic scale (blue dots) with linear fit in the tail (solid red line). The fit reveals exponential behavior in the tails of the velocity distribution.

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