# Diffusion and drift in a medium with randomly distributed traps

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The long-time properties of biased diffusion in media with randomly distributed traps is discussed. For any bias the asymptotic decay is exponential, contrary to the unbiased case. We find a sharp transition between a small-bias behavior, for which particles are effectively localized, and a large-bias behavior, for which the particles drift with the bias.

The problem of diffusion in a medium with randomly distributed traps serves as a model for processes occurring in a number of contexts. While it is by now a classical model[1] for diffusion-controlled chemical reactions, it appeared only relatively recently in solid-state physics.[2]

Denote by $\rho_c(\vec{r},t)$ the density of particles of type $C$ which diffuse in a medium with a particular realization of a random distribution of particles of type $S$ (sinks). Particles $C$ are trapped on particles $S$. One is interested in $n_c(\vec{r},t) \equiv \langle \rho_c(\vec{r},t) \rangle_s$ which is the number of particles not yet trapped, at time $t >> 0$, averaged over all trap distributions. Naively, one could expect that $n_c(t)$ decays exponentially at long times. It was only very recently that this was found to be false.[3,4] In fact, we have shown[4] that at long times the decay is described by the following behavior:

$$n_c(t) \sim \exp(-\mathrm{const}\, t^{d/d+2}) \quad , \tag{1}$$

where $d$ is the spatial dimensionality. The physical reason for this behavior is that at long times the surviving particles are in large trap-free regions. These regions are rare; their probability of occurrence goes like $\exp(-n_s V)$ where $n_s$ is the average trap concentration and $V$ the volume of the region. However, the survival probability is so strongly enhanced that regions with diameter $l \sim (Dt/n_s)^{1/d+2}$ contribute dominantly to the particle number $n_c(t)$, leading to Eq. (1).

In the present Brief Report we discuss the modification of this behavior when a drift term is added to the diffusion equation. We were intrigued by some statements[3,5] in the literature, concerning the behavior in one-dimension (1D) [where an $\exp(-t^{1/3})$ behavior has been known for a while], that a constant drift term restores an exponential decay, *if the drift velocity exceeds a threshold value.* The above explanation of Eq. (2) suggests that this would be wrong. Any nonzero constant drift should lead to exponential decay, as we argue below. However, we have found an interesting transition in the average drift velocity as a function of the bias field, and we wish to report this observation here.

We first argue that the decay is exponential for any value of the bias field. The physics is as follows: A particle which happens to be in a trap-free region of diameter $l$ has two essential pathways for survival. Either it resists the drift motion and stays in its region or it lets go with the drift. Both pathways lead to exponential decay, but with different decay constants. If the particle stays in the trap-free region, its decay would be governed by the solution of a Fokker-Planck equation

$$\left( \frac{\partial}{\partial t} - D\nabla^2 + \vec{v}\cdot\vec{\nabla} \right) \rho_c(\vec{r},t) = 0 \quad , \tag{2}$$

with effective boundary conditions $\rho_c = 0$ on the boundary of the trap-free region. Here $\vec{v}$ is the drift velocity in a trap-free medium. The asymptotic decay is governed by the lowest eigenvalue $\epsilon_0(\vec{v})$ of the correspondent eigenvalue problem $[-D\nabla^2 + \vec{v}\cdot\vec{\nabla} - \epsilon(\vec{v})]\rho_c = 0$, which can be written as

$$\left[ -D\left( \vec{\nabla} - \frac{\vec{v}}{2D} \right)^2 + \frac{v^2}{4D} - \epsilon(\vec{v}) \right] \rho_c = 0 \quad . \tag{3}$$

From this, one sees immediately that the $\epsilon_n$'s are shifted up as

$$\epsilon_n = \epsilon_n(\vec{v}=0) + v^2/4D \quad . \tag{4}$$

The contribution to $n_c(r,t)$ at long times comes from large trap-free regions. Since $\epsilon_0(\vec{v}=0) \rightarrow 0$ in large regions, $n_c(\vec{r},t)$ would decay as

$$n_c(\vec{r},t) \sim n_c(\vec{v}=0,t)\exp(-v^2 t/4D) \quad . \tag{5}$$

On the other hand, if the particles roam out of the trap-free region, we expect the decay to be governed by the mean-field behavior. In a three-dimensional continuum model with perfect spherical traps, this is Smoluchowski theory corrected for the drift. The effect of one single trap is described by Eq. (2) with boundary condition

$$\rho_c(\vec{r}) = \begin{cases} 0, & \text{for } |\vec{r}| = a \\ \rho_c(\infty), & \text{for } |\vec{r}| \rightarrow \infty \end{cases} \quad . \tag{6}$$

By expanding $\rho_c$ into spherical harmonics, one obtains for the flux into the trap

$$J = 4\pi\rho_c(\infty) D a f\left(\frac{va}{2D}\right) , \tag{7}$$

with

$$f(x) = \frac{\pi}{2x}\sum_{l=0}^{\infty}(-1)^l(2l+1)\frac{I_{l+1/2}(x)}{K_{l+1/2}(x)}$$
$$\approx \begin{cases} 1 + x - x^2/3 \pm \cdots , & x \ll 1 \\ x/2 , & x \gg 1 \end{cases} . \tag{8}$$

($I_n$ and $K_n$ are spherical Bessel functions.) Assuming that this calculation is not invalidated by the existence of other traps, this leads to an asymptotic decay

$$n_c(t) \sim e^{-kt} , \tag{9}$$

$$k \approx \begin{cases} 4\pi n_s a D + 2\pi n_s a^2 v - \cdots , & v \ll D/a \\ \pi n_s a^2 v , & v \gg D/a \end{cases} . \tag{10}$$

In $d$ dimensions and/or with other (e.g., lattice) specific models, we generally expect the mean-field behavior to be

$$k \propto \begin{cases} n_s a^{d-2} D, & v \ll D/a \\ n_s d^{d-1} v, & v \gg D/a \end{cases} . \tag{11}$$

Thus both pathways lead necessarily to exponential decay without threshold. However, another kind of transition becomes now apparent: At small velocities $\vec{v}$, the decay (5) is slower and therefore advantageous for "survival strategy." For large $\vec{v}$ the behavior, respectively, (10) and (11), is advantageous. As behavior (5) is associated with roaming within the trap-free cavities, we expect that the mean velocity $\vec{v}_{av}$ of a cluster of particles would be zero. If the velocity $\vec{v}$ is large, such that the second behavior is dominating, the cluster velocity $\vec{v}_{av}$ should be of the order of $\vec{v}$. We should stress that here $\vec{v}_{av}$ is *not* the average velocity of individual particles in this cluster, but the mean rate of change of its center of gravity. The difference between these two arises due to the higher absorption rate of the faster moving particles. A critical velocity $v_{cr}$ is determined by the conditions $k = v^2/4D$ or

$$v_{cr} \sim D(n_s a^{d-2})^{1/2} . \tag{12}$$

At asymptotically large times, a sharp transition in mean behavior is expected then at $v_{cr}$.

At large but finite times, this transition is, of course, smoothed out. It is also shifted towards a somewhat smaller value of $v$, since for finite time $t$ the decay for $v < v_{cr}$ is governed by Eq. (4), with

$$\epsilon_0(\vec{v}=0) \propto D n_s l^{-2} \propto D\left(\frac{n_s}{Dt}\right)^{2/d+2} , \tag{13}$$

where $l$ is the typical diameter of trap-free regions contributing at time $t$.

We found this predicted behavior sufficiently interesting to look for it in Monte Carlo simulations. The two-dimensional model used was the same as in Ref. 4. A drift motion along the diagonal was generated by choosing the probabilities for steps in the positive $x$ and $y$ directions to be $(1+p)/4$, and those for steps in the negative directions to be $(1-p)/4$.

Figure 1 shows the results of runs with several values of $p = v\sqrt{2}$, each consisting of $\sim 10^2 - 10^3$ walks of 800 steps. The exponential decay was approximately compensated by adding a first-order birth process with a suitable rate. In Fig. 1(a) we show the observed effective decay constant $k$, averaged over $400 < t < 800$ as a function of $v$. The continuous curve is the parabola $v^2/4D + \epsilon_0(v=0)$, with $\epsilon_0$ chosen such as to fit the data at small $v$. The parabola cuts the linear function (10) at $v \simeq 2$. *At the same point* we observe a dramatic change in the function $v_{av}$ shown in Fig. 1(b). This is the transition indicated in the above discussion.

Four final comments are in order: (i) The asymp-

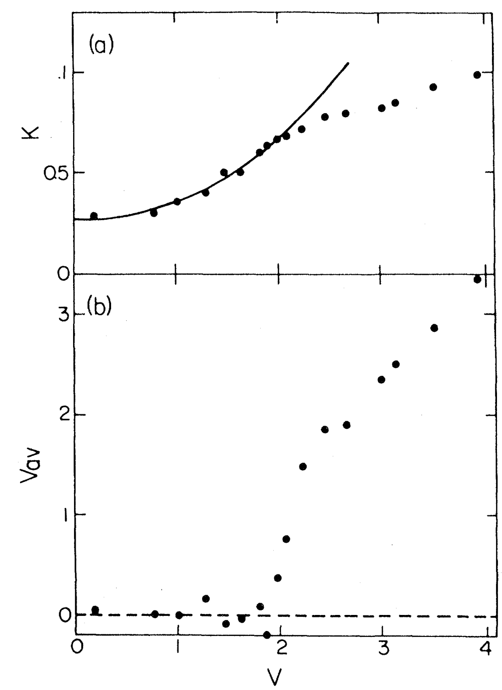


FIG. 1. Transition in observed behavior. (a) Observed decay rate as a function of the bias. The quadratic curve is the theoretical prediction for small $v$. The points, resulting from Monte Carlo simulation, show the transition to a different behavior at higher-bias value. (b) Observed transition in the average cluster velocity as a function of the bias. The points come from the same Monte Carlo simulation. Note that the transition occurs at the same value of the bias in panel *a*.

totic behavior can be found exactly in one-dimension, assuming perfectly absorbing pointlike traps. Using the method of Ref. 4 we find indeed

$$n_c(t) \sim n_c(t;v=0)\exp[-(v^2/4D)t]$$

for all velocities (there is no analog to the mean-field behavior in this model). (ii) The phenomena discussed in this report is reminiscent of the breakdown of Anderson localization[6] in a strong applied electric field. (iii) In an ac electric field, the particle number should decay according to Eq. (2) for sufficiently large $t$, when the drift length is smaller than the diameter $l$ of the dominating trap-free regions. (iv) Our discussion deals with the very long-time tail of $n_c(t)$. It is thus not directly related to measurements of mean trapping times of carriers in electric fields.[5]

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[1]M. V. Smoluchowski, Phys. Z. 17, 557, 585 (1976).

[2]P. M. Richards, Phys. Rev. B 20, 2964 (1979); M. Nechtstein *et al.*, Phys. Rev. Lett. 44, 356 (1980).

[3]B. Movaghar, G. W. Sauer, and D. Würtz, J. Stat. Phys. 27, 473 (1982).

[4]P. Grassberger and I. Procacica, J. Chem. Phys. (in press).

[5]D. Haarer and H. Möhrwald, Phys. Rev. Lett. 34, 1447 (1975).

[6]P. W. Anderson, Phys. Rev. 109, 1492 (1958).