

Superdiffusion in a Model for Diffusion in a Molecularly Crowded Environment

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Abstract

We present a model for diffusion in a molecularly crowded environment. The model consists of random barriers in percolation network. Random walks in the presence of slowly moving barriers show normal diffusion for long times, but anomalous diffusion at intermediate times. The effective exponents for square distance versus time usually are below one at these intermediate times, but can be also larger than one for high barrier concentrations. Thus we observe sub- as well as super-diffusion in a crowded environment.

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I. INTRODUCTION

One of the important issues in biology is to understand how diffusion is affected by the environment. This understanding is needed to correctly describe the passive intracellular transport as this process may regulate important cellular properties: signal transduction [1], gene transcription [2], kinetics of reactions [3] and regulation of cell polarization [4].

The interior of biological cells [5] represents a very dense and crowded environment with a specific molecular mobility. Intracellular diffusion is hindered by barriers consisting of large molecules sometimes even immobile tethered large molecules, binding and collisional interactions. One way of interpreting such a system is to view it as a disordered system. In general for random walks [11] in media with disordered microscopic substructures one expects anomalous diffusion [6, 7, 8] where the mean-square displacement $\langle \Delta \mathbf{r}(t)^2 \rangle$ no longer is proportional to the time t :

$$\langle \Delta \mathbf{r}(t)^2 \rangle = C_\alpha t^\alpha \quad (1)$$

with $C_\alpha > 0$. If $0 < \alpha < 1$ then we call the diffusion sub-diffusive, and if $\alpha > 1$ super-diffusive; normal diffusion has $\alpha = 1$. In biological systems as well as for models of biological system, so far only sub-diffusive behavior has been observed [6] except if the transport is facilitated or restricted. For example if the diffusion is directed by a motor protein, non-random super-diffusion can be observed but not for free diffusion. However, super-diffusion has been observed in a two-dimensional complex plasma [9] and in two-dimensional Yukawa liquids [10]. Thus super-diffusion does exist and its existence in the cell needs to be discussed.

Sub-diffusion occurs if the mobility of diffusing particle or molecule is impaired by obstacles (mobile and immobile) or attractive forces. Under these premises it seems unlikely to find super-diffusion.

From a physical point of view the disorder in the cell has a characteristic time scale. If the diffusing particle has diffused long enough, such that the time scale has been explored, one expects normal diffusion. If there is no characteristic time (in fractal media) then the diffusion is always anomalous [8]. However, this picture does not take into account the (im)mobility, collision, attractive forces etc. To study the effect produced by immobile as well as mobile barriers we have developed a model mimicking the molecularly crowded environment with mobile as well as immobile barriers taking into account particular length

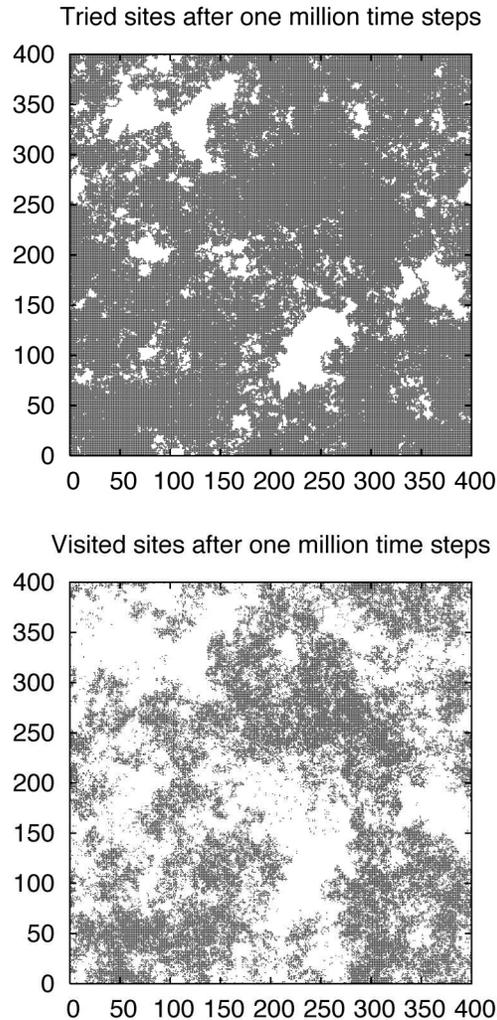


FIG. 1: Illustration in small square lattice: Tried (part a) and visited (part b) sites after one million time steps.

scales.

II. THE MODEL

In percolation theory [12], each site on a large lattice is randomly either occupied, with probability p , or empty, with probability $1 - p$. For percolative diffusion, a random walk starts on an occupied site and then on each time step selects randomly a direction to move to. It actually moves one unit distance (lattice constant) into this direction if that neighbor site is occupied. Empty sites are prohibited for the walker. For $p < p_c$ the walk can extend

$d \log \langle r^* r \rangle / d \log t$; $d = 2$, $a = 0.5$, $p_c - p = 0, 0.1, \dots, 0.5$

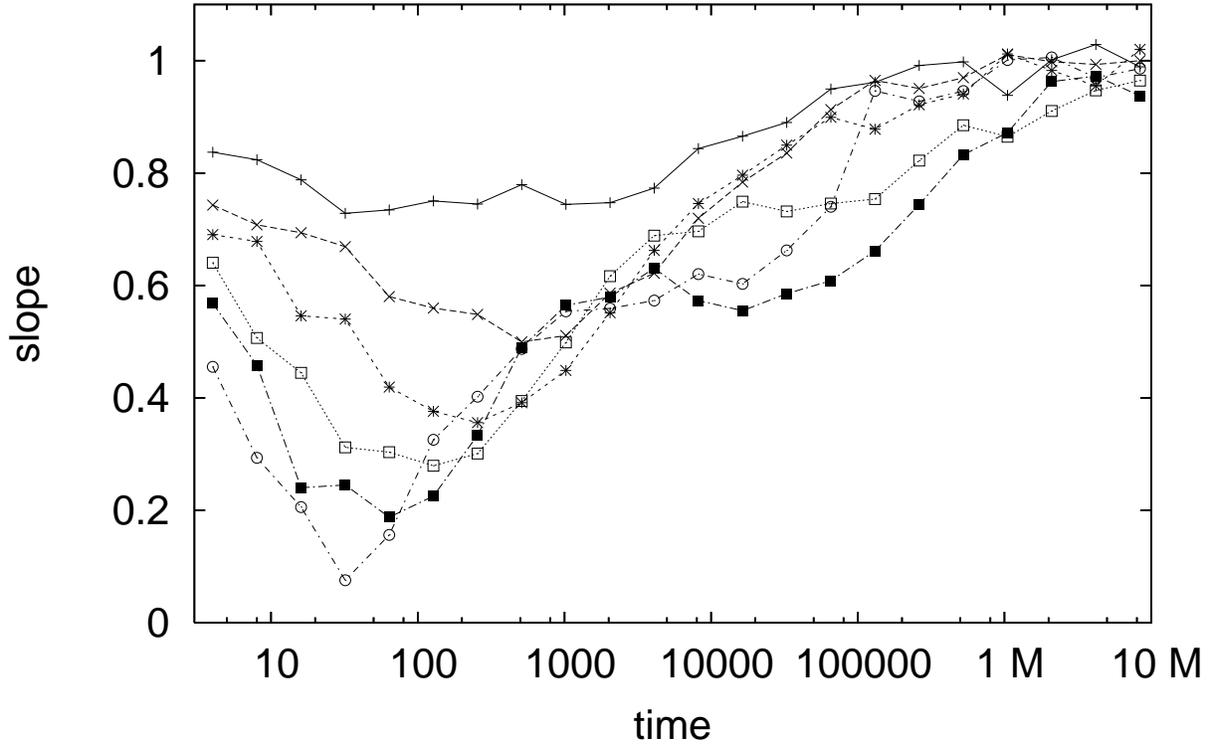


FIG. 2: Effective exponent for 8000 walks on 7001×7001 , $a = 1/2$, $A = 0.01$. The concentration p of allowed sites decreases from top to bottom: $p_c - p = 0$ (+), 0.1 (\times), 0.2 (stars), 0.3 (open squares), 0.4 (full squares), 0.5 (circles).

only over the finite cluster in which it started, while for $p > p_c$ it can diffuse towards infinity if it started on the infinite cluster. Right at $p = p_c$ anomalous diffusion takes place with a mean square distance increasing to infinity but with an exponent $\alpha < 1$ [12].

In biological applications, the prohibited sites may be more or less mobile biomolecules. Their effect can be taken into account approximately by assuming that also a prohibited site i allows the walker to move through, with some probability q_i . The reciprocal probability $1/q_i$ then can be interpreted as the lifetime of the barrier, in the sense that about once during that lifetime the barrier moves away for one time step before returning to that site. Thus we have still a quenched disorder; with annealed disorder where all lifetimes are the same, we have normal diffusion, squared distance proportional to time, with a diffusivity reduced by the (slowly) moving barriers. We now assume that the probability distribution

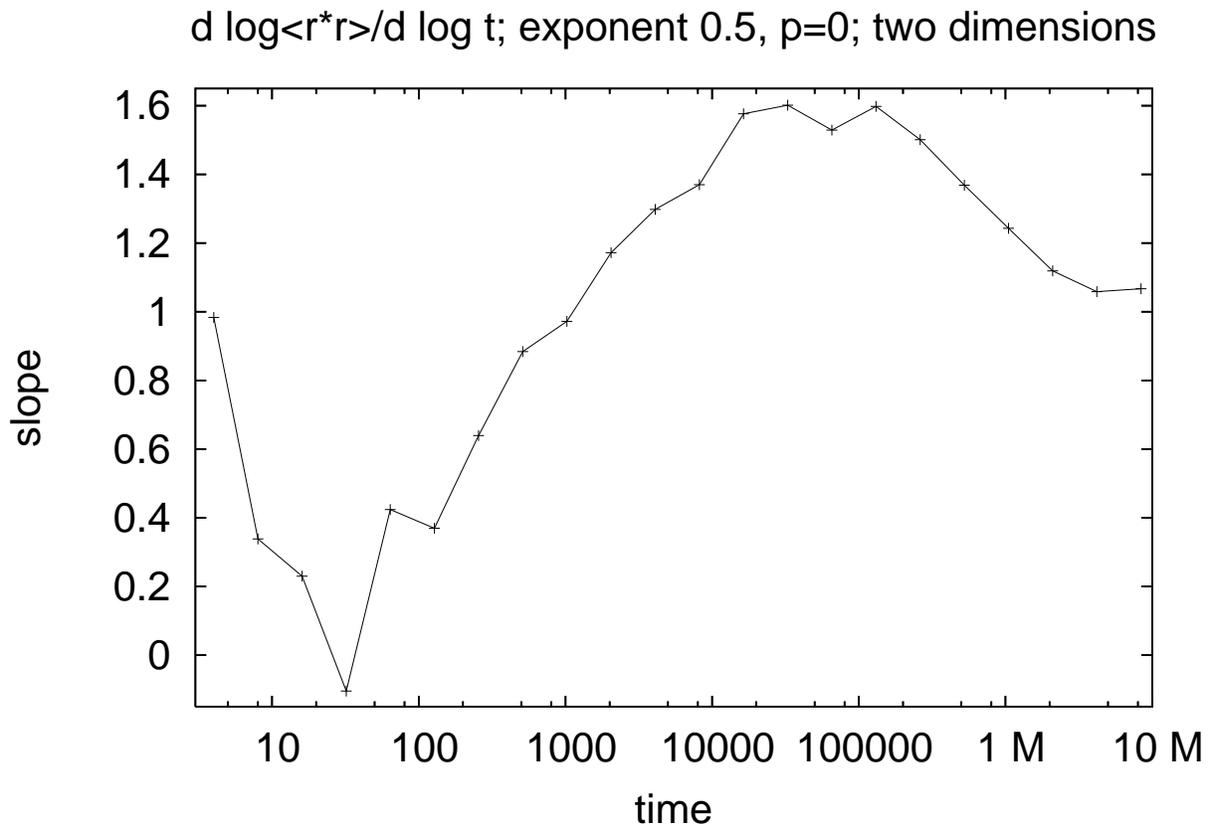
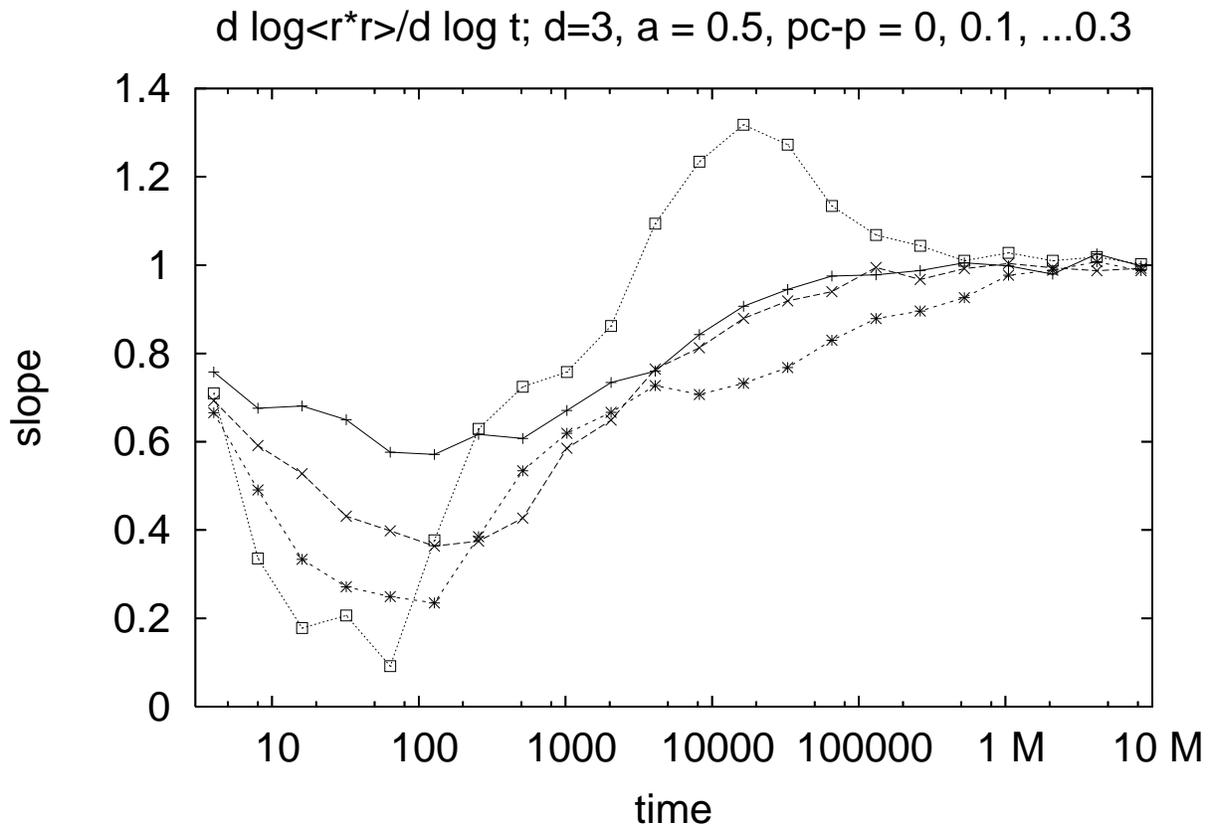


FIG. 3: Effective exponent for 8000 walks on $401 \times 401 \times 401$ (part a, symbols as in Fig.2) and 7001×7001 , (part b); $a = 1/2$, $A = 0.01$. 5

30,000 (+) and 8,000 (x) walks, $d = 3$, $p\text{-pc} = 0.3$

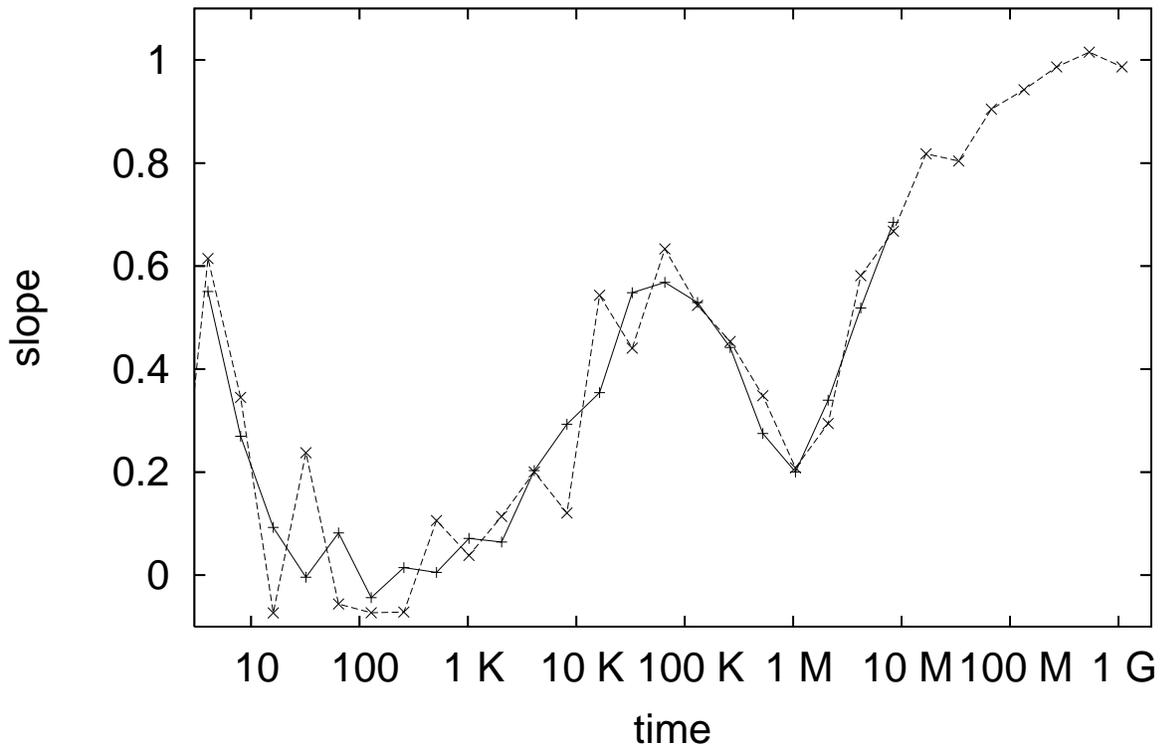


FIG. 4: As Figure 3 but $A = 0.0001$ and better statistics or longer times.

function $f(q)$ for the q_i is a power law,

$$f(q) \propto 1/q^a \quad (2)$$

with some exponent a between zero and infinity. More quantitatively, for each prohibited site we determine, when it is visited for the first time by the walker, a random number r , homogeneously distributed between 0 and 1, and then fix q_i for that site i as

$$q_i = Ar^{1/(1-a)} \quad (3)$$

with some free parameter A .

III. RESULTS

Figure 1 illustrates for two dimensions at $p = p_c - 0.5 = 0.0927$ and exponent $a = -1/2$ the results of one walk after one million time steps. Part a shows the set of sites which

have been tried at least once, and part b shows those sites which have actually been visited inspite of the barriers. After 8 million steps, all sites were tried, and after 64 million steps, all sites were visited. One can get anywhere, provided one has enough time.

For 7001×70001 square lattices, where $p_c \simeq 0.593$, our simulations show for $A = 0.01$ and 0.0001 that the squared distance is a complicated function of the time. (For $A = 1$ and $a > 1$ the q_i are larger than one which makes little sense, and for $a = 0$ and 0.5 at $A = 1$ the squared distances are close to $t/2$; not shown.) We thus look for smaller A at the slopes in the log-log plots, i.e. at the effective exponents

$$\alpha_{\text{eff}} = d \ln \langle \Delta \mathbf{r}(t)^2 \rangle / dt. \quad (4)$$

In each case we simulate $p = p_c, p_c - 0.1, p_c - 0.2, \dots$ down to $p_c - 0.5 \simeq 0.093$. We see for short times different slopes in our log-log plots, but for long times the effective slopes approach unity: Normal diffusion with mean squared distance proportional to time. For $a = 2$, for an exponentially decaying distribution $f(q)$, and for a Weibull distribution (stretched exponential) the time variations of the effective exponents were similar but less pronounced.

Experimentally more relevant are three instead of two dimensions, and some results are shown in Figure 3 a, rather similar to two dimensions in Figure 2. Now $p_c = 0.3116$. For very small $p = 0.0116$, squares in Figure 3, we see an overshooting with an effective exponent α_{eff} above unity at intermediate times; this is not a statistical fluctuation and shows up in all 20 simulated samples (not shown). It also was seen in two dimensions at very low p , Figure 3 b. One may call this effect superdiffusion since for more than one order of magnitude the exponent is above unity.

Basically, the positive probability of each barrier to move away and to let through the random walker means that for sufficiently long times we always get normal diffusion, $\alpha = 1$. For times which are not long enough to see this moving-away of the barriers, but long enough for the walker to explore the whole finite cluster for $p < p_c$ on which it started, we have $\alpha = 0$. For our moderately small $A = 0.01$ these different regimes cannot be reliably separated; that works better for much less mobile barriers: $A = 0.0001$ in Figure 4. There the effective exponents are about zero for $t \sim 10^2$, show a maximum but no longer overshooting below $t \sim 10^5$, and approach unity above $t \sim 10^8$.

IV. DISCUSSION

In summary, we see a non-monotonic variation of the effective exponents with time, showing both subdiffusive and superdiffusive behavior. Asymptotically, however, the exponent always seems to approach unity for $t \rightarrow \infty$. In experiments with more limited variation of times, this variation of α_{eff} with time could wrongly be interpreted as asymptotic subdiffusion or asymptotic superdiffusion; long times [13] are needed.

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