Diffusion in disordered media as a process with memory

Michele Vendruscolo[1] and Matteo Marsili[2]
[1] Istituto Nazionale per la Fisica della Materia (I.N.F.M.) and International School for Advanced Studies (S.I.S.S.A.), Via Beirut 2-4, 34014 Trieste, Italy
[2]Institut de Physique Téorique, Université de Fribourg, CH-1700 Fribourg, Switzerland
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The problem of a random walk in disordered media is mapped into a model of a random walk with memory. The latter model, as opposed to the former one, does not make reference to a particular realization of the disorder. The equivalence of the two models implies that the latter model retrieves dynamically a realization of disorder; the only one which is consistent with its dynamics. In this latter approach to the dynamics in disordered media, effects of memory, aging and the peculiar localization properties of the random walker, appear quite natural. [S1063-651X(96)50808-1]

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The dynamics of disordered systems is a very active subject of research of statistical physics. In nonequilibrium systems, such as driven interface growth [1] and charge density waves, [2] disorder leads to very interesting effects, such as depinning transitions, creep phenomena, and self-organization. In out of equilibrium systems, like spin glasses, aging effects arise which, at least at a mean field level, has been related to the lack of time translational invariance and the failure of fluctuation dissipation relations [3]. The main complication brought by the presence of disorder is that, in order to compute a physical quantity, apart from the ''dynamic'' average over different stochastic time evolutions, quenched dynamics requires a second average over the realizations of disorder. This, operationally, implies that one has to evolve the system in several disorder configurations and at the end average the result over the realizations of disorder. On one hand, the dynamics explicitly depends on the particular realization of the disorder (typically through transition rates). On the other, in most systems, one expects the physical quantities to be self-averaging and therefore to depend weakly on the disorder configuration. This situation is rather unsatisfactory, in our opinion, because only after this second average over disorder it is possible to appreciate the general features of the dynamics. It has recently been pointed out [4] that this problem can be overcome in nonequilibrium models based on extreme dynamics, by appealing to an annealed dynamics (we shall use this term as opposed to quenched dynamics) which does not make reference to a particular realization of disorder. The advantage of this point of view is that only the average over different stochastic time evolutions needs to be taken: the effective dynamics is indeed such that the averages over disorder are taken in ''run time,'' i.e., at each time step, by the process itself. Moreover, this approach provides also the statistical weight of the history of the process, which is hardly available in dynamics with disorder. The key point, in the derivation of such annealed dynamics, is that the future evolution has to be statistically consistent with the past history. The mathematical translation of this principle relies on the concept of conditional probability. The process thus acquires time dependences, which naturally explain the emergence of memory effects in quenched dynamics. It has also been shown that, from this point of view, the relation between extremal dynamics and self-organization is a simple consequence of a more general relation between dynamical processes with memory and self-organization [5].

The purpose of this paper is to apply the same considerations to an equilibrium system. We shall deal with the simplest such system, i.e., a one-dimensional random walk in random environment. For this we will derive the exact corresponding annealed dynamics. This dynamics, by definition, does not depend on any particular realization of the disorder. However, as we shall see, the process has the same statistical properties. Asymptotically, for large times, the process singles out a particular realization of the disorder, which is the only one which is consistent with the past history of the process. A simple generalization of the dynamics with memory we find, shows that, interestingly enough, the disordered dynamics lies on the borderline between random dynamics and deterministic dynamics. The random walker, in the latter case, will sooner or later localize on some site. Finally, we shall generalize our arguments to the problem of a random walk with traps and draw some conclusions.

The random random walk (RRW) on a line is defined by assigning at each site $i=0,\pm 1,\pm 2,\ldots$ a random variable $p_i\in[0,1]$ drawn from a distribution $P\{p\leqslant p_i<p+dp\}=\phi(p)dp$. The evolution of the position x_t of the RRW is defined by $x_{t+1}=x_t+1$ with probability p_{x_t} and $x_{t+1}=x_t-1$ otherwise. In spite of its simplicity this model has been studied by many authors as a toy model for localization, [6] depinning transitions, [7] and aging effects [8]. The most striking feature is that the diffusion is extremely slow: the typical size visited by the walker after a time t is $\delta x\sim(\ln t)^2$. Comparing this result, originally derived rigorously by Sinai, [9] with the diffusion of a random walk without disorder, $\delta x\sim\sqrt{t}$, suggests that disorder has really dramatic effects on the dynamics.

In order to introduce our model, let us consider the case of a uniform distribution $\phi(p)=1$. Imagine observing the walker in its motion, without knowing the realization $\{p_i\}$ of the disorder. The only information available is what one sees, namely, the number $n_{i,t}$ of times that the random walker has visited site i and the number $k_{i,t}$ of times in which it has moved from site i to site $i+1$. As we shall now show, it is possible, using this information, to describe a

RRW even if the values of p_i are not known. This is accomplished by observing that the probability that the number of right jumps $i \to i+1$ is k, given that site i has been visited n times and the transition probability is $p_i = p$, is simply given by the binomial distribution

$$P(k|n,p) = \binom{n}{k} p^k (1-p)^{n-k}, \tag{1}$$

where the notation $P(A|B)$ stands for the probability of the event A, conditional to the occurrence of B. Regarding k as the ''effect'' of the ''cause'' p, we can invert this statistical relation to obtain the probability $dP(p|n,k)$ that $p \leq p_i < p + dp$ given k and n. Using Bayes rule of causes (see, [10] p. 124), it is easy to find that $dP(p|n,k) = (n+1)P(k|n,p)dp$. From this we can obtain an ''effective'' transition probability

$$p^a_{n,k} = \int dP(p|n,k) p = \frac{k+1}{n+2}, \tag{2}$$

where the last equality holds for $\phi(p) = 1$ (see later). The content of Eq. (2) is that, among all the processes and all the realizations of the disorder, the probability that the random walker will jump from site i to site $i+1$, given that it has made the same jump k times after the n previous visits, is $p^a_{n,k}$. This is the transition probability, which is consistent, in a conditional way, to the past history of the process. The history of the process is in general encoded in the effective distribution of the variable p_i at time t, which was named ''run time statistics'' in [4]. In our case the distribution of p_i is parametrized by only two numbers n_i and k_i, and therefore a direct expression of the effective dynamics in terms of k_i and n_i only is possible. The structure of the memory can be described by placing a Polya urn on each site [10].

The model defined by Eq. (2) will be hereafter called a random walk with memory (RWM). Its evolution is defined as follows: define on each site i of the lattice two integer ''dynamical'' variables $n_{i,t}$ and $k_{i,t}$, which count the number of visits on site i and the number of jumps $i \to i+1$. At time $t=0$, $n_{i,0} = k_{i,0} = 0$ and the walker is at site $i=0$. At time t, if the random walker is at site i, then with probability $p^a_{n_{i,t},k_{i,t}}$ it will move to site $i+1$ and $k_{i,t+1} = k_{i,t} + 1$. Otherwise the walker moves to site $i-1$ and $k_{i,t+1} = k_{i,t}$. In either case $n_{i,t+1} = n_{i,t} + 1$ increases by one. This process, by construction, is expected to reproduce the same results of the RRW with a random realization of $\{p_i\}$. In the RWM, the transition probabilities depend on the dynamical variables $\{k_{i,t}, n_{i,t}\}$ and therefore evolve in time. On the other hand, in the RRW, the transition probabilities p_i are fixed before the process starts. The equivalence of the dynamics of the two walkers results from the fact that each realization of the RWM asymptotically singles out a realization of the disorder, in the sense that $p^a_{n_{i,t},k_{i,t}} \to p_i$ as $t \to \infty$, where p_i is a uniform random number in $[0,1]$. This has been explicitly checked in numerical simulations, but it can also be argued from the distribution $dP(p_i|n,k)/dp$ of p_i. This is indeed sharply peaked around the mean value $p^a_{n,k}$ with a width of order $1/\sqrt{n}$. The statistics of the asymptotic value of $p^a_{n,k}$ as $n \to \infty$ can be explicitly shown to be that of uniform random variables by analyzing the moments of the effective transition probability $p_i(n_i) = p^a_{n_i,k_i}$. Dropping the i index for the moment, one observes that at the $(n-1)$st visit $p(n-1)^q$, with probability $p(n-1)$, increases to $[(n+1)p(n-1)+1/n+2]^q$ while with probability $1-p(n-1)$ it becomes $[(n+1)p(n-1)/n+2]^q$. Taking the average over realizations leads to a recursion relation for the moments of $p(n)$ which, with a little algebra, can be solved to find

$$M_q(n) = \langle p(n)^q \rangle = \frac{1}{n+1} \sum_{k=1}^{n+1} \left(\frac{k}{n+2} \right)^q. \tag{3}$$

Note that $M_1(n) = 1/2$ for all n. Moreover, all central moments $\langle [p(n) - \langle p(n) \rangle]^q \rangle$ with q odd vanish identically. For $n \gg 1$, one easily finds $M_q(n) = (1+q)^{-1} + O(n^{-1})$, i.e., the moments of $p(n)$ tend indeed to those of a uniform distribution in $[0,1]$. Therefore, the distribution of the transition probabilities, for a RWM in a box of size L with periodic boundary conditions, will asymptotically tend to a δ function around a random value p_i whose statistics is uniform in $[0,1]$. However, strictly speaking, even with periodic boundary conditions, the random walk will never reach a stationary state. This is reminiscent of systems out of equilibrium.

Another interesting observation is that one can easily calculate the probability of a realization of the process, i.e., of a given history $\{x(\tau): \tau = 1,t\}$. This is indeed given simply by $P\{n_{i,t}\} = \Pi_i [n_{i,t}+1]^{-1}$ [11]. Note that to obtain such a quantity in the RRW, one needs to evaluate it for a given realization of the disorder and then average over all realizations.

The diffusion law $\delta x \sim (\ln t)^2$ can be understood, in the context of the RWM, with the following argument. First we note that the values of k_i and n_i on different sites are not independent. For example it is easy to check that $t = \Sigma_i n_i$ and $x_t = \Sigma_i (2k_i - n_i)$. In general $n_i = k_{i-1} + n_{i+1} - k_{i+1}$. In this relation the k's are distributed uniformly between 0 and the n's. Then, approximately, this relation has the form $n_{i+1} \simeq C_i n_i$ with C_i a random variable. In other words, the variable $\ln n_i$ will have the shape of a random walk over i, which means that typically the maximum value of n_i for $i \in [0, L(t)]$ will be $n_{\max} \sim \exp \sqrt{L(t)}$. Since this value will also dominate the sum $\Sigma_i n_i = t$, we can conclude that $L(t) \sim (\ln t)^2$.

One striking feature of the RRW is the lack of time translational invariance. It was pointed out [8] that two times correlation functions are not functions of the difference of the times, as is normally the case, but also depend on the ''waiting'' time (i.e., the smallest time). This was related in Ref. [8] to the aging phenomena observed in spin glasses and glasses. The calculation of $\langle A_t A_{t+\tau} \rangle$, where A_t is any observable, depends only on processes between times t and $t+\tau$. If the transition probabilities involved in these process are constant in time, time translation invariance follows naturally. The lack of time translational invariance is no surprise in the RWM, because the transition probabilities explicitly depend on the ''waiting'' time t. This point can hardly be appreciated in the framework of the RRW, where the transition probabilities are fixed from the beginning. The absence of quenched disorder in the RWM evidences the fact that aging effects result from local memory effects. These effects, as shown by the equivalence of the RRW and RWM, are also present in disordered dynamical systems.

One might wonder what happens if instead of a uniform distribution one considers a general distribution $\phi(p)$. It is not difficult to show that all the above considerations hold the same, apart from the specific form of the moments and of the distribution of $p_i(n)$. Indeed Eq. (1) still holds. However, when one inverts it to find the distribution $dP(p|n,k)$ one has to account for the fact that the probability that $p \leqslant p_i < p + dp$ is $\phi(p)dp$ with $\phi(p) \neq 1$ in general. In practice Eq. (2) is slightly modified, but only up to factors of order n^{-1}. For example, if

$$\phi(p) = \Gamma(\alpha+\beta)x^{\alpha-1}(1-x)^{\beta-1}/[\Gamma(\alpha)\Gamma(\beta)],$$

one finds $p^a_{n,k} = (k+\beta)/(n+\alpha+\beta)$. Our numerical check of the diffusion as a function of α for $\beta=1$ confirms the depinning transition for $\alpha > 2$ found by Derrida [12].

To address the problem of localization we note that on each site the RWM can create a barrier. If the walker has failed to pass a site after n visits, its probability to overcome it at the next visit is $p^a_{n,0} = 1/(n+2)$. Even though this probability decreases, it decreases so slowly that any barrier will sooner or later be overcome. This results from a straightforward application of the Borel Cantelli lemma [10]. It is worth observing that this behavior is the probabilistic counterpart of the ''marginal'' localization properties of the RRW [6]. Indeed it is easy to show, by the same argument, that if $np^a_{n,0} \to 0$, as $n \to \infty$ the RWM would surely localize, sooner or later on some site. This marginality seems to be even stronger as suggested by the following argument. For any regular distribution $\phi(p)$, we found $np^a_{n,0} \to 1$ as $n \to \infty$. Let us therefore generalize our model by taking

$$p^a_{n,k} = \frac{k+1}{n+2} + a\sin\left(2\pi\frac{k+1}{n+2}\right). \qquad (4)$$

This describes a generalized symmetric ($p^a_{n,k} + p^a_{n,n-k} = 1$) random walk with memory. Note that $np^a_{n,0} \to 1 + 2\pi a$. We expect that for $a<0$ the walker localizes, whereas for $a>0$, for large times, the dynamics becomes that of a random walker without disorder (i.e., $p_i = 1/2$). This expectation is based on the fact that the function $f(x) \equiv p^a_{n,xn}$ seen as a map [i.e., $x_{n+1} = f(x_n)$] has two stable fixed points (0 and 1) and one unstable fixed point (in $x=1/2$) in the first case ($a<0$) while in the second case the stability is reversed (0,1 are unstable and 1/2 is stable). Our problem is not a map, but it is similar (it has also randomness). However, numerical investigation shows that our expectation is correct. For $a<0$ the walker localizes, whereas for $a>0$ all the transition probabilities $p_i \to 1/2$ as $t \to \infty$. In other words, as shown in Fig. 1, the dynamics recovers different distributions of the disorder in the three cases:

$$\phi(p) = \tfrac{1}{2}\delta(p) + \tfrac{1}{2}\delta(p-1) \quad \text{for} \quad a<0,$$

$$\phi(p) = 1 \quad \text{for } a=0,$$

$$\phi(p) = \delta(p - \tfrac{1}{2}) \quad \text{for} \quad a>0. \qquad (5)$$

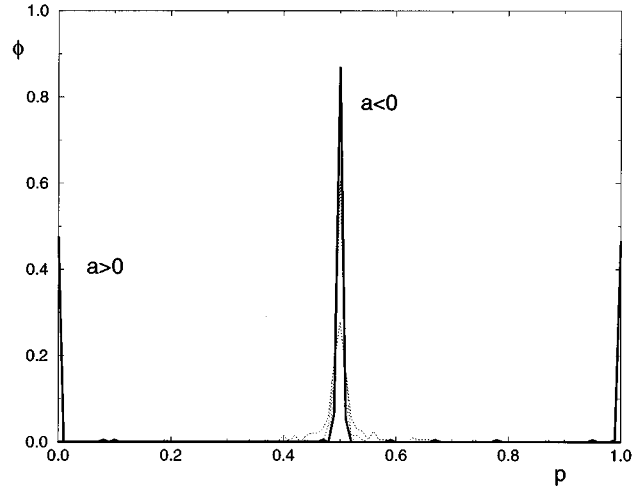

FIG. 1. Probability density $\phi(p)$. The solid curve centered in $p=0.5$ is obtained for $a=0.1$ and is reminiscent of a random walk. The dotted lines are previous stages of simulation. The solid curve with two peaks in $p=0$ and $p=1$ refers to the $a=-0.1$ case where localization takes place.

From this point of view the case $a=0$ is very peculiar. It is the only case for which the distribution which is recovered by the dynamics is continuous. The case $a<0$ bears some resemblance to systems, such as the Hopfield model [13] or folding proteins, [14] where the phase space has a peculiar organization and the dynamics ''localizes'' on a particular low energy state.

The above model can be generalized straightforwardly to higher dimensions d. This only requires the introduction of d dynamical variables $k_i^{(j)}$, $j=1,\ldots,d$, one for each direction on each site. An even simpler generalization is the case of a d dimensional random walker with random traps: Assign a uniform variable $p_i \in [0,1]$ to each site of the lattice. If the walker is on site i at time t, with probability p_i it remains on the same site at $t+1$, and with probability $1-p_i$ it diffuses to one of the neighbor sites. Still we can use $p^a_{n_i,k_i}$ for the probability of jumping out of site i, conditional to n_i visits, and k_i previous jumps out of the trap. It is easy to see how the diffusion law is modified in this case. Indeed, apart from the fact that the walker can spend a time $n_i > 1$ over a given site before jumping to the next one, the diffusion is the same. This means that $\delta x^2 \sim N$ where N is the number of sites visited (i.e., the number of jumps). This is related to the time t by summing all the times spent on different sites: $t = \Sigma_{i=1}{}^N n_i$. This sum is dominated by the large n_i values. The probability that the walker has been trapped for n_i steps on site i is $(n_i+1)^{-1}$. The probability that it will jump out of the trap is $p^a_{n_i,0} = 1/(n_i+2)$. Therefore the distribution of n_i is $D(n) = [(n+1)(n+2)]^{-1}$. This means that, for $N \gg 1$, $t = \Sigma_{i=1}{}^N n_i \sim N \ln N$, which yields the diffusion law $t \sim \delta x^2 \ln \delta x^2$. We checked the logarithmic corrections to the diffusion numerically. In this case, using the generalized model of Eq. (4), it is easy to find that $D(n) \sim n^{-2-2\pi a}$. Therefore, for $a>0$, the above argument yields the standard diffusion $\delta x^2 \sim t$, whereas for $a<0$ one finds anomalous diffusion $\delta x^2 \sim t^{1+2\pi a}$. Also in this case, therefore, disorder dynamics appears to be a borderline case.

In conclusion, we have derived and discussed some simple models of random walks which reproduce the behavior of diffusion in disordered media *without* specifying the disorder. We have seen that the dynamics itself retrieves a realization of the disorder with the proper statistical properties. Our results may well be used to generate dynamically a random realization of the disorder in any model with quenched variables. It is tempting to conjecture that such an algorithm could provide an alternative to the simulated annealing [15] procedure used to find optimal configurations in disordered systems. The annealing procedure has indeed the drawback that, once the disorder realization is fixed, the starting configuration of the dynamical variables may be ''far'' from a reasonably good optimal state. Using the above results would instead produce dynamically a realization of the disorder which is ''consistent'' with the configuration of the dynamical variables.

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