Dynamics of active run and tumble and passive particles in binary mixture

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We study a binary mixture of disk-shaped active run and tumble particles (ARNPs) and passive particles on a two-dimensional substrate. Both types of particles are athermal. The particles interact through the soft repulsive potential. The activity of ARNPs is controlled by tuning their tumbling rate. The system is studied for various sizes of passive particles keeping size of ARNPs fixed. Hence the variables are, size ratio (S) of passive particles and ARNPs, and activity of ARNPs is $v$. The characteristics dynamics of both ARNPs and passive particles show a crossover from early time ballistic to later time diffusive. Furthermore, we observed that passive particles dynamics changes from diffusive to subdiffusive with respect to their size. Moreover, late time effective diffusivity $D_{eff}$ of passive particles decreases with increasing their size as in the corresponding equilibrium Stokes systems. We calculated the effective temperatures, using $D_{eff}$, $T_{a,eff}(\Delta)$ and also using speed distribution $T_{a,eff}(v)$ and compared them. The both $T_{a,eff}(\Delta)$ and $T_{a,eff}(v)$ increases linearly with activity and are in agreement with each other. Hence we can say that an effective equilibrium can be establish in such binary mixture. Our study can be useful to study the various biological systems like; dynamics of passive organels in cytoplasm, colloids etc.

I. INTRODUCTION

In the recent years, researchers have paid a lots of attention in the field of active matter [1–6] because of their unusual properties in comparison to their equilibrium counterparts. Examples of active systems ranges from microscale such as bacterial colonies, cell suspension, artificially designed microparticles [7–12], etc. to the larger scale; fish school, flock of birds [13–15], etc. Active system continuously evolve with time which leads to non equilibrium class with intresting features i.e; pattern formation [17], nonequilibrium phase transition [18–21], large density fluctuations [22], enhanced dynamics [9, 23, 24], motility induced phase separation [25–28] etc. In recent years, the motion of passive particles in the presence of an active medium is used to explore the nonequilibrium properties of the medium. In such mixtures passive particles exhibit enhanced diffusivities $D_{eff}$ greater than their thermal (Brownian) diffusivity $D_0$ [29, 30]. In the experiment of [31], passive Brownian disks in active bacterial solution show enhanced diffusivity. The enhanced diffusivity $D_{eff}$ increases linearly with increasing concentration of bacteria in the solution [32, 34]. A variety of studies have focused on the role of bacterial concentration on passive particle diffusion. The effect of passive particles size is still not clear. In the absence of bacteria, or the equilibrium fluid the diffusivity of a sphere follows the Stokes-Einstein relation [35]. To understand the role of particle size on their dynamics in the active medium, we introduce a binary mixture of active run and tumble ARNPs and passive particles. ARNPs move in a straight line for some time and then undergo a random rotation (tumble event). Hence activity can also be tuned with tumbling rate. A large tumbling rate means smaller run time and hence more random motion.

We studied the mixture for different sizes of passive particles and the activity of ARNPs. Effective diffusity $D_{eff}$ of ARNPs does not change significantly whereas it decreases linearly with size for the passive particles: similar to their equilibrium counterparts-Stokes system [35]. We calculated the effective temperatures, using $D_{eff}$, $T_{a,eff}(\Delta)$ and using speed distribution of ARNPs, $T_{a,eff}(v)$. The both increases linearly with increasing activity for all size ratios. Hence although the system is active, an effective equilibrium can be established in such mixtures.

The rest of paper is organized as follows. In section II we discuss the model with simulation details. In section III we discuss the results followed by conclusion in IV at the end.
II. MODEL

We consider a binary mixture of \( N_a \) small run and tumble particles \( ARNPs \) of radius \( r_a \), and \( N_p \) passive particles of radius \( r_p \) moving on a two-dimensional (2D) substrate of size \( L \times L \). The size of the \( ARNPs \) particle is kept fixed whereas the size of passive particles is tuned. We define the size ratio \( S = r_p/r_a \). The position vector of the centre of the \( i^{th} \) \( ARNPs \) and passive particle at time \( t \) is given by \( \mathbf{r}_i(t) \) and \( \mathbf{r}_j(t) \), respectively. The orientation of \( i^{th} \) \( ARNPs \) is represented by a unit vector \( \mathbf{n}_i = (\cos \theta_i, \sin \theta_i) \). The dynamics of the \( ARNPs \) particle is governed by the overdamped Langevin equation

\[
\partial_t \mathbf{r}_i^a = v_0 \mathbf{n}_i + \mu_1 \sum_{j \neq i} \mathbf{F}_{ij}
\]

The first term on the right-hand side (RHS) of Eq. 1 is due to the activity of the \( ARNPs \), and \( v_0 \) is the self-propulsion speed. The second term, the force \( \mathbf{F}_{ij} \) is the soft repulsive interaction among the particles. It is obtained from the binary soft repulsive pair potential \( V(r_{ij}) = \frac{k(r_{ij} - 2\sigma)^2}{2} \) and \( \mathbf{F}_{ij} = -\nabla V(r_{ij}) \), for \( r_{ij} \leq \sigma \) and zero otherwise. \( \sigma = a_i + a_j \), where \( a_i,j \) is the radius of \( i^{th} \) and \( j^{th} \) particle respectively. \( r_{ij} = |r_j - r_i| \) is the distance between particle \( i \) and \( j \). The smallest time step considered is \( \Delta t = 5 \times 10^{-4} \), much smaller than the elastic time scale \( \tau \) (for \( \mu = 1 \) and \( k = 1 \)).

The summation runs over all the particles. \( \tau = (\mu k)^{-1} \) sets the elastic time scale in the system. Further, the orientation of \( ARNPs \) is controlled by run and tumble events. The particles orientation is updated by Eq. 2 introducing a uniform random number \( r_\nu \). A tumbling rate \( \lambda \) is defined such that if \( \lambda > r_\nu \) then the particle undergoes a tumble event with a random orientation \( \eta_i \in (-\pi, +\pi) \). Else it undergoes run event with the same angle as in previous step. Hence large tumbling rate \( \lambda \) means frequent change in particle orientation. Hence the orientation update of \( ARNPs \) is given by:

\[
\theta_i(t + \Delta t) = \theta_i(t) + \eta_i(t)
\]

The position of the passive particles is also governed by the overdamped Langevin equation,

\[
\partial_t \mathbf{r}_i^p = \mu_2 \sum_j \mathbf{F}_{ij}
\]

The \( \mathbf{F}_{ij} \) has the same form as defined in Eq. 1. There is no translational noise \( \mathbf{S} \) in Eqs. 1 and 3, therefore, both \( ARNPs \) and passive particles are athermal in nature.

III. RESULTS

A. Dynamics of the particles in the mixture

We characterise the dynamics of both types of particles in the mixture for different system parameters (size ratio \( S \) and activity \( v \)). We first calculate the displacement of \( ARNP \), and passive particles and calcu-
late their mean-square displacement (MSD); \( \Delta_{a,p}(t) = \langle |r(t + t_0) - r(t_0)|^2 \rangle \). The subscript \( a \) and \( p \) resemble the active and passive particles respectively. \(< .. >\), implies average over different reference times \( t_0 \)'s, for all the particles of respective types and over 50 independent realizations.

The Fig. 2(a-b) shows the plot of MSD of ARNPs, \( \Delta_a(t) \) for different size ratio \( S = 2, 4, 6, \) and \( 8 \) keeping fixed activities \( v = 5 \times 10^4 \) and \( v = 1.2 \times 10^4 \) respectively. We find that \( \Delta_a(t) \) is independent of the size ratio \( S \) in all the cases and shows an early time superdiffusive to late time diffusive dynamics. In general the particle follows the persistent random walk (PRW) and MSD can be approximated as -

\[
\Delta(t) = 2dD_{eff}t[1 - \exp(-t/t_c)]
\]

where \( D_{eff} \) is the effective diffusivity in the steady state and \( t_c \) is the typical crossover time from superdiffusion to diffusion. The effective diffusivity of ARNPs, \( D_{a,eff} \) shows weak dependence with size as shown in Fig. 3(a).

In Fig. 2(c-d) we show the plot of MSD of passive particles \( \Delta_p(t) \) for different size ratio. The dashed and solid lines are with slope 2 and 1 respectively. For small size ratio, the MSD is diffusive at the late time and slowly becomes subdiffusive for large \( S \). The typical crossover time \( t_{p,c} \) (as marked by two vertical arrows at the top and bottom curves). The crossover time \( t_{p,c} \) increases linearly with \( S \) for both activities as shown in Fig. 3(c). Hence bigger passive particles spend more time in superdiffusion. We further calculated the dependence of effective diffusivity of passive particles, \( D_{p,eff} \) on size ratio \( S \). The \( D_{p,eff} \) decreases inversely as a function of size ratio as shown in Fig. 3(b). It matches with the earlier results for the diffusion of Brownian disk moving in the equilibrium Stokes fluid.

We also explored the system for fixed size ratios \( S = 1 \) and \( S = 8 \) and varying the activity \( v \). For all activities the ARNPs show the persistent random walk (PRW) as given in Eq. 4 and MSD shows a crossover from early time ballistic to the late time diffusive behaviour. In Fig. 4(a-b) we shows the plot of MSD of ARNPs particles, \( \Delta_a(t) \) for different \( v \) and fixed size ratios \( S = 1 \) and \( 8 \) respectively. The data points from the numerical simulation and lines are fit from the expression of MSD as given in Eq. 4 for \( v = 5 \times 10^4 \). The crossover time \( t_{a,c} \) increases by increasing activity. The \( t_{a,c} \) is obtained by fitting the MSD \( \Delta_a(t) \) of ARNPs with the expression of PRW as given in Eq. 4. In Fig. 5 we plot the crossover \( t_{a,c} \) vs. \( v \). The \( t_{a,c} \) increases linearly with increasing \( v \) as shown in Fig. 5. We also calculated the \( D_{a,eff} \), obtained from the fitting. The variation of \( D_{a,eff} \) with activity will be discussed later.

We show the scaling collapse of MSD by plotting on the \( x \)-axis the scaled time \( t/t_{a,c} \) and \( y \)-axis the scaled MSD, \( \Delta_a(t)/D_{a,eff}t_{a,c} \). We find scaling collapse of data for both size ratios and for all activities as shown in the inset of Fig. 4(a-b).

We also calculated the MSD of passive particles \( \Delta_p(t) \) for different activities and for the two size ratios \( S = 1 \) and \( S = 8 \) as shown in Fig. 4(c-d). For small activity \( S = 1 \), the passive particles also show a crossover from early time ballistic to late time diffusive behavior and fitted well with the expression for the PRW as given in
\[\Delta p(t) \propto t^\beta(t)\]

(a) Plot of variation of \(t_{a,c}\) with \(v\) for different size ratios \(S\).

Eq. 4 Data shows a scaling collapse when we plot the scaled time \(t/t_{a,c}\) vs. scaled MSD, \(\frac{\Delta_x}{D_{p,eff}t_{a,c}}\). For large size ratio, \(S = 8\), passive particles show an early time ballistic but late time subdiffusion as we can see in the Fig. 4(d). Hence the MSD can not no longer be compared with the PRW.

We also investigated the dynamics of particles by extracting the dynamic MSD exponent \(\beta(t)\) defined by \(\Delta(t) \sim t^\beta(t)\), hence

\[\beta(t) = \frac{\log_{10}[\Delta(10^t)]}{\log_{10}[\Delta(t)]}\] (5)

The Fig 6 is plotted for the same parameter as in 4. For the ARNPs \(\beta_{a}(t)\) shows crossover from superdiffusive \(\beta_a(t) > 1\) to diffusive \(\beta_a(t) \sim 1\) regime. For the passive particles for \(S = 1\), early time dynamics is superdiffusive \(\beta_p(t) > 1\) and becomes diffusive \(\beta_p \sim 1\) at late time. Whereas for the size ratio 8 passive particles show superdiffusion \(\beta_{p}(t) > 1\) to subdiffusive \(\beta_{p} < 1\) motion.

B. Diffusivity and effective temperature of active particles in the mixture

In order to further explore the concept of effective temperature \([40-43]\) of the medium. Assuming an effective equilibrium, a relation between an effective temperature (calculated from the speed distribution) and effective diffusivity calculated from MSD of active particles can be written as: \(T_{a,eff}(\Delta) = D_{a,eff}/k_B\), where \(k_B\) is a constant factor used as the fitting parameters.

We calculated the speed distribution \(P(s)\) of ARNPs. The particle speed distributions determine the mean kinetic energy of the particles. If the distribution follows a Maxwell-Boltzmann (\(MB\)) form as always the case in fluids at equilibrium, the mean kinetic energy is related to the thermodynamic temperature via the equipartition theorem [40]. We calculate the \(p(s)\) and it follows the \(MB\) distribution for different parameters. Comparing it with standard \(MB\) distribution we calculated the effective temperature \(T_{a,eff}(v)\) as a function of activity \(v\) for different size ratio \(S\).

In Fig. 7 we plot the variation of \(T_{a,eff}(v)\) and \(T_{a,eff}(\Delta)\) vs. \(v\) for different \(S\). The data shows good match of both the effective temepartures. In active run and tumble particle system [44] \(D_{eff} = v_0^2/d\lambda = v_0 v r_a/d\). Where \(d\) is the dimensionality of space. Hence \(T_{a,eff}(\Delta)\) varies
IV. DISCUSSION

We studied the dynamics of a binary mixture of disk-shaped active run and tumble and passive particles on a two-dimensional substrate. Both types of particles are athermal in nature. The activity of active particles is controlled by their tumbling rate. The size of ARNPs is fixed whereas it is varied for passive particles. Further, in the mixture of ARNPs particles, the MSD show the early time ballistic behavior and late time diffusive motion with increasing value of \( v \) and size ratio \( S \). The passive particles show the crossover from late time subdiffusive to diffusive dynamics on increasing \( v \) and decreasing \( S \). The late time effective diffusivity of passive particles \( D_{p,\text{eff}} \) decay monotonically with their size as found in equilibrium passive Stokes fluid [35]. The effective diffusivity of ARNPs increases linearly with their activity and shows a good match with the effective temperature obtained from the steady-state speed distribution with the Maxwell-Boltzmann distribution. Hence our study explores dynamics and steady-state of ARNPs and passive particles in the mixture and shows an effective equilibrium in the system. Our particle-size dependence of MSD of passive particles in the presence of active run and tumble particles has important applications in particle sorting in different types of fluids like-microfluidic devices [45].

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