Clearing out a maze: The hungry random walker and its anomalous diffusion

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We study chemotaxis in a porous medium using as a model a biased (“hungry”) random walk on a percolating cluster. In close resemblance to the 1980s arcade game Pac-Man®️, the hungry random walker consumes food, which is initially distributed in the maze, and biases its movement towards food-filled sites. We observe that, on the percolating cluster, the mean-squared displacement of the pacman process shows anomalous dynamics, which follow a power law with a dynamical exponent different from both that of a self avoiding random walk as well as that of an unbiased random walk.

The change in dynamics with the propensity to move towards food is well described by a dynamical exponent that depends continuously on this propensity, and results in slower differential growth when compared to the unbiased random walk.

Consider a random walker confined by a disordered environment of obstacles (see Fig. 1). Let the walker be free to move in the void space between the obstacles, with its movement biased to nearby places where it encounters a resource (“food”), which it then consumes. On a two-dimensional square lattice the sites of which are randomly blocked (with probability $1-p$), this process resembles the motion of Pac-Man®️ known from the famous 1980’s arcade game.

The unbiased random walk on such a lattice with obstacles is one of the simplest models for transport in porous media [1,2]. It is known to show “anomalous” dynamics, i.e. non-trivial power laws in the transport properties that are caused by the fractal structure of the accessible sites. When the probability for a site not to be blocked, $p$, crosses the critical probability $p_c$, a system-spanning (“percolating”) cluster of accessible sites first appears in the infinite system. The mean-squared displacement (MSD) of an unbiased random walker that is confined to the percolating cluster follows the asymptote $\delta r^2(t) \sim t^{2\nu}$ with an exponent $\nu < 1/2$ given by the walk dimension $d_w$, $\nu = 1/d_w$. For the 2D square lattice, $d_w \approx 2.878$ and $p_c \approx 0.592746$ [3]. (In the following we will reserve the term “random walk” to refer to this unbiased walk.)

Following a food bias resembles the chemotactic motion of bacteria in porous media. The dynamics of microswimmers in crowded environments of obstacles is of obvious importance for the physics of biological systems [4,5], and also for applications such as groundwater decontamination (where food to the bacteria is an unwanted pollutant) or microbial enhanced oil recovery (where microbes feed on long hydrocarbon chains, breaking them up into valuable light crude oil) [6]. Two aspects of bacterial motion are important in this context: the first is the bacteria’s starvation behavior, either because they die, or because starved bacteria tend to increase their efficiency in seeking food. The second is the interplay between anomalous diffusion and chemotaxis, in particular concerning the exploration (and subsequent clogging) of dead ends in the percolating structure. Lattice-based random-walk models of starving walkers have recently been discussed [7,8], albeit in the homogeneous medium. Our model focuses on the second aspect, the chemotactic exploration of the porous medium.

We model the motion as a discrete process on the lattice. At every time step, the walker at position $i$ has a probability to move to any of its allowed nearest-neighbor sites $j$ given by

$$p_{j \leftarrow i} = \frac{\exp F_j}{\sum_{k \sim i} \exp F_k},$$

(1)

where $F_k$ is the propensity to move towards food at site $k$, $F_k = 0$ if $k$ is blocked, and the sum runs over all nearest neighbor sites $k$. Initially, all accessible lattice sites are assigned a homogeneous propensity $F$. As the process evolves, food is removed from all the sites $j$ that

![FIG. 1. Sketch of the model. Blue squares are obstacles, small yellow circles are food and the large yellow symbol is the random walker (pacman).](image-url)
the walker encounters, setting $F_0 = 0$. This describes a non-Markovian transient process that clears out an increasingly large portion of the accessible space. In this sense, it is a near-sighted version of Pac-Man®. (We do not attempt to model the behaviour of a human player who would bias his steps based on the known structure of the maze [10].)

At first glance, the model is quite similar to generalizations of the self-avoiding walk (SAW). In the SAW the walker is free to move to any not-yet visited site, but never allowed to revisit an already encountered site. On a lattice without obstacles (free SAW), its MSD grows as $\delta r^2(t) \sim t^{2\nu}$ with an anomalous exponent $\nu_{\text{SAW}} > 1/2$, i.e. faster than the free random walk. In 2D, $\nu_{\text{SAW}} = 3/4$ has been conjectured as the exact value [11] [12]. The SAW on the percolating cluster is a model for linear polymers in heterogeneous media. Its exponent $\nu_{\text{pcSAW}}$ is larger than that of the free SAW [13], specifically $\nu_{\text{pcSAW}} \approx 0.78$ in 2D [14] [15]. Thus, while the random walk slows down when constrained to the percolating cluster, the SAW speeds up.

Variants of the SAW that merely suppress repeated visits to the same site instead of disallowing them are quite similar to our model [1]. They have been termed “true” [10] or myopic self-avoiding walks [17]. On the percolating cluster, their MSD are also found to grow faster than that of the random walk [13] [20].

The surprising result from our simulations is that the MSD of the hungry walker on the percolating cluster grows less efficiently than that of the random walker at long times: it is described by a different walk dimension $d_{\text{pcman}}$ that is larger than that of the unbiased random walk, $d_w$ (i.e. by an exponent $\nu_{\text{pcman}} < 1/2.878$).

We have performed Monte Carlo simulations of the process described by Eq. (1). Random matrices for $p = 0.592746$ were created with lateral dimensions between $L = 10000$ and $L = 25000$, and periodic boundary conditions were employed for the trajectories. Wrapping site-percolating clusters were identified by the Hoshen-Kopelman algorithm [21]. The random walks were started on a random location on the (largest) percolating cluster, and results are typically averaged over 90000 runs of up to $5 \times 10^5$ steps each (using $N = 100$ walks with random starting points on each of $M = 900$ matrix realizations). Jump probabilities are calculated by keeping track of already visited sites in a hash table [22]. We have checked for finite-matrix-size effects in some runs up to $10^{10}$ steps [23] and in matrices with sizes up to $L = 120000$. The robustness of our long-time extrapolations was checked to be compatible with a few runs up to $10^{12}$ steps for $F = 10$.

Figure 2 shows the MSD obtained for walks on the percolating cluster with different food propensities. The case $F = 0$ (random walk) is included for reference. It displays the expected asymptotic law $\delta r^2 \sim t^{2/d_w}$. The MSD with $F > 0$ increase faster initially: After the first step, the walker remains strongly biased towards exploring new sites. Indeed, for large $F$, the initial increase in the MSD is $\sim t^{2/d_w}$, the power law expected from the free SAW, since at short times, the fractal structure of the percolating cluster is not yet explored. After this transient, anomalous subdiffusion manifests itself. Remarkably, the power-law increase of the $F > 0$ curves is slower than that of the $F = 0$ reference. Up to the longest time accessible in our simulations, $t = 10^{10}$, the MSD for $F = 10$ appears to be well described by a power law $\delta r^2 \sim t^{2/d_{\text{pcman}}}$ with an exponent $d_{\text{pcman}}$ that is larger than $d_w$. This is emphasized by the dash-dotted line in Fig. 2 that represents the power-law with $d_{\text{pcman}} = 3.03$, the exponent that best describes our $F = 10$ data.

The power-law growth becomes clearer when looking at the logarithmic derivative of the mean-squared displacement, $\alpha(t) = d \ln \delta r^2/d \ln t$. If the SAW follows a power law, $\alpha(t)$ is a constant and its value is the power-law exponent. As shown in Fig. 3, the effective exponent $\alpha(t)$ for $F = 10$ indeed remains close to $2/d_{\text{pcman}}$, and stays significantly below the value $2/d_w$ expected for $F = 0$, over 6 orders of magnitude in time. Remarkably, the thus estimated exponent $d_{\text{pcman}}$ is close to the known value of the dynamical critical exponent for the random walk, $z \approx 3.036$, obtained from the all-cluster averaged MSD [3] (i.e. for a set of walkers that starts out on any non-blocked site rather than just the sites of the percolating cluster). Recall that for the latter, trajectories contribute that eventually localize, with a weight given by the cluster-size distribution [24] [25]; this leads to $z = 2d_w/d_f$ in 2D, where $d_f = 91/48$ is the fractal dimension of the percolating cluster.

Our finding can be rationalized by the following con-
jecture: any random walk on the percolating cluster will perform random excursions that leave the backbone of the cluster and explore culs-de-sac out of which the process has to return. These culs-de-sac are dangling clusters that have a fractal size distribution (the same as the overall cluster size distribution \[25\]). While the random walk on the percolating cluster sees some effect of these dangling clusters, the effect of food bias is to draw the walker more deeply into any cul-de-sac whose entrance it randomly samples. Thus, over sufficiently long time scales, the “pacman” process will perform excursions that slow down the overall growth of the MSD as compared to the random walk.

That the dangling ends have an effect on the walk dimension is known from the case of the random walk in 2D. If the walker is restricted to explore only the backbone of the percolating cluster, \(d_{wb}^{gb} \approx 2.70 < d_w\) \[26\], i.e., the MSD grows faster than on the full cluster. \[27\]

To further test whether the pacman dynamics is indeed described by a power law with an exponent different from \(d_w\), let us discuss the number of distinct sites \(S\) visited by the walker as a function of time. For a random walk that is homogeneous, ergodic, and fulfills detailed balance, one expects this number to scale with the dimensionality of the available space, i.e., \(S \sim R^{d_w}\) for a walk of typical lateral extension \(R\). The left panel of Fig. 4 reveals that for times \(t > 10^7\) and up to at least \(t = 10^{12}\), the quantity \(S\) grows faster than \((\delta r^2)^{d_f/2}\). Since \(S \sim R^{d_f}\) is an upper bound for the growth law, this implies that (at least in this time window) the MSD is not a good indicator of the typical area covered by the walk. A possible explanation in line with our rationale of the slower growth observed in the MSD is that indeed, the pacman process first traverses the dangling ends of the percolating cluster in a low-dimensional fashion similar to a SAW, followed by a more space-filling exploration of the dangling ends that leads to the faster growth in \(S\) with \(\delta r^2\) that we observe. Since dangling ends have a power-law size distribution, a power-law-like increase in \(S\) results.

Still, the observed behavior in \(S(\delta r^2)\) might suggest a cross-over to ordinary random-walk dynamics at times much larger than those that we can access in our simulation, and that the values of \(\alpha(t)\) discussed in Fig. 3 are the result of such a cross-over. We therefore present a further estimate of \(d_{gb}^{pacman}\) based on the growth of \(S\). Following an argument by Leyvraz and Stanley \[28\], consider the average number \(G\) of possible growth sites for \(S\) at a given time, i.e., the average number of unvisited nearest-neighbor sites. Since \(G\) only changes when \(S\) changes, one would estimate \(dG/dS \sim S^{-1/2}\) if \(G\) were composed of identically independently distributed random increments. Assume that relevant correlations (introduced both by the structure of the percolating cluster and by the non-Markovian jump rates) change this to \(dG/dS \sim S^{-x}\) with some \(x \neq 1/2\). The rate of increase in the number of sites visited \(S\) will scale with the prob-
ability to step onto a growth site; one thus estimates $S/(dG/dS) \sim t$, which is well fulfilled by our numerical data. Assuming now that asymptotically, $S \sim t^{d_f/d_{w}}$, plus corrections to scaling that are likely to cancel out in $S/(dG/dS)$, we get $\mu(t) = t \, dG/dS(t) \sim t^{d_f/d_{w}}$, where $d_{w} = d_f(1+x)$ is the walk dimension of the process to be determined. We estimated $dG/dS$ by counting the average number of unvisited nearest-neighbor sites seen at every step, and show $\beta(t) = \mu(t)^{1/d_f} / t^{1/d_{w}}$ in the right panel of Fig. 4. The lower set of curves assumes $d_{w} = 2.878$ and $z \approx 3.036$. Error bars indicate standard deviations from different realizations for the fixed time interval.

Since there is no obvious intrinsic time scale characterizing the $F$-dependence of the motion, the observed exponent itself can change continuously with $F$. In Fig. 5 we show the values of $\alpha(F)$ estimated from our simulations, obtained by averaging the logarithmic derivatives of the MSD for times $t \gtrsim 1.4 \times 10^7$. The values depend somewhat on the time window chosen for averaging, but the continuous increase from $F = 0$ to $F \to \infty$ is robust. Such a continuously changing exponent is best rationalized by observing that the efficiency with which the walker is drawn into the culs-de-sac also depends on $F$. As $F$ increases, the size-distribution of dangling ends is probed with a weight function that depends on $F$. In this respect, our model differs from, e.g., the change in universality classes incurred by a change in microscopic dynamics in the three-dimensional Lorentz model [29].

Our statement that this kind of model shows a continuously changing exponent, is also supported by the case of the hungry walker on the one-dimensional lattice with an absorbing boundary at the origin, for which the survival probability has been shown to scale as a power law in time, with an exponent that depends on $F$ [30].

In summary, we have studied a model for chemotaxis in a random medium that resembles the game Pac-Man®: the non-Markovian random process of moving a food-consuming (hungry) walker on the percolating cluster on a 2D square lattice. It shows anomalous sub-diffusion that is well described by a propensity-dependent dynamical exponent. Its mean squared displacement follows a power-law that is slower than that of the unbiased walker. For increasing $F$, the walker initially moves farther from the origin than the random walk, but then becomes less effective in exploring area. We argue that this results from the fact that the hungry walker “gets lost” in the culs-de-sac: it tends to explore the dangling ends of the percolating cluster in more depth than the unbiased walker. Qualitatively, this matches the observation that chemotactic bacteria tend to get stuck in the “dead zones” of porous media. The dependence of the dynamics on food propensity is better described by assuming a $F$-dependent exponent, rather than by a cross-over behavior between two fixed power laws. Our model hence provides a simple example of continuously changing dynamical exponents.

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