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**Clustering in anomalous files of independent  
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O. FLOMENBOM

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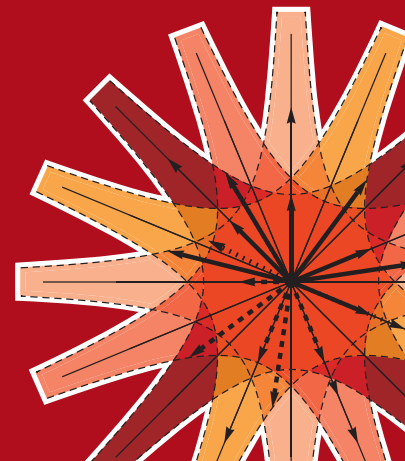


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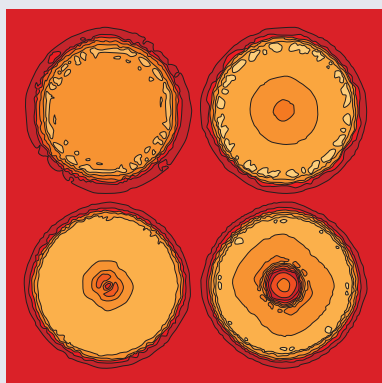
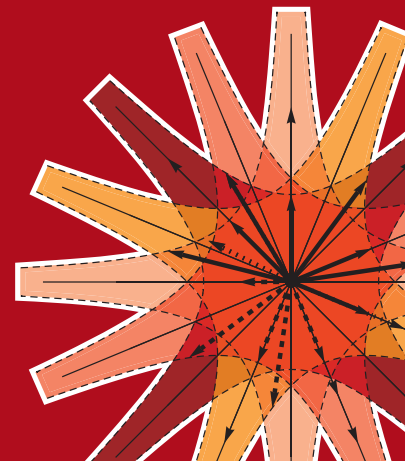
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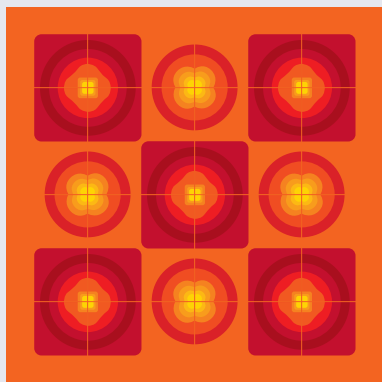
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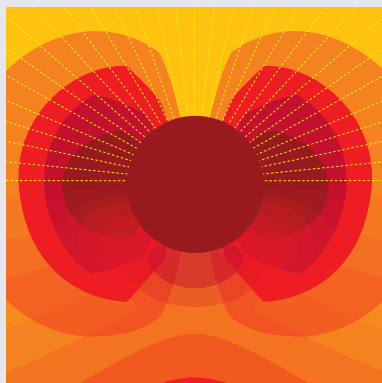
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# Clustering in anomalous files of independent particles

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**Abstract** – The dynamics of classical hard particles in a quasi-one-dimensional channel were studied since the 1960s and used for explaining processes in chemistry, physics and biology and in applications. Here we show that in a previously undescribed file made of anomalous, independent, particles (with jumping times taken from,  $\psi_\alpha(t) \sim t^{-1-\alpha}$ ,  $0 < \alpha < 1$ ), particles form clusters. At steady state, the percentage of particles in clusters is about,  $\sqrt{1-\alpha^3}$ , only for anomalous  $\alpha$ , characterizing the criticality of a phase transition. The asymptotic mean square displacement per particle in the file is about,  $\log^2(t)$ . We show numerically that this phenomenon of a dynamical phase transition is very stable, and relate it with the mysterious phenomenon of rafts in biological membranes, and with regulation of biological channels.

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**Introduction.** – File dynamics (sometimes called, single file dynamics) is the diffusion of  $N$  ( $N \rightarrow \infty$ ) identical Brownian hard spheres in a quasi-one-dimensional channel of length  $L$  ( $L \rightarrow \infty$ ) [1–19], such that the spheres do not jump one on top of the other, and the average particles' density is about fixed. The most well-known statistical property of this process is that the mean square displacement (*MSD*) of a tagged particle in the file follows,  $MSD \approx t^{1/2}$ . Indeed, file dynamics were used in modeling numerous microscopic processes [20–26]: the diffusion within biological and synthetic pores and porous material [20,21,25], the diffusion along 1D objects, such as in biological roads [26], the dynamics of a monomer in a polymer [22], etc. Nevertheless, in real files, one, or several, of the conditions defining the *basic* file may break down. Studies of generalizations of basic files show a rich spectrum of properties. For example, when the particles can bypass each other with a constant probability upon encountering [9], an enhanced diffusion is seen. When the particles interact with the channel, a slower diffusion is observed [16]. For Brownian files with an initial particles' density law that is not fixed, the diffusion is enhanced [10]. Moreover, in heterogeneous files with diffusion coefficients drawn from a density that diverges like a power law around the origin, slower dynamics are almost always obtained [12–14]. (See part A in the supplementary material (SM), presented in [27], for further mathematical description on the files introduced in this paragraph and

in the next one.) Generalizations of the basic file are important since these models represent reality much more accurately than the basic file.

## The model. –

*Anomalous files of independent particles.* Only recently, files that are anomalous were studied [17,18]; in such files, the jumping times of the particles are taken from a jumping time probability density function (PDF) of the form:  $\psi_\alpha(t) \sim t^{-1-\alpha}$ ,  $0 < \alpha < 1$ . In [16], it was shown that in renewal-anomalous files, were all the particles attempt a jump together, the *MSD* scales as the *MSD* of the corresponding Brownian file in the power of  $\alpha$ . Here, we study previously undescribed anomalous files made of independent particles. In such files, a random anomalous time is independently assigned for each particle. The fastest particle attempts a jump, and then, all the random times are adjusted. Finally, the particle that attempted jumping receives a new random time. This system has  $N$  independent anomalous clocks, where a renewal-anomalous file has only one clock. This is the origin for very different dynamical behaviors: Since the clocks are anomalous and independent, the particles are further connected in space, causing further slowness, even relative to renewal-anomalous files. Mathematically, the reason is that at large times, the order of the jumps that enables motion is exponentially small (with the number of particles that try moving). The basic manifestation of this is a logarithmic scaling with the time of the *MSD* per particle,  $MSD \sim \ln^2(t)$ .

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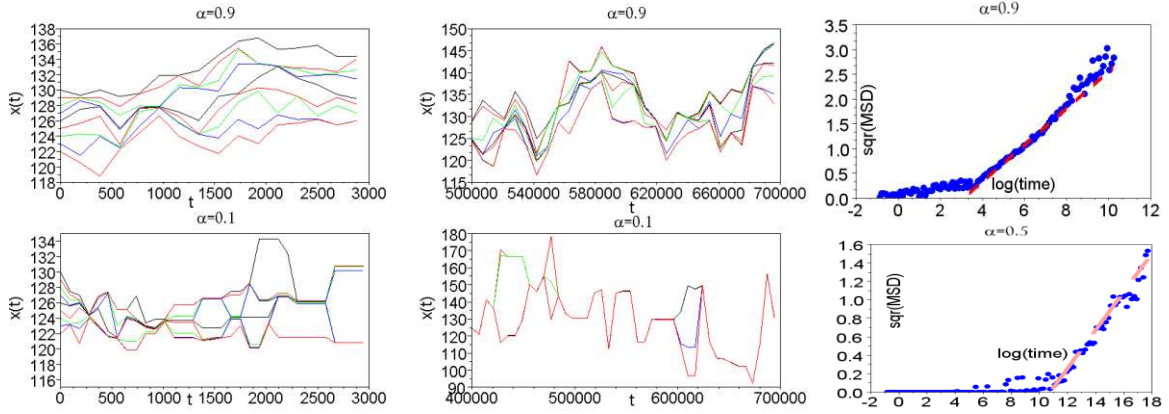


Fig. 1: Nine trajectories from an anomalous file of independent particles plotted as a function of the cycle index,  $t$ ; note that the actual time obeys the formula:  $t = t^{1/\alpha}$ . Particles are initially positioned at the integers, here shown particles located initially in the range, 122–130. In the simulations,  $N = 501$ ,  $\Delta = 1$  (the initial distance among particles),  $D = 1$  (the diffusion coefficient of the particles),  $dt = 0.13$ , and the jumping distance obeys,  $\sqrt{2D dt}(2q-1)$ , where  $q$  is a random number uniform in the unit interval. (Here, we use units without dimensions.) The upper panels show trajectories for  $\alpha = 9/10$  and the lower panels for  $\alpha = 1/10$ . Left panels show high-resolution trajectories at the initial stage of the process. Right panels show trajectories at low resolution at the last third of the simulation (we plot the trajectory every seven thousand cycles). Trajectories in a cluster look in this plot as one trajectory. Clearly, the attraction's strength among trajectories increases when  $\alpha$  decreases. This is evident at short times and at large times. We also show the  $MSD$  for two values of  $\alpha$  with fitting functions taken from eq. (3), on a square-root logarithmic scale.

Moreover, and even more exciting, we find a unique phenomenon in such files: the formation of clusters. We characterize the criticality of this dynamical phase transition showing that the number of particles in clusters at steady state follows,  $\sqrt{1-\alpha^3}$ . We also prove in many numerical tests that this phenomenon is indeed stable. Finally, we also suggest a link of this phenomenon with the mysterious phenomenon of rafts in membranes [24], and with the regulation of biological channels [25].

### Results. –

#### *Scaling law for anomalous files of independent particles.*

Here, we study anomalous files of independent particles using scaling laws. Firstly, we write down the scaling law for the mean absolute displacement ( $MAD$ ) in a renewal file with a constant density [10,14,18]:

$$\langle |r| \rangle \sim \langle |r| \rangle_{free} / n. \quad (1)$$

Here,  $n$  is the number of particles in the covered length  $\langle |r| \rangle$ , and  $\langle |r| \rangle_{free}$  is the  $MAD$  of a free anomalous particle,  $\langle |r| \rangle_{free} \sim t^{\alpha/2}$ . In eq. (1),  $n$  enters the calculations since all the particles within the distance  $\langle |r| \rangle$  from the tagged one must move in the same direction in order that the tagged particle will reach a distance  $\langle |r| \rangle$  from its initial position. Based on eq. (1), we write a generalized scaling law for anomalous files of independent particles:

$$\langle |r| \rangle \sim \frac{\langle |r| \rangle_{free}}{n} f(n), \quad 0 < f(n) < 1. \quad (2)$$

The first term on the right-hand side of eq. (2) appears also in renewal files; yet, the term  $f(n)$  is unique.  $f(n)$  is the probability that accounts for the fact that for moving  $n$  anomalous independent particles in the same

direction, when these particles indeed try jumping in the same direction (expressed with the term,  $\langle |r| \rangle_{free}/n$ ), the particles in the periphery must move first so that the particles in the middle of the file will have the free space for moving, demanding faster jumping times for those in the periphery.  $f(n)$  appears since there is not a typical timescale for a jump in anomalous files, and the particles are independent, and so a particular particle can stand still for a very long time, substantially limiting the options of progress for the particles around him, during this time. Clearly,  $0 < f(n) < 1$ , where  $f(n) = 1$  for renewal files since the particles jump together, yet also in files of independent particles with  $\alpha > 1$ , since in such files there is a typical timescale for a jump, considered the time for a synchronized jump. We calculate  $f(n)$  from the number of configurations in which the order of the particles' jumping times enables motion; that is, an order where the faster particles are always located towards the periphery. For  $n$  particles, there are  $n!$  different configurations, where one configuration is the optimal one; so,  $\frac{1}{n!} \leq f(n)$ . Yet, although not optimal, propagation is also possible in many other configurations; when  $m$  is the number of particles that move, then,  $f(n) \sim \binom{n}{m} (n-m)! \frac{1}{n!}$ , where  $\binom{n}{m} (n-m)!$  counts the number of configurations in which those  $m$  particles around the tagged one have the optimal jumping order. Now, even when  $m \sim n/2$ ,  $f(n) \sim e^{-n/2}$ . Using in eq. (2),  $f(n) \sim e^{-n/n_0}$  ( $n_0$  a small number larger than 1), we see,

$$MSD \sim \left( \frac{\alpha}{n_0} \right)^2 \ln^2(t). \quad (3)$$

(In eq. (3), we use,  $MSD \sim MAD^2$ .) In fig. 1, we show that results from simulations coincide with eq. (3), for various

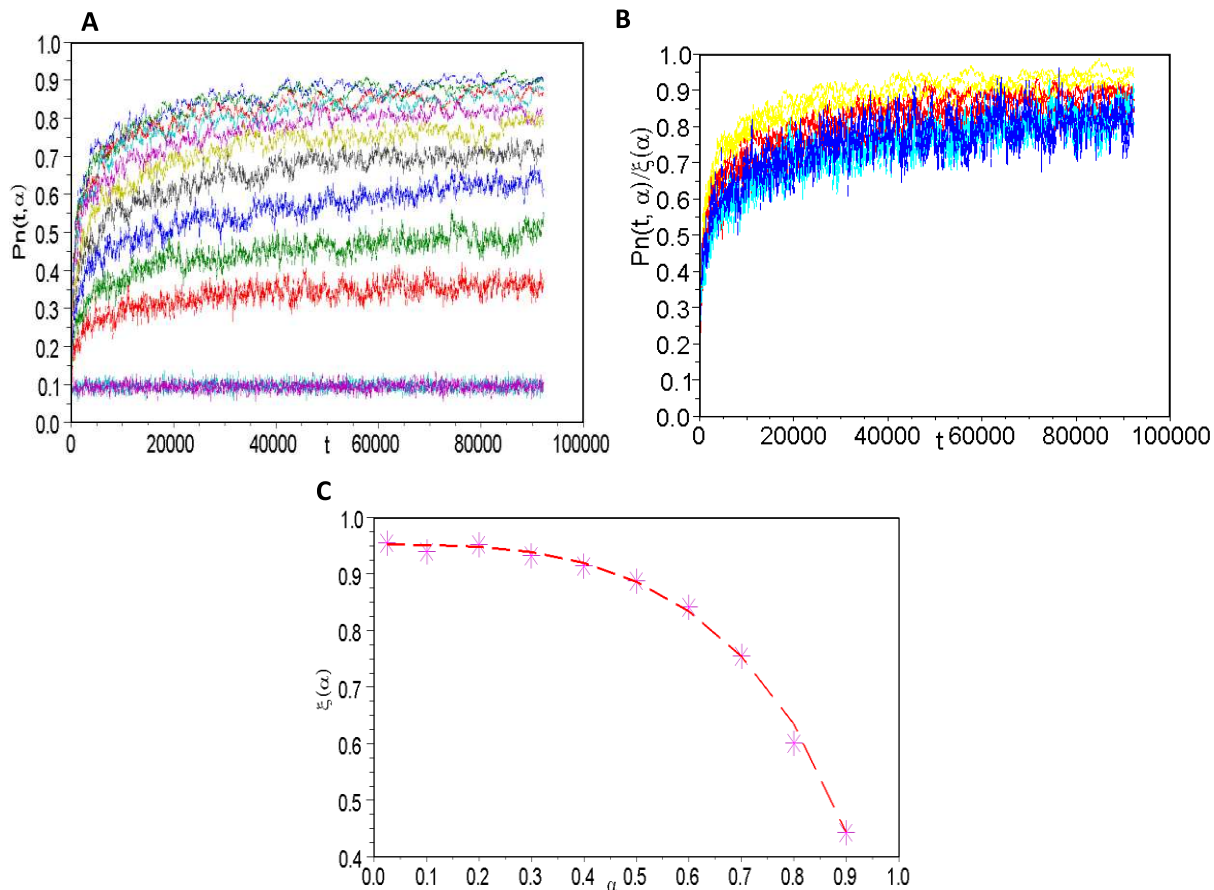


Fig. 2:  $p_n(t, \alpha)$ , its normalized form and  $\xi(\alpha)$ . (A)  $p_n(t, \alpha)$  as a function of the event index  $t$ , for 10 values of anomalous  $\alpha$ ,  $\alpha = 0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3, 0.2, 0.1, 0.024$ , for the third (from the bottom) and on curves, respectively, and the control curves: an anomalous file with  $\alpha = 3.37$  and a normal dynamics file (these curves fluctuate around,  $p_n(t, \alpha) = 0.1$ ). The clustering phenomenon is unique for anomalous files of independent particles, representing a phase transition depending on  $\alpha$ . (B) Normalizing  $p_n(t, \alpha)$  with its asymptotic value  $\xi(\alpha)$ , all anomalous curves follow pretty much the same route. (C)  $\xi(\alpha)$  with its fitting curve,  $\xi(\alpha)$ . As  $\alpha$  goes to zero, about 97% of the particles are in clusters.

values of  $\alpha$ . Equation (3) shows that asymptotically the particles are extremely slow in anomalous files of independent particles.

*Numerical results of anomalous files of independent particles.* For understanding this slowness even better, we perform extensive numerical simulations. In the simulations,  $N = 501$ , and the initial density is constant with a distance of unity among the point particles. At the edges, reflecting boundaries are positioned at points,  $\pm 253$ . (We use units without dimensions all over). Random jumping distances are distributed uniformly in about a unit interval centered on the origin, and the reflection method is used in moving the particles, namely, a jump is made and the particles' order remains. Simulations were performed for seven values of  $\alpha$  in the range of anomaly,  $0.024 \leq \alpha \leq 0.9$  (in this range, the average of  $\psi_\alpha(t)$  is infinite). In addition, we performed two control simulations: one for a file of independent particles with  $\alpha = 3.37$  (that has a finite average for  $\psi_\alpha(t)$ ) and one for normal dynamics. Trajectories obtained from simulations are shown in fig. 1 as a function

of the number of the cycles  $t$ , where a cycle contains  $N$  attempts of jumping. The trajectories exhibit the phenomenon of clustering: namely, particles attract each other and then move pretty much together. It is also evident that the value of  $\alpha$  and the number of cycles determine the degree of clustering in the system. We note that the results presented here are independent of the value for  $N$  and are qualitative identical for files with finite size particles (see part B of the SM, presented in [27]).

Characterizing the formation of the clusters, fig. 2(A) shows  $p_n(t, \alpha)$ : the percentage of particles in a cluster at  $t$  for a particular  $\alpha$  (namely, the number of particles in clusters above the total number of particles). Here, when adjacent particles are at a distance not larger than 0.1, they are considered clustered. The curves height depends on  $\alpha$ , yet when normalizing  $p_n(t, \alpha)$  with  $\xi(\alpha)$  ( $\equiv p_n(t \rightarrow \infty, \alpha)$ ), the curves pretty much coincide with each other (fig. 2(B)). (In action,  $\xi(\alpha)$  is the average of  $p_n(t, \alpha)$  calculated from the last 10% of the trajectory.)  $\xi(\alpha)$  is shown in fig. 2(C) with the optimal (4-parameter) fitting function,  $\xi(\alpha) = 0.98(1 - (\frac{\alpha}{0.99})^{3.09})^{0.537} - 0.028$ .

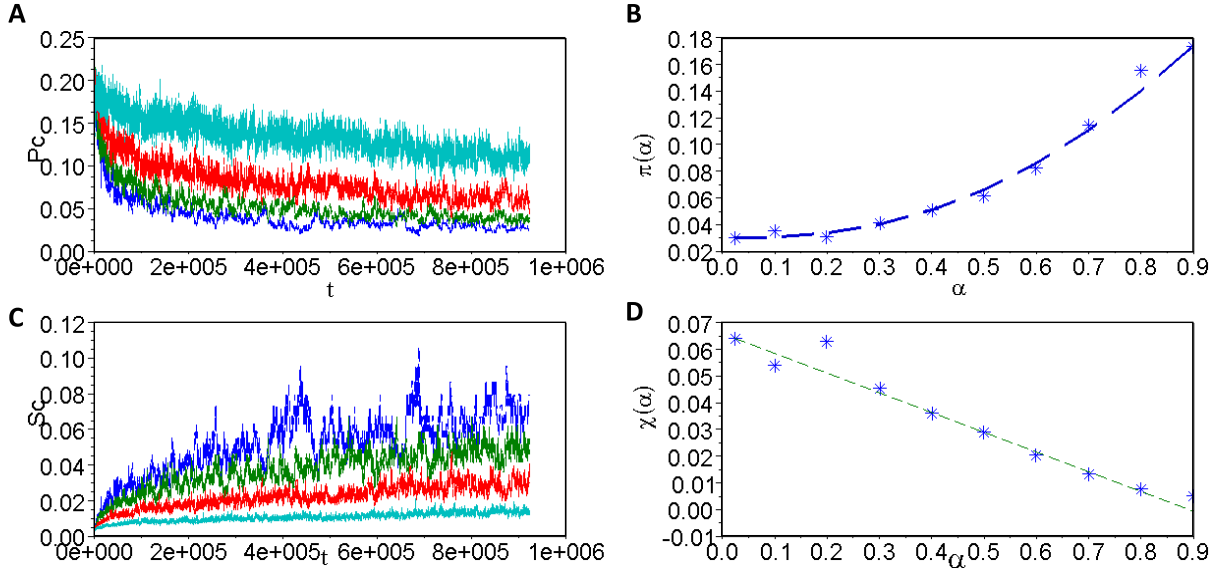


Fig. 3:  $p_c(t, \alpha)$ ,  $\pi(\alpha)$ , and  $S_c(t, \alpha)$  and  $\chi(\alpha)$ . (A)  $p_c(t, \alpha)$  as a function of the event index  $t$ , for 4 values of anomalous  $\alpha$ ,  $\alpha = 0.7, 0.5, 0.3, 0.024$ , counting from the top curve. The percentage of clusters is smaller when  $\alpha$  is small, since the clusters are larger at small  $\alpha$ . (B)  $\pi(\alpha)$ , the steady-state value for the number of clusters in percentages is shown with its fitting curve,  $\tilde{\pi}(\alpha)$ . As  $\alpha \rightarrow 0$ , the percentage of clusters is 3%. (C)  $S_c(t, \alpha)$  as a function of the event index  $t$ , for the 4 values of anomalous  $\alpha$  in (A), counting from the lower curve. The average size of a cluster is large when  $\alpha$  is large. Here, the average cluster can contain, momentarily, about 10% of the particles. (D)  $\chi(\alpha)$ , the steady-state value for the average size of a cluster (in percentage) with its simple fitting curve,  $\tilde{\chi}(\alpha)$ . As  $\alpha \rightarrow 0$ , the average cluster's size is 33.

This fitting function is of the form of

$$\tilde{\xi}(\alpha) \approx \sqrt{1 - \alpha^3}. \quad (4)$$

When  $\alpha \rightarrow 0$ , almost all particles are in clusters. The fluctuations in  $\xi(\alpha)$  are about 5% for  $\alpha = 0.9$ , and are about 0.5% for  $\alpha = 0.024$  (with about a linear interpolation with  $\alpha$ ). The fluctuations in  $\xi(\alpha)$  represent the motion of particles among clusters. Namely, for a small value of  $\alpha$  at steady state, the particles in a cluster move together, where at larger values of  $\alpha$ , about 5% of the particles diffuse among clusters. Since clustering occurs only for anomalous  $\alpha$ ,  $\tilde{\xi}(\alpha)$  describes the criticality of a phase transition. Indeed,  $\tilde{\xi}(\alpha)$  has a typical form for a scaling function in critical phenomena [28] (see the next paragraph for further discussion about this point). Complementary information about the clustering is obtained from two additional functions:  $p_c(t, \alpha)$  and  $S_c(t, \alpha)$ . Figure 3(A) presents  $p_c(t, \alpha)$ : the percentage of clusters (measured in terms of the number of particles) at  $t$  for a particular  $\alpha$ . For relatively large values of  $\alpha$ , the number of clusters is also large (yet, the clusters are smaller in size). The fluctuations in the number of clusters is also larger when  $\alpha$  is larger. This is in accordance with the behavior of  $p_n(t, \alpha)$ . Figure 3(B) shows  $\pi(\alpha) (\equiv p_c(t \rightarrow \infty, \alpha))$  vs.  $\alpha$  for all anomalous values of  $\alpha$ . The optimal fitting function has the form  $\tilde{\pi}(\alpha) = 0.78(1 + (\frac{\alpha}{1.19})^{2.49})^{0.42} - 0.75$ .  $\tilde{\pi}(\alpha)$  follows closely a function of the form

$$\tilde{\pi}(\alpha) \approx 0.6 \left( \sqrt{1.7 + \alpha^3} - 1.25 \right). \quad (5)$$

$\tilde{\xi}(\alpha)$  and  $\tilde{\pi}(\alpha)$  have complementary physical interpretation, seen in their scaling laws following (about),  $\sqrt{1 \pm \alpha^3}$ .  $\tilde{\xi}(\alpha)$  quantifies particles in clusters, where the same number of particles can exist for a small or a large number of clusters.  $\tilde{\pi}(\alpha)$  simply counts clusters, and can have the same value when these are either small clusters or large clusters. Importantly, when clustering occurs, we see a small number of large clusters as  $\alpha$  becomes smaller, where in a system without clustering, we may see about 10% of small clusters. Figure 3(C) presents the average size of a cluster,  $S_c(t, \alpha) (\equiv p_n(t, \alpha)/p_c(t, \alpha))$ . Here, fluctuations are larger when  $\alpha$  is small. Figure 3(D) shows  $\chi(\alpha) (\equiv S_c(t \rightarrow \infty, \alpha))$ , the asymptotic value of a cluster's size, with its simple fitting function

$$\tilde{\chi}(\alpha) = (33 - 37\alpha)/N. \quad (6)$$

Interestingly, the average size of a cluster is limited with about 33 particles when  $\alpha \rightarrow 0$ , where clustering disappears when  $\alpha \rightarrow 1$ , further quantifying the phase transition.

### Discussion and conclusions. –

*Characterizations of the clustering.* Firstly, we recall that slowness is expected in files of anomalous independent particles since the order of the jumps that enables motion is exponentially small (with the number of particles that try moving) and the dynamics are without a typical timescale. For further explaining the clustering, we look on the actual values of the jumping times of the particles after the process has been going on for a while; see fig. 4.

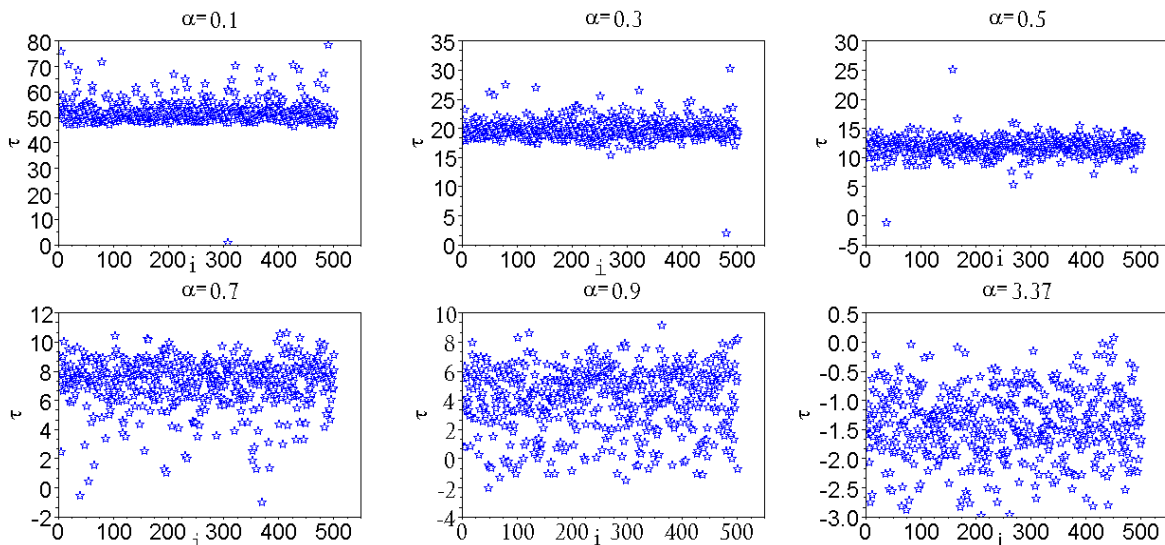


Fig. 4: The band of jumping times ( $\tau$ ) after about 7 hundred thousand cycles for a system of about 500 point particles for several values of  $\alpha$  on a log-linear scale.

(These are the quantities discussed in the derivation of the *MSD*.) It is clear from fig. 4 that when  $\alpha$  decreases the typical value for the jumping time increases (here, the typical time is the jumping time of most of the particles). The interesting issue here is that when  $\alpha$  decreases there is a phenomenon that only a few particles are significantly faster relative to all the others. This tells the story of the clustering and the phase transition: when one particle jumps over and over and over again, it clusters the particles in its vicinity, since when only a particular particle moves repeatedly several times, it closes the gap among the particles in its vicinity, such that they are eventually clustered.

How can we explain the form of the fitting functions? Firstly, we note that the fitting function of  $\xi(\alpha)$  has a standard form for a scaling function at criticality of a phase transition [28]:  $f(\alpha) \sim (1-\alpha)^\mu$  (where a function in  $\alpha$  can replace  $\alpha$  in generalizations), and  $\chi(\alpha)$  and  $\pi(\alpha)$  pretty much follow from  $\xi(\alpha)$ .  $\pi(\alpha)$  is complementary to  $\xi(\alpha)$ , since it has such a physical interpretation, and  $\chi(\alpha)$  is the ratio of the previous ones.

Now, for further supporting the form of the fitting function of  $\xi(\alpha)$ , we calculate the PDF of slowest jumping time when there are  $n+1$  jumping times in the band:

$$f_{s.t.}(t; n+1) = \psi(t) \left( \int_0^t \psi(s) ds \right)^n \sim t^{-1-\alpha} e^{-nt^{-\alpha}}. \quad (7)$$

We emphasize the following three points: 1)  $f_{s.t.}(t; n+1)$  is very small for times smaller than,  $t^* \equiv n^{1/\alpha}$ , that is the time when the argument of the exponent  $e^{-nt^{-\alpha}}$  is unity. 2)  $t^*$  is the typical timescale for most of the particles in the file, in the limit of many cycles. This is indeed seen in fig. 4. The reason is very simple: after many cycles, most of the particles are extremely slow, since only the fast ones move and after several jumps the anomalous

properties of  $f_{s.t.}(t; n+1)$  “assign” the particle a very slow jumping time. 3) When calculating the first and the second moments of  $f_{s.t.}(t; n+1)$  in the range  $t \leq t^*$ , we find,  $\langle t \rangle \sim n^{1/\alpha-1}$  and  $\langle t^2 \rangle \sim n^{1/\alpha-2}$ . This should reflect the properties of the fast particles until the time  $t^*$ . It is evident that a transition occurs in the second moment when  $\alpha > 1/2$ :  $\langle t^2 \rangle$  vanishes when  $\alpha > 1/2$ , yet scales with  $n$  when  $\alpha < 1/2$ . Namely, for  $\alpha < 1/2$  many of the fast particles are slower than  $t^*$ , yet when  $\alpha > 1/2$ , most of the fast particles are indeed faster than  $t^*$ . This behavior is indeed seen in fig. 4: when  $\alpha < 1/2$  fewer and fewer particles are seen in the range  $t \leq t^*$ , yet when  $\alpha > 1/2$  we see many particles in this range. This is the origin for many small clusters when  $\alpha > 1/2$  and only a few clusters, yet larger, when  $\alpha < 1/2$ .  $\tilde{\xi}(\alpha)$  and  $\tilde{\pi}(\alpha)$  capture this property.

*Anomalous files, rafts and channels.* Now, we also find that clustering is seen in anomalous files embedded in two-dimensions, creating a network of isotropic files, like streets and junctions. Indeed, this system is a generalization of a 1-dimensional file, and is defined with two free parameters: the percentage of intersections (without directional preference in intersections) and the length of the interval until an intersection occurs. We study files that intersect each other for 1% every interval of 10 (see part C in the SM, presented in [27], for a comprehensive analysis). Among other results, we find that in such a system 50% of the particles are in clusters when  $\alpha \rightarrow 0$ . Indeed, the results are sensitive to the branching parameters: when branching occurs in smaller intervals, clustering decreases, and we can speculate that when diffusion happens in two dimensions (not in a network of one-dimensional files), the clustering phenomenon is not observed when the density is reasonable (not too high). This is in accordance with known results showing that the slower diffusion so typical for a particle in a file in one-dimension does not hold for



diffusion of hard particles in two-dimensions, where in such a system a standard diffusion is seen (when the density is not too high). Still, we have chosen here reasonable parameters for the branching: the average size of a jump is 0.25, and the branching occurs every interval of 10; this is not too small an interval so that branching indeed has a role (seen also in the results), still the branching happens after frequent enough jumps and the clustering is indeed seen.

An isotropic network of files embedded in two-dimensions enables relating the clustering with rafts: a raft in a (two-dimensional) membrane is a dense patch of specific lipo-molecules [24]. The mechanism of the formation of these patches is still not clear, yet it is known that rafts do not largely occur due to an electrostatic attraction. We think that the phenomenon of clustering in anomalous files of independent particles can explain rafts in membranes: given that the lipo-molecules diffusion is anomalous (anomalous diffusion is common in membranes), they will form rafts, since diffusion in biological membranes is describable with the model of an isotropic network of files in two dimensions.

Finally, we expect that the clustering phenomenon is universal and holds in a wide range of external conditions, since the diffusion coefficient of the particles does not affect this phenomenon, yet  $\alpha$ , the only other external parameter here, is the control parameter. Since clustering is expected to be universal, it may be used in regulating biological channels, an important topic in biophysics, *e.g.* [25]; this is achieved when controlling the phase of the anomalous particles in the channel (clustered or diffusing), using one of two possibilities: changing  $\alpha$  (smaller or larger than 1) or controlling the synchronization of the particles (synchronized or independent, with anomalous  $\alpha$ ).

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