Chapter 3

Dynamics of passive particle in active run and tumble medium

3.1 Introduction

In the previous Chapter 2, we explored the dynamics of the active particles on the patterned surface and draw a phase diagram of the system, and also verified the Green-Kubo relation. In this Chapter, we numerically studied the effect of size of passive particle on their dynamics in the sea of active run and tumble particles (RTPs). We varied the size of passive particles comparable to RTPs to much larger. The density of passive particles is kept small. System is also studied for different activities of RTPs. We explored the dynamics from short to large time limit and found that dynamics is superdiffusive for short times and shows a crossover from diffusion to subdiffusion for large times. Interestingly crossover time increases on increasing size.

In recent years, researchers have paid a lot of attention in the field of active matter [Bechinger et al. (2016); Cates & Tailleur (2013); Fily et al. (2018); Marchetti et al. (2013); Solon et al. (2015); Toner et al. (2005); Vicsek & Zafeiris (2012)] because of their unusual properties in comparison to their equilibrium counterparts. Examples of active systems range from microscale such as bacterial colonies, cell suspension, artificially designed microparticles [Patteson et al. (2016); Semwal et al. (2021); Shaebani et al. (2020)] etc. to the larger scale; fish school, flock of birds [Giannini & Puckett (2020); Kumar et al. (2014)] etc. Active system continuously evolve with time which leads to nonequilibrium class with interesting features i.e; pattern formation [Bechinger et al. (2016); Denk & Frey (2020); Zhang et al. (2017)], nonequilibirum phase transition [Bhattacherjee et al. (2015); Gowrishankar & Rao (2016); Pattanayak & Mishra (2018); Singh et al. (2021)], large density fluctuations [Mandal et al. (2020)], enhanced dynamics [Kumar et al. (2021); Semwal et al. (2021); Shaebani et al. (2020)], motility induced phase separation [Bechinger et al. (2016); Gonnella et al. (2015); Kümmel et al. (2013); Solon et al. (2015)] etc. In recent years, the motion of passive particles in the presence of an active medium has been used to explore the nonequilibrium properties of the medium. In such mixtures, passive particles exhibit enhanced diffusivities, greater than their thermal (Brownian) diffusivity [Leptos et al. (2009); Shaebani et al. (2020)]. In the experiment of [Wu & Libchaber (2000)] passive Brownian disks in active bacterial solution show enhanced diffusivity. The enhanced diffusivity increases linearly with increasing concentration of active particles in the solution [Kim & Breuer (2004); Kumar et al. (2021); Leptos et al. (2009)]. While most of the previous experimental and numerical studies have focused on the effect of concentration of active medium or activity of active particles respectively [Dolai et al. (2018); Thiffeault & Childress (2010); Vutukuri et al. (2020); Wu & Libchaber (2000); de Castro et al. (2021)]. In recent experiment of Alison *et. al.* [Patteson et al. (2016)] showed that the diffusivity of passive particles in active bath shows a non-monotonic dependence on size. Most of numerical simulations of active passive systems have focused on the mixture of active Brownian particles (ABPs) and passive particles. Although statistically steady state dynamics of RTPs and ABPs are similar [Solon et al. (2015)], but the detail dynamics of passive particles in RTPs medium is not yet explored. To understand this we explored the short and late time dynamics of passive particles in RTPs mixture. We explored the dynamics for different sizes of passive particles and activities of RTPs. The activity of RTPs is tuned by varying their tumbling rate. We find that the size of passive particles does not influence the dynamics of RTPs, but the dynamics of passive particles depends on their size as well as activity of RTPs. The dynamics of passive particles is ballistic for short times for all parameters and shows a crossover to diffusion for intermediate times and late time subdiffusion for large size ratios. The crossover time increases by increasing size of passive particles and activity of RTPs. The late time dynamics of RTPs are always diffusive and found in previous studies [Solon et al. (2015)]. Our numerical study show the detail dynamics of passive particles in active RTP medium. The early time dynamic is superdiffusion due to the active medium but the late time asymptotic dynamics and crossover from early to late time dynamics very much depends on the system parameters. Hence our study provide a detail understanding of passive objects dynamics in active medium. The rest of paper is organised as follows. In section 3.2 we discuss the model with simulation details. In section 3.3 we discuss the results followed by conclusion in section 3.4 at the end.

3.2 Model

We consider a binary mixture of N_a small run and tumble particles RTPs of radius a_a, and N_p passive particles of radius a_p moving on a two-dimensional (2D) substrate of size $L \times L$. The linear dimension of the system is fixed to $L = 150a_a$. The size of the RTPs is kept fixed whereas the size of passive particles is varied and we define the size ratio S $= a_p/a_a$. The position vector of the centre of the i^{th} RTPs and passive particle at time t is given by $\mathbf{r}_i^a(t)$ and $\mathbf{r}_i^p(t)$, respectively. The orientation of i^{th} RTPs is represented by a unit vector $\mathbf{n}_i = (\cos\theta_i, \sin\theta_i)$. The dynamics of the RTPs particle is governed by the overdamped

Langevin equation [Fily & Marchetti (2012); Semwal et al. (2021)]:

$$\partial_t \mathbf{r}_i^a = v_0 \mathbf{n_i} + \mu_1 \sum_{j \neq i} \mathbf{F}_{ij} \tag{3.1}$$

The first term on the right-hand side (RHS) of eqn. 3.1 is due to the activity of the RTPs, and v_0 is the self-propulsion speed. The second term, the force F_{ij} is the soft repulsive interaction among the particles. It is obtained from the binary soft repulsive pair potential $V(r_{ij}) = \frac{k(r_{ij}-\sigma)^2}{2}$ 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 summation runs over all the particles, k is the force constant, and μ is the mobility of the particle, such that $\tau = (\mu k)^{-1} = 0.01$ sets the elastic time scale in the system. Further, the orientation of RTPs is controlled by run and tumble events. The particles orientation is updated by eqn. 3.2 introducing a uniform random number r_n where $r_n \in (0,1)$. A tumbling rate λ is defined such that if $\lambda > r_n$ 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 λ means frequent change in particles orientation. Hence the orientation update of RTPs is given by:

$$\theta_i(t+\Delta t) = \begin{cases} \theta_i(t) + \eta_i(t) & \text{with rate } \lambda \\ \theta_i(t) & \text{with rate 1-}\lambda \end{cases} \tag{3.2}$$

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

$$\partial_t \mathbf{r}_i^p = \mu_2 \sum_{i \neq j} \mathbf{F}_{ij} \tag{3.3}$$

The $\mathbf{F}_{ij}$ has the same form as defined in eqn. 3.1. The dynamic of both types of particles is, athermal because we do not have any thermal noise in the translational motion eqn. 3.1 and 3.3. Although experimental system always have some thermal fluctuations present, but we studied the purely athermal system to see the role of activity in the mixture. The smallest time step considered is $\Delta t = 5 \times 10^{-4}$, much smaller than the elastic time scale $\tau = 0.01$. All the physical quantities are averaged over 50 independent realizations. The self-propulsion speed v_0 is kept fixed to 0.5 and activity is varied by tuning tumbling rate λ from 10^{-4} to 2×10^{-3}. For λ larger than these values, no interesting results are found [–3490 (tex)]. We define the dimensionless activity as $v = v_0/\lambda a_a$ and it varies from 5×10^3 to 5×10^4. We start with random initial positions and orientation directions of all the particles. Once the update of the above two equations is done for all $N = N_a + N_p$ particles, it is counted as one simulation step. We simulated the system for total 2×10^5 steps. Packing fractions of RTPs and passive particles is fixed $\frac{\pi(N_a a_a^2 + N_p a_p^2)}{L^2} = 0.6$. In all the cases, the packing fraction of RTPs and passive particle are kept fixed to 0.5 and 0.1 respectively. The current study mainly focus on the effect of activity and size ratio, hence we keep the total packing fraction close to the random close packing in two dimensions [Shaebani et al. (2020)]. Also the packing fraction of passive particles are kept low to understand their dynamic due to the background majority RTPs and the passive-passive interaction can be ignored.

3.3 Results

3.3.1 Results for different size of passive particles

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 RTPs, and passive particles and calculate their mean-square displacement (MSD); $\Delta_{a,p}(t) = \langle |\mathbf{r}(t+t_0) - \mathbf{r}(t_0)|^2 \rangle$. The subscript a and p resembles 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. To understand the effect of size ratio on RTPs, Fig. 3.1(a-b) shows the plot of MSD of RTPs, $\Delta_a(t)$ for different size ratios $S = 2, 4, 6$, and 8 keeping fixed activities $v = 5 \times 10^4$ and $v = 1.2 \times 10^4$ respectively. We found that $\Delta_a(t)$ shows a very weak dependence on the size ratio S in all the cases and shows an early time superdiffusive to late time diffusive dynamics. Which suggest that the dynamics of RTPs is not much affected due to the presence of passive particles. For all system parameters, the RTPs show the Persistent Random Walk (PRW) and MSD can be approximated as [Romanczuk et al. (2012); Semwal et al. (2021); Shaebani et al. (2020)]:

$$\Delta(t) = 2dD_{eff}t[1 - \exp(\frac{-t}{t_c})] \tag{3.4}$$

where D_{eff} is the effective diffusivity in the steady state, $(d = 2)$ is dimensionality of the space and t_c is the typical crossover time from superdiffusion to diffusion.

In Fig. 3.2 we show the variation of effective diffusivity of RTPs, $D_{a,eff}$ vs. size S for three different activities $v = 5 \times 10^4, 2.5 \times 10^4$ and 1.6×10^4. For all the cases, the $D_{a,eff}$ shows a very weak dependence on the size of passive particles.

We further explore the MSD of passive particles in the mixture. In Fig. 3.1(c-d) we show the plot of MSD of passive particles $\Delta_p(t)$ for different size ratios. We further explore the dynamics of passive particles for short and late times. The solid line is line with slope 2, hence early time dynamic of passive particles is superdiffusive and then in shows a crossover to late time diffusion to subdiffusion. To explore the late time behaviour we define the dynamic exponent $\beta(t)$ by:

$$\beta(t) = log_2 \frac{[\Delta(2t)]}{[\Delta(t)]} \tag{3.5}$$

In Fig. 3.3 we plot the dynamic exponent $\beta_p(t)$ (for passive particle) for different S for two different activities $v = 5 \times 10^4$ and 1.2×10^4. We find that for all size ratios, the very early time dynamic is superdiffusive with $\beta_p(t) > 1$, then it decay to value $\beta_p(t) < 1$. The deviation from late time $\beta_p(t) \approx 1$ to smaller than 1 increases on increasing S. The late time $\beta_p(t)$ decreases on increasing S for both activities. We further calculate the crossover time $t_{p,c}$ from early time superdiffusive to late time subdiffusion. The crossover time is defined as the time at which $\beta_p(t)$ crosses the $\beta_p(t) = 1$ first time. The crossover time $t_{p,c}$ increases with S for both activities as shown in Fig. 3.4(b). We find that crossover time of passive particles $t_{p,c}$, very strongly depends on their size and activity of RTPs. For large size and activity the crossover time is larger. In Fig. 3.4(b) we show the variation of $t_{p,c}$ for two different activities $v = 5 \times 10^4$ and 1.6×10^4 as a function of size S. We find that the variation is non-linear and slope of $t_{p,c} \simeq S^n$, where $n \in (1/2, 1)$. Which matches very well with the previous experimental systems [Wu & Libchaber (2000)] and deviation from the equilibrium result [Patteson et al. (2016)]. Increase in $t_{p,c}$ for large size ratio suggests that the bigger passive particles experiences persistent motion for larger period due to the clustering of RTPs present around them.

3.3.2 Results with varying activity of RTPs

We also explored the system for size ratios $S = 1$ and $S = 8$ and varying the activity v. For all activities the RTPs show the persistent random walk (PRW) as given in eqn. 3.4 and MSD shows a crossover from early time superdiffusive to the late time diffusive behaviour. In Fig. 3.5(a-b) we shows the plot of MSD of RTPs, $\Delta_a(t)$ for different v and fixed size ratios $S = 1$ and 8 respectively. We observe dynamics increases monotonically on increasing v. The small activity, means larger tumbling rate, hence the more frequent random reorientation of particle, which leads to the small translational displacement and hence slower dynamics. The data points from the numerical simulation and lines are fit from the expression of MSD as given in eqn. 3.4. The crossover time $t_{a,c}$, increases by increasing activity, The $t_{a,c}$ is obtained by fitting the MSD $\Delta_a(t)$ of RTPs with the expression of PRW as given in eqn. 3.4. In Fig. 3.4(a) we plot the crossover $t_{a,c}$ vs. v. The

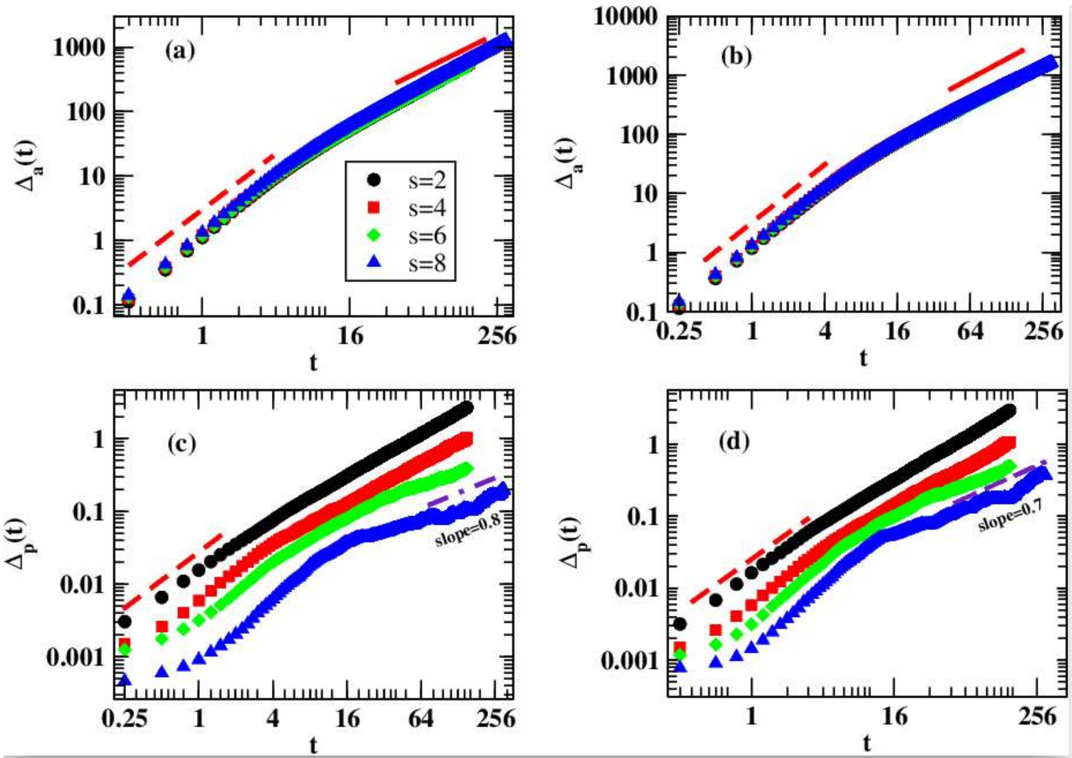


Fig. 3.1 (color online) Plot for $\Delta_a(t)$ vs. t for active (a-b) and passive particles $\Delta_p(t)$ (c-d), left panel is for activity $v = 5 \times 10^4$, and right is for 1.2×10^4 with variation of size ratios S. Dashed and solid lines are lines with slope 2 and 1 respectively. The dashed line in (c-d) is of slope 2. The dotted dashed line in (c) and (d) is of slope 0.8 and 0.7 respectively.

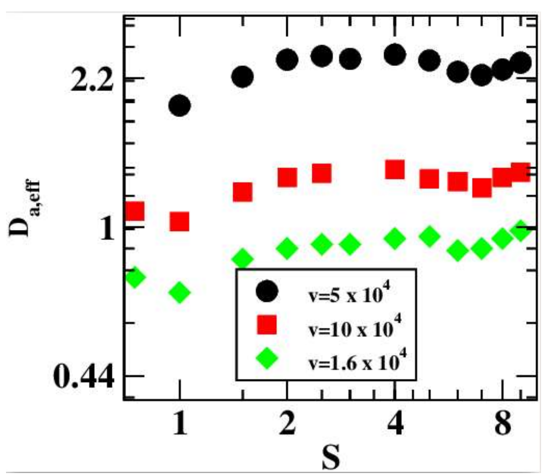


Fig. 3.2 (color online) Plot shows variation of $D_{a,eff}$ with size ratio S for three different activities of RTPs.

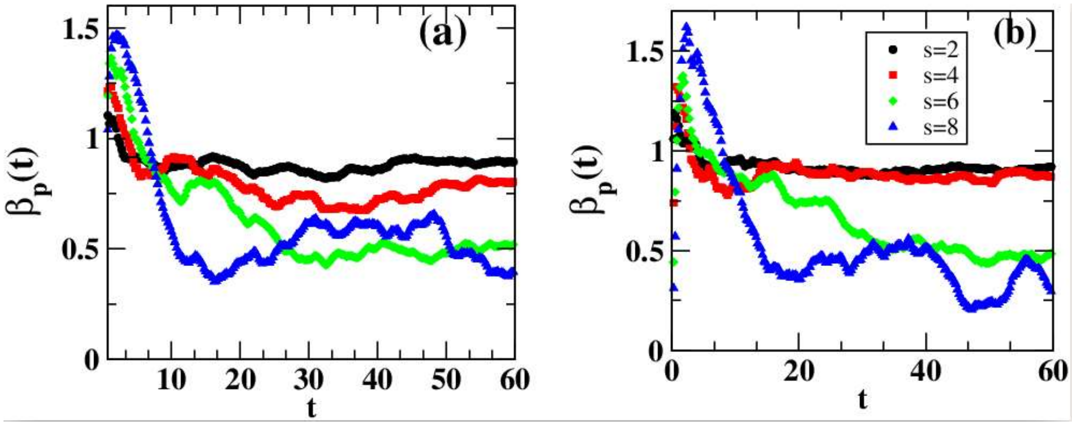
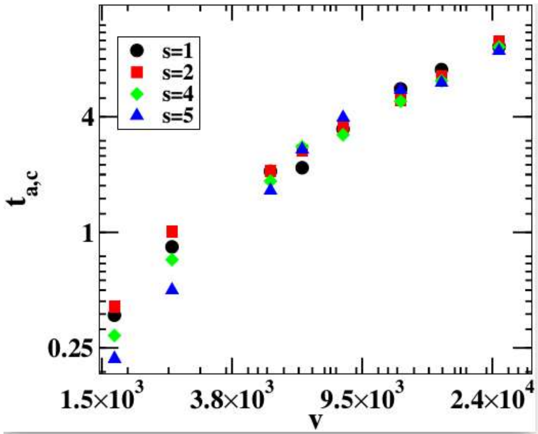


Fig. 3.3 (color online) Plot of $\beta_p(t)$ vs. t for passive particle for different size ratios for two different activities 5×10^4 and 1.2×10^4 other parameters are same as mentioned in Fig. 3.1(c-d).

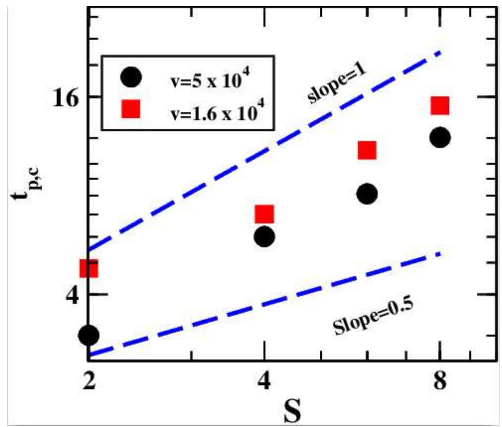
$t_{a,c}$ increases linearly with increasing v.

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, $\frac{\Delta_a(t)}{D_{a,eff}t_{a,c}}$. Where $D_{a,eff}$ is obtained by fitting the data for $\Delta_a(t)$ with the eqn. 3.4. We find scaling collapse of data for both size ratios and for all activities as shown in the inset of Fig. 3.5(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. 3.5(c-d). For small size ratio $S = 1$ and all activities, the MSD shows an early time superdiffusion to late time diffusive behaviour, whereas for larger size ratio $S = 8$, it is superdiffusive for early time and then goes to the late time subdiffusion regime. Interestingly for small size ratio we find weaker dependence of activity on the dynamics of passive particles, but strong dependence of activity for larger size ratio $S = 8$. This is due to the relatively larger number of RTPs required to move the passive particle for large size ratio. Whereas for the small size ratio even a single RTP can change dynamics of passive particle. Hence more random motion. To further confirm the dynamics of passive particles we calculated the effective dynamic exponent $\beta_p(t)$ as defined in eqn. 3.4. In Fig. 3.6, we show the variation of $\beta_p(t)$ vs. time t for size ratio



(a)



(b)

Fig. 3.4 (a) Plot of variation of $t_{a,c}$ with v for different size ratios S. (b) $t_{p,c}$ for passive particles with size ratios S for two different activities. The two line are of slope 1 and 0.5 respectively (Error of the order of symbol size).

$S = 1$ and $S = 8$ respectively. For small size ratio $S = 1$ Fig. 3.6(a), for all activities, $\beta_p(t)$ is close to 1.1 for early time and then approaches to value close to 1 for large times. For larger activities the late time $\beta_p(t)$, fluctuates around 1 and deviation from 1 is found for different activities. For larger size ratio $S = 8$ Fig. 3.6(b) for all activities the early time $\beta_p(t)$ is superdiffusive with $\beta_p(t) \simeq 1.5$ and then approaches to value smaller than 1 for late time. Hence for all activities the late time dynamic is subdiffusive for large size ratio.

3.4 Summary

We studied in detail the dynamic of passive particles in the presence of RTPs in binary mixture on a two-dimensional substrate. Both types of particles are athermal in nature. The activity of active particles is controlled by their activity v. The size of RTPs is fixed whereas it is varied for passive particles. The MSD of RTPs show the early time ballistic behavior and late time diffusive motion for all values of v and size ratios S. The dynamics of RTPs show very weak dependence on the size ratio S, whereas it shows enhance dynamics for larger activity. MSD for RTPs shows the good scaling collapse of data for different activity.

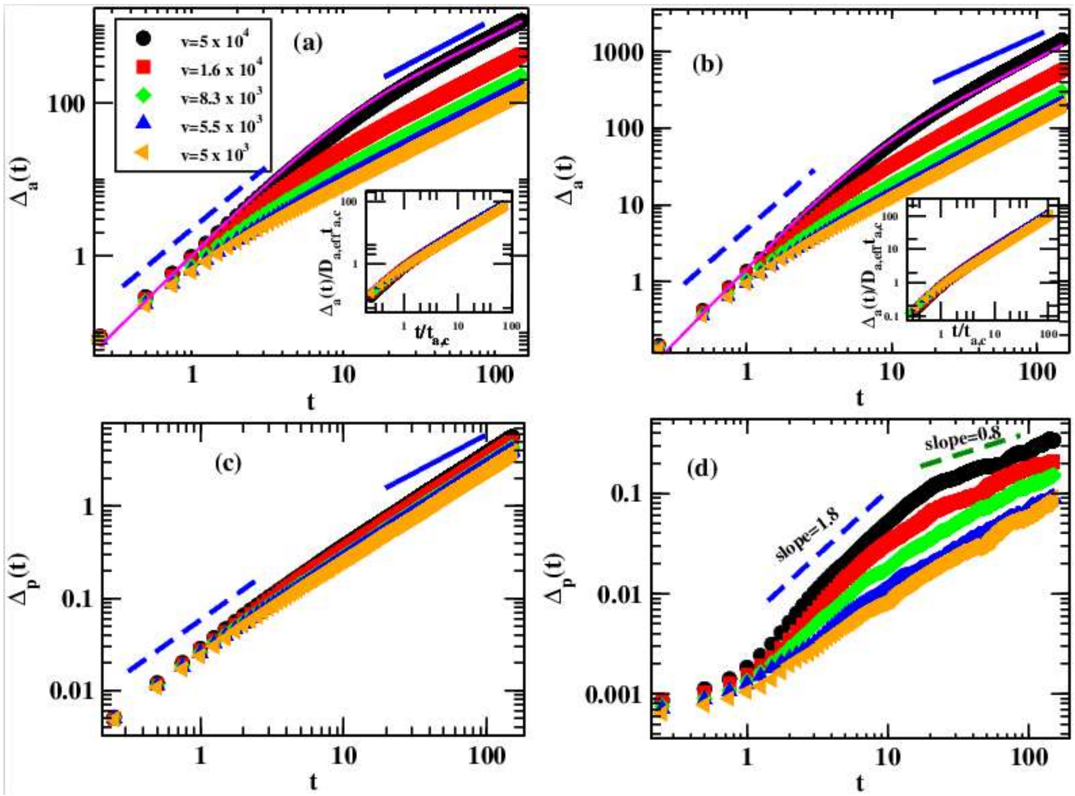


Fig. 3.5 (color online) The Plots (a)-(d) show the $\Delta(t)$ vs. t for active $\Delta_a(t)$ (a-b) and $\Delta_p(t)$ passive particles (c-d),left panel is for S= 1 and right panel is for S=8 with different v (inset shows the scaling plot of MSD for RTPs). lines are fitting function using eqn. 3.4. solid and dashed lines in (a-b-c) are of slope 1 and 2 respectively.

For small size ratios and large activity the MSD of passive particles in the mixture shows a crossover from early time superdiffusion to late time diffusion, whereas it goes to late time subdiffusive behaviour for large size ratio and lower activity. Hence the dynamics of passive particles show a change in dynamics from late time diffusive to subdiffusive dynamics on decreasing v and increasing S.

Hence our study explores the detail dynamics and behaviour of RTPs and passive particles in the mixture. Current study is focused on the small packing density of passive particles, where passive-passive interaction can be neglected. The study of mixture with passive particles packing fraction comparable to the active RTPs is an interesting problem to explore in future. Our particle-size dependence of MSD of passive particles in the presence

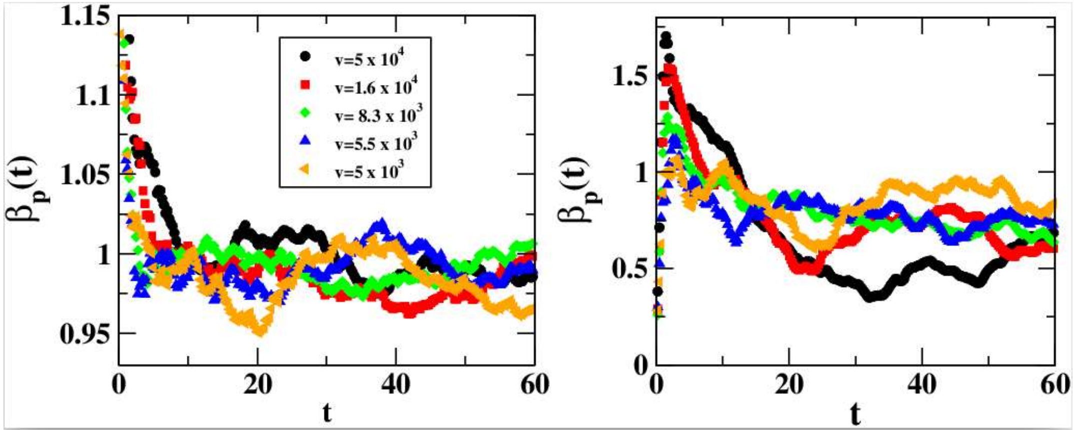


Fig. 3.6 (color online) The Plots (a)-(b) show the $\beta_p(t)$ vs. t for two different size ratio s=1(left panel) and s=8 (right panel) for different activities, other parameter are same as in Fig. 3.5(c-d).

of active run and tumble particles has important applications in particle sorting in different types of fluids like-microfluidic devices [(Abeylath & Turos, 2008)].

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