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How rare are diffusive rare events?

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Abstract – We study the time until first occurrence, the *first-passage time*, of rare density fluctuations in diffusive systems. We approach the problem using a model consisting of many independent random walkers on a lattice. The existence of spatial correlations makes this problem analytically intractable. However, for a mean-field approximation in which the walkers can jump anywhere in the system, we obtain a simple asymptotic form for the mean first-passage time to have a given number k of particles at a distinguished site. We show numerically, and argue heuristically, that for large enough k , the mean-field results give a good approximation for first-passage times for systems with nearest-neighbour dynamics, especially for two and higher spatial dimensions. Finally, we show how the results change when density fluctuations anywhere in the system, rather than at a specific distinguished site, are considered.

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Introduction. – Rare events control the kinetics of many physical systems. They are frequently associated with *activated* processes, corresponding to the crossing of a high free-energy barrier, as happens, for example, in nucleation processes [1]. On the other hand, in diffusive systems, where particles undergo Brownian motion, there are no such energy barriers. Here, questions arise such as: what is the time required for a particle to first reach a particular region of space, or for a pair of particles to meet for the first time? Depending on the circumstances, such events can be very rare, in which case they may be the limiting step in the dynamics of the system. It is then crucial to understand when such events will occur.

Diffusive systems exhibit universality, in the sense that their behaviour is often independent of the microscopic details. It is then convenient to study simple models, in the hope that the results will extend to more complicated systems. A common choice is that of particles undergoing a *random walk* on a lattice [2]. For a single-particle random walk, first-passage times to a given site in an infinite system have long been studied [3], and much is now known about their statistics [2,4]. Recent progress in this direction was made by Condamin *et al.*, who

studied first-passage times and distributions for a single particle diffusing from a source site to a destination site in a confined region [5–7]. Other properties, however, are relevant only when many walkers are present, for example the sequence of times for each to arrive at a given point [8], and the territory covered after a given number of steps [9,10].

In this letter, we study the following first-passage problem for systems containing many random walkers on a periodic lattice: how long does it take for k of the walkers to accumulate at a given site? For k much larger (or much smaller) than the mean density, this corresponds to a large local density fluctuation, and is thus a rare event. A related quantity was studied numerically in [11], as a model of particles traversing a membrane pore. Special cases have also been studied in relation to Ritort's backgammon model [12,13], and another related model was recently used in a study of cooperativity in chemical kinetics [14]. The general problem has, however, received scant attention, despite its relevance for many physical systems.

Indeed, the problem pertains to any systems whose dynamics may be affected by the accumulation of diffusing particles in a given region. A particular physical example that we have in mind is a fluid of hard discs exhibiting *glassy* behaviour. When the density of discs is close to the fluid-solid transition, configurations become “jammed”,

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resulting in slow, glass-like dynamics [15]. However, even in this situation, each disk can be surrounded by a small amount of “free volume” in which the disks “rattle” about. This limited disk motion gives rise to an effective free volume transport, which, on large scales, may be viewed as diffusive. When enough free volume accumulates in a region of the system, a neighbouring disc can move into the resulting space, causing a large local rearrangement of the jammed structure. The dynamics of these rearrangements is thus controlled by the rare accumulation events, which can be viewed as density fluctuations of the free volume.

In this work, we focus on the simple multiple random walker problem, which still poses rather formidable challenges. Actually, for systems containing many random walkers, exact results are known for first-passage times from one configuration to another, in terms of eigenvalues and eigenvectors of the transition matrix, for the case where a single walker moves at each time step [16,17] or where all walkers can move simultaneously [18]. But these results do not extend easily to the case of interest here, where we are concerned with transitions from a large set of rather disparate configurations (*i.e.* all configurations having k walkers at a given site) to another.

Since diffusive processes give rise to spatial and temporal correlations that render the problem analytically intractable, we also consider a mean-field version of this problem, in which particles can jump not only between neighbouring sites, but to *any* of the sites in the system with equal probability, which reduces the problem to a type of Ehrenfest urn model [13,19]. We show numerically that this approximation provides a qualitative explanation of the behaviour of the mean first-passage time also for diffusive dynamics.

The model. – We consider N independent random walkers on a lattice with volume (= number of sites) V and periodic boundary conditions. In this paper we study only regular “cubic” lattices of spatial dimension d (a ring for $d=1$, square lattice for $d=2$ and simple cubic lattice for $d=3$). In 1D, at each time step a single walker is selected to move right, move left, or stay where it is, with probabilities p , q , and $r = 1 - (p + q)$, respectively. For 2D square and 3D simple cubic lattices, we study only the case in which the chosen walker moves one lattice spacing in any direction with equal probability.

We are interested in the event (*i.e.* the set of configurations) S_k that a distinguished site, labelled by 0, is occupied by exactly k particles; in particular, we are interested in the *first time* at which this event occurs, that is, when the system configuration lies inside the set S_k . The mean particle density (number of particles per site) $\rho := N/V$ plays a crucial role here: for k either much larger or much smaller than this mean density, the event S_k is *rare*. From the static point of view, this means that the probability that the event occurs is small. From the dynamical point of view of interest here, it means that the time needed to actually see the event occur is, on average, very long.

Starting from an initial condition with the particles distributed randomly, the main question of interest is thus *how long it takes for the rare event to occur* —that is, we are interested in the mean *first-passage time* τ_k^{FP} for the system to reach S_k , averaged over all random initial conditions which are *not in* S_k [6]. In this paper we consider the case of relatively low mean density, of order $\rho = 1$, and fluctuations to large local densities $k \gg \rho$. In systems where the density is high, a fluctuation in which a site becomes nearly empty is also a rare event with important physical applications, such as in Ritort’s backgammon model [12]. This case can also be studied using the methods described here, as we will discuss elsewhere.

Mean-field approximation. – In order to make analytical progress, we consider a mean-field version of the model, in which the walkers may jump to *any* other site, with equal probability $1/(V-1)$; this is equivalent to considering dynamics on a completely-connected graph. The model then reduces to an Ehrenfest *urn model* [13].

In this case, the particles which are not at the distinguished site “0” can be regarded as belonging to a reservoir containing $N - n_0$ particles, the locations of which are irrelevant. The occupation number n_0 of site “0” then undergoes a Markovian random walk whose hopping probabilities depend on its current position, for which exact results are known [20,21]. In the context of urn models, further results were found in [19,22]. We approach the problem from within this context.

We denote the mean first-passage time from S_l to S_m by $\tau_{l \rightarrow m}$. It is convenient to first study $\tau_k^+ := \tau_{k \rightarrow k+1}$, the mean first-passage time from S_k to S_{k+1} . Suppose that at a given time step, there are k particles at the distinguished site, so that the system is in S_k . There are then three possibilities, whose probabilities depend explicitly on k : with probability β_k , a walker from the reservoir lands at the distinguished site, thereby reaching S_{k+1} ; with probability γ_k , a walker from the distinguished site leaves to the reservoir, giving S_{k-1} ; and with probability $\alpha_k := 1 - \beta_k - \gamma_k$, a walker moves around inside the reservoir, without affecting site 0, so that the system remains in S_k . In the mean-field case, these probabilities are independent of the microscopic configuration, and are given by

$$\beta_k = \frac{N-k}{N} \frac{1}{V-1} (1-r), \quad \gamma_k = \frac{k}{N} (1-r). \quad (1)$$

Here, k/N is the probability of choosing a *site* containing k of the N walkers. The factor $(1-r)$ appears in all such probabilities, and results in a factor $1/(1-r)$ in the expressions for mean times; for simplicity, we omit it in the following, considering the case where the particle must jump, *i.e.* $p+q=1$.

After a given step, which takes time 1, if the system finds itself in some S_i , then the subsequent mean first-passage time to S_{k+1} is $\tau_{i \rightarrow k+1}$. By conditioning on the

outcome of a step starting at S_k , we obtain

$$\tau_k^+ = \alpha_k(1 + \tau_k^+) + \beta_k(1 + \tau_{k+1 \rightarrow k+1}) + \gamma_k(1 + \tau_{k-1 \rightarrow k+1}). \quad (2)$$

Since only one walker moves at each step, to reach S_m from S_l , we must first pass through all intermediate S_i . We thus have additivity of mean first-passage times: $\tau_{l \rightarrow m} = \sum_{i=l}^{m-1} \tau_i^+$ for $l < m$. In particular, to reach S_{k+1} from S_{k-1} , we must pass through S_k , so that $\tau_{k-1 \rightarrow k+1} = \tau_{k-1}^+ + \tau_k^+$. Furthermore, we have $\tau_{m \rightarrow m} = 0$ for any m . Inserting these results in eq. (2), we get

$$\tau_k^+ = 1 + \alpha_k \tau_k^+ + \gamma_k (\tau_{k-1}^+ + \tau_k^+), \quad (3)$$

and hence, by rearranging, we obtain a first-order recurrence relation giving τ_k^+ in terms of τ_{k-1}^+ :

$$\tau_k^+ = \frac{1}{\beta_k} + \frac{\gamma_k}{\beta_k} \tau_{k-1}^+; \quad (4)$$

this result was first derived in [20] by a different method. The boundary value τ_0^+ is the mean of a geometric distribution with parameter α_0 , and is hence given by $\tau_0^+ = \frac{1}{1-\alpha_0} = \frac{1}{\beta_0}$. By interchanging β_k and γ_k , we find a similar recurrence relation in the other direction for the mean time $\tau_k^- := \tau_{k \rightarrow k-1}$, obtaining $\tau_k^- = (1 + \beta_k \tau_{k+1}^-) / \gamma_k$.

An important related concept in random processes is the *recurrence time* to a set A , that is, the time required for the system to return to A , given that it started there [23]. The mean recurrence time τ_k^{rec} to the set S_k is found, again by conditioning, to satisfy

$$\tau_k^{\text{rec}} = 1 + \beta_k \tau_{k+1}^- + \gamma_k \tau_{k-1}^+. \quad (5)$$

In the situation that we are considering, for fluctuations to $k \gg \rho$, the mean times τ_k^- to decrease k are small, whereas the times τ_k^+ to increase it are large. We thus obtain the following approximate relation between the recurrence time and the first-passage time:

$$\tau_{k-1}^+ \simeq \frac{1}{\gamma_k} \tau_k^{\text{rec}} = \frac{N}{k} \tau_k^{\text{rec}}. \quad (6)$$

The mean first-passage time to the set S_k from a *random* initial condition, denoted τ_k^{FP} , is now given by a sum of the $\tau_{m \rightarrow k}$, each weighted by the probability of starting in S_m . This is dominated by the largest term, $\tau_{0 \rightarrow k}$, which in turn is dominated by τ_{k-1}^+ , giving the approximate result

$$\tau_k^{\text{FP}} \simeq \tau_{k-1}^+ \simeq \frac{1}{\gamma_k} \tau_k^{\text{rec}}. \quad (7)$$

Asymptotics. – The recurrence relations given above yield closed-form results for mean first-passage times, expressed as sums [21]. That representation does not, however, allow us to easily understand the behaviour as a function of the system parameters. Instead, we focus on asymptotic results which give the dominant behaviour. To do so, we use the Kac recurrence theorem [6,23,24].

This states that the mean recurrence time to a set A in an ergodic system is given exactly by $\tau_A^{\text{rec}} = \frac{1}{\mathbb{P}[A]}$, where $\mathbb{P}[A]$ is the stationary probability that the system is in A . By using the results of the previous section, this will then provide information on mean first-passage times. We remark that this result of Kac is apparently still not well known in the physics literature: for example, refs. [16–18] resorted to much more complicated techniques to calculate Poincaré cycles (*i.e.* mean recurrence times) in these systems; see also [5,6].

We denote the set of microscopic configurations by Ω . These are given by vectors of size N containing the positions of all walkers. Each such configuration is equally likely, since the transition probabilities between them are symmetric, so that the Kac formula gives the exact mean recurrence time to the set S_k as

$$\tau_k^{\text{rec}} = \frac{1}{|S_k|/|\Omega|} = \frac{V^N}{\binom{N}{k}(V-1)^{N-k}}, \quad (8)$$

where $|A|$ denotes the number of configurations in the (finite) set A , obtained by combinatorial arguments, and $\binom{N}{k}$ is a binomial coefficient.

For large N and V , fixed density $\rho = N/V$, and fixed $k \ll N$, we substitute the asymptotic results $N!/(N-k)! \sim N^k$ and $1 - \frac{1}{V} \sim \exp(-1/V)$ into the exact recurrence time expression (8), to obtain the asymptotics

$$\tau_k^{\text{rec}} \sim k! \left(\frac{V}{N}\right)^k \exp\left(\frac{N-k}{V}\right), \quad (9)$$

and hence

$$\tau_k^{\text{rec}} \sim k! \rho^{-k} \exp(\rho). \quad (10)$$

Physically, the total number of particles present should not affect the dynamics of a given particle, so that the *physical time* is the number of steps per particle (*i.e.* the physical time unit corresponds to one “sweep” through the N particles in the system). Since $\tau_k^{\text{FP}} \simeq \frac{N}{k} \tau_k^{\text{rec}}$, we finally obtain the following approximate asymptotic expression for the per-particle first-passage time to S_k :

$$\frac{1}{N} \tau_k^{\text{FP}} \simeq (k-1)! \rho^{-k} \exp(\rho). \quad (11)$$

Asymptotically, the mean-field first-passage time thus depends on N and V only via the density ρ of walkers for k small compared to the total number of particles.

Figure 1 compares the exact and asymptotic mean-field first-passage times per particle (from initial occupation number 0 to final occupation number k) for several system sizes at fixed density. The times are indeed independent of system size, provided that k is not close to N . The curvature visible in the plot shows that the growth is faster than exponential: indeed, asymptotically $\log(k!) \sim k \log k - k$, giving a logarithmic correction on a semi-log plot. For larger values of k , a different approach is needed; however, Arora *et al.* [19] showed that for $k = N$ the asymptotic result is $\tau_N^{\text{FP}} \sim V^N$, which coincides with the asymptotic behavior of our result when we put $V = N/\rho$.

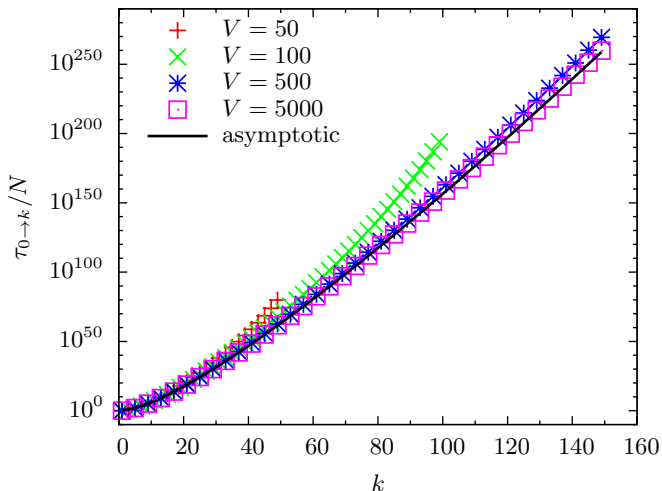


Fig. 1: Exact results for mean first-passage times $\tau_{0 \rightarrow k}$ per particle in mean field for different system sizes V , compared to the asymptotic result (11), as a function of the size k of the fluctuations. The mean density is fixed at $\rho = 1$.

Comparison between mean-field and spatial cases.

— The relation between the mean first-passage time τ_{k-1}^+ and the mean recurrence time τ_k^{rec} was derived in the mean-field approximation. Nonetheless, the following argument shows that it should also provide a reasonable approximation in the case of diffusive dynamics. If we start in S_k for a large k , then it is unlikely that we will add another particle to the distinguished site. Rather, after a waiting time, we will likely drop down to S_{k-1} , and from there most likely to S_{k-2} , and so on — that is, we can assume that once we have left S_k , we escape from there back to a “random” condition, from where the system will reach S_{k+1} via a first-passage process. Thus, conditioning on whether we stay in, or leave, S_k , we obtain

$$\tau_k^{\text{rec}} \simeq (1 \times \mathbb{P}[\text{stay}]) + (\tau_k^{\text{FP}} \times \mathbb{P}[\text{leave}]) \quad (12)$$

$$\simeq 1 + \gamma_k (\tau_k^{\text{FP}} - 1). \quad (13)$$

Neglecting the fast escape process, we obtain the same approximate relation $\tau_k^{\text{FP}} \simeq \tau_k^{\text{rec}} / \gamma_k$ as before, so that the mean-field result should also describe qualitatively the behaviour in the spatial case. This also explains why higher dimensions are closer to mean field: once the system has left S_k , it is much harder to return to it, since even if we choose a particle in a neighbouring site, it has many more ways not to return (probability $1 - (1/2d)$) than to return (probability $1/2d$) to the distinguished site.

Figure 2 compares the mean-field results to unbiased nearest-neighbour single-particle motion on “cubic” lattices with dimensions $d = 1, 2, 3$ and a fixed number of lattice sites. We see that the mean-field results reproduce very well the qualitative dependence of the first-passage time on k . Note that due to the very rapid increase in the first-passage time as a function of k , we are unable to

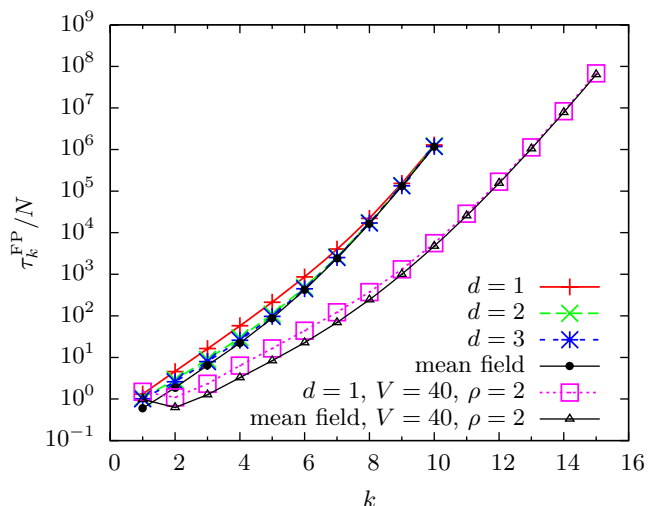


Fig. 2: Mean first-passage times τ_k^{FP} as a function of k for cubic lattices of spatial dimension $d = 1, 2, 3$, for system size $V = 729 = 27^2 = 9^3$ and density $\rho = 1$, compared to the mean-field result. Data are also shown for a 1D diffusive chain with $V = 40$, $\rho = 2$, and the corresponding mean-field result. Error bars are smaller than the size of the symbols, and lines are shown as a guide for the eye.

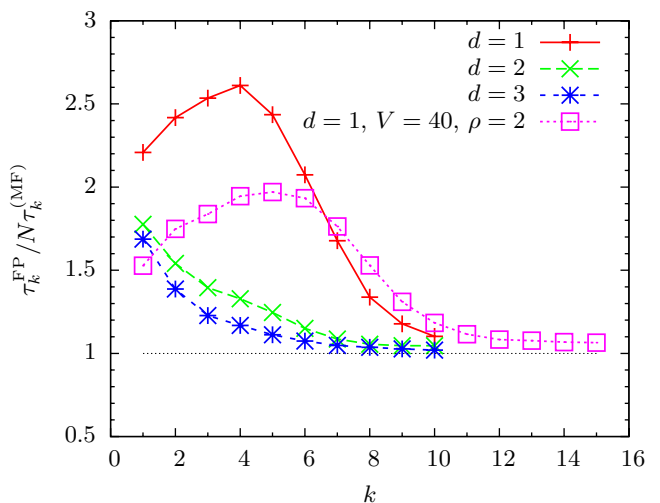


Fig. 3: The diffusive data of fig. 2, divided by the corresponding mean-field first-passage times for the same system parameters.

reach large values of k with brute-force simulations¹. We also show sample results for a higher density and smaller system size, for which larger values of k can be reached.

For a quantitative comparison, the ratio of the diffusive to mean-field results is shown in fig. 3. As expected, mean field is closer to the spatial results for higher spatial dimension. Surprisingly, for $d = 2$ spatial dimensions the mean-field result is also a *quantitatively* good estimate,

¹We have explored the possibility of using a more efficient algorithm along the lines of partial-path sampling [25] to evaluate these large first-passage times. Although these methods work very well for the mean-field case, for diffusive dynamics the strong spatial correlations present make their implementation a difficult task.

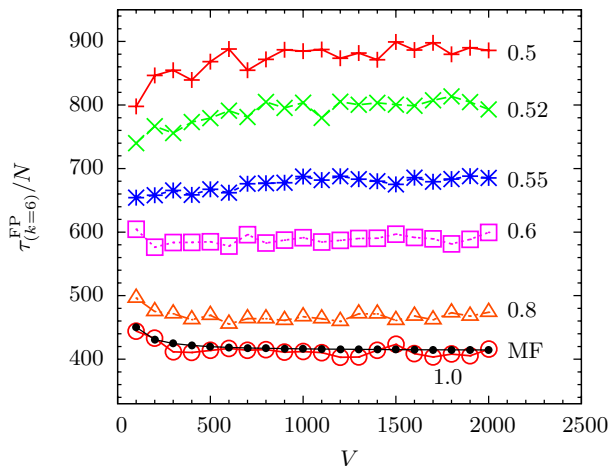


Fig. 4: Mean first-passage times per particle to occupation number $k=6$ at a distinguished site, on a 1D lattice as a function of system size V , for different values (labelled) of the bias parameter p , with density $\rho=1$. The mean-field (MF) result is shown for comparison (black dots).

provided the event is actually rare, *i.e.* for moderate k . Thus spatial correlation effects are very strong in 1D, but much less so in higher dimensions, in agreement with the above discussion.

Furthermore, in all cases, the mean-field results become increasingly accurate for larger k . This can be explained as follows. For small k , in the mean-field case, particles can arrive rapidly at the distinguished site from any part of the system and quickly cause the required fluctuation. In the diffusive case, however, the arrival of particles at the site is controlled by slow diffusive processes, for which the distance a particle is able to move in a time t scales only like \sqrt{t} . For large k , on the other hand, the first-passage event takes so long that each particle has enough time to explore the whole (finite) system by diffusion, and the problem is reasonably independent of the spatial details.

This independence can also be explained in terms of a recent result due to Condamin *et al.* [7]. Our many-walker problem can be mapped onto the motion of a single walker in an (Nd) -dimensional hypercubic domain with an appropriate target set. The result of ref. [7] shows that the first-passage time for the applicable case of “non-compact” exploration of the domain should depend rather weakly on the distance to the target, and hence on whether the dynamics is diffusive or mean field. We intend to explore this approach in future work.

Effect of bias. – To further study the relation between the spatial and mean-field cases, we studied in 1D the effect of the bias parameter p , which is the probability that a particle jumps to the right, always fixing $p+q=1$, so that the chosen particle always jumps. Figure 4 shows the result of varying p between 0.5 (symmetric case with no bias) and $p=1$ (totally asymmetric motion to the right). As p varies between these two extremes, the first-passage time curve interpolates smoothly between

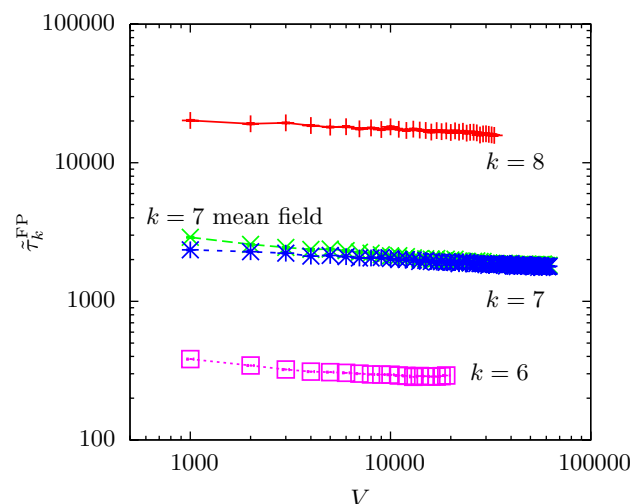


Fig. 5: First-passage times τ_k^{FP} , as a function of system size V , to reach occupation number $k=6, 7, 8$ anywhere in the system, starting from random configurations where no sites have this occupation number. Times shown are numbers of steps.

the symmetric and mean-field cases, with the numerical data falling on top of the mean-field curve for $p=1$. We can understand this as reflecting the decreasing influence of spatial correlations. When $p=1$, spatial correlations propagate to the right only, so that the incoming particles to the distinguished site have, in effect, no information about these spatial correlations, just as in mean field.

Fluctuations anywhere in the system. – Finally, we study the problem of the first-passage time τ_k^{FP} for *any* site in the system to reach occupation number k . Even in mean field, exact calculations for this case are very difficult: we are aware of solutions only for $V=2$ sites [22] and for the special case in which $k=N$ [19], *i.e.* in which all particles collect at one site, solved using a clever method which unfortunately does not appear to generalise to other values of k . Solving the case $k=0$ would yield an exact solution for zero-temperature glassy relaxation in the Ritort backgammon model [12,19].

Instead of an exact solution, we can relate this case to that with a distinguished site. The set of configurations \tilde{S}_k forming the rare event is now approximately V times larger than before, since configurations with k particles on *any* of the V sites are included in the event. The Kac method then shows that recurrence, and hence first-passage, times are approximately V times *smaller* than before. Alternatively, we can argue that the sites are roughly independent, with exponentially distributed first-passage times. The minimum of these times — the time until the first site reaches occupation number k — is then also exponentially distributed, with a mean V times smaller.

To test this, we plot in fig. 5 the first-passage time to reach occupation number $k=6, 7, 8$ somewhere in the system. In this figure, the times have *not* been divided by

N as in the previous graphs, and hence they correspond to ρV times the physical mean first-passage time to the event. Since in the distinguished case, for a fixed density, the times per particle converge to a constant as $V \rightarrow \infty$ (as seen, for example, in fig. 4), the above argument would imply that the raw total number of steps should converge to a constant in the current case. In fact, we see that the numerically-determined times decay slightly *faster* than the $1/V$ expectation, apparently by a small inverse power of V , the exponent of which is roughly independent of the value of k . (For $k=6$ the times are very short, and the apparent saturation is not relevant.)

This observation can be explained as follows. As the system size $V \rightarrow \infty$, configurations with k particles on some site are much more likely to occur. Each such configuration contributes 0 to the calculation of the mean first-passage time. However, the probability of lying outside the set \tilde{S}_k of such configurations decays exponentially with V . Including them in the calculation thus results in an exponential decay of the mean first-passage time with V , which merely measures the volume of \tilde{S}_k rather than the dynamics of the system, and for this reason we disallow such initial conditions. Nevertheless, as V grows, there is still an ever greater probability that some sites have occupation numbers *close* to k . These sites can be reached more easily by other particles, thus lowering the mean first-passage time from its expected $1/V$ behaviour.

Conclusions. – In summary, we have shown how the mean first-passage time to rare events in a many-particle random walk model depends on the system parameters. We found that the first-passage time to have k particles at a distinguished site grows asymptotically as $k!/\rho^k$ for the mean-field case, and we showed that this agrees increasingly well with the spatial results for increasingly rare events. We also showed how the results change for fluctuations anywhere in the system.

In the future, we intend to study the full probability distribution of first-passage times. A further interesting extension would be to study the statistics of first passage to large density fluctuations for diffusive processes on heterogeneous —*e.g.* scale-free— network structures.

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