Non-Equilibrium Disordering Processes in a Binary System due to a Brownian Agent: Exact Lattice Calculation

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ABSTRACT

We study the disordering processes of the model of a binary system due to a Brownian agent in one dimension (d = 1). In this model, the spin at each site can take either the value 1 or -1. We choose the initial configuration to be all spins up or equal to 1 and let the random walker disorder the system as time progresses. We use a exact discrete lattice calculation approach to calculate the average magnetization density (m 0 (t)) at the origin. By taking into account the inhomogeneity of the spin- rate or coupling rate we find that the predicted results agree well with the Monte Carlo simulation results.

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Abstract

We study the disordering processes of the model of a binary system due to a Brownian agent in one dimension ($d = 1$). In this model, the spin at each site can take either the value 1 or -1. We choose the initial configuration to be all spins up or equal to 1 and let the random walker disorder the system as time progresses. We use a exact discrete lattice calculation approach to calculate the average magnetization density ($m_0(t)$) at the origin. By taking into account the inhomogeneity of the spin-flipping rate or coupling rate we find that the predicted results agree well with the Monte Carlo simulation results.

1 Introduction

Brownian motion is one of the fundamental processes of nature. It was originally observed in the irregular motion of pollen grains by the botanist Brown [1], and cast into the language of the diffusion equation by Einstein [2]. It has been applied to an enormous variety of processes in the mathematical framework of random walks [3]. A very rich field of research has been built around the behavior of a random walk(RW) coupled to a disordered environment [4], a good example being the anomalous diffusion of electrons in a disordered medium [5]. Also, one can consider a random walker, i.e. some type of defect, *being* the disordering agent in its environment. Applications of the latter include the tagged diffusion of atoms in a crystal [6, 7, 8] and magnetic disordering mediated by wandering vacancies [9]. Motivated by the important role of such processes in a myriad of real systems, we shall study some specific models for the interactions between the walker and its environment, namely how a system disorders when its kinetics is mediated by a walker.

In our previous papers [10, 11], we introduced this model in the context of binary data corruption which can be thought of as an example of a RW or as a Brownian agent(BA) disordering its bistable environment [i.e, consisting of elements which can

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take one of two possible states such as a binary data system(bits) or a magnetic system(Ising spins)] . In other words, the BA interacts with its environment by corrupting(switching) the data bits(spins) with probability or coupling rate, q as it wanders. Thanks to the solubility of its dynamics equation mostly obtained by the continuum theory approach, we were able to study a variety of its statistical properties as well as their physical nature e.g. magnetization density , global magnetization, two point correlation function, and probability of magnetization density.

In this paper we will instead apply the exact analytic calculation namely lattice calculation to study the magnetization density of the Binary system with quenched random coupling(time independent couplings in contrast to annealed disorder) drawn from a uniform distribution.

The paper is organized as follows. In Sec. II we formulate the discrete model in d dimensions. We derive the average magnetization density at the origin without averaging over q [i.e., we only average over the BA paths]. In Sec. III , a relatively straightforward average over q is done to obtain asymptotic results of magnetization density for the uniform distribution $S[q]$. We make a comparison between the theory and the results from simulations in Sec. IV. The conclusions are in Sec. V.

2 Discrete Formulation of the Model

We start with the binary spin system on a hypercubic lattice of dimension d. We represent each spin by an Ising spin variable $\sigma_{\mathbf{r}}$, where $\mathbf{r}$ denotes a discrete vector. $\sigma_{\mathbf{r}}$ may take the value $+1$ for up spin and (-1) for down spin. The position of the BA is denoted by a lattice vector $\mathbf{R}$. At each time step, the BA has a probability p to make a jump to one of its nearest neighbors. On a given jump, there is a probability q that the spin at the site it is leaving is switched. Given the above rule, the master equation is

$$P(\mathbf{R},\{\sigma_{\mathbf{r}}\},t+\delta t) = (1-p)P(\mathbf{R},\{\sigma_{\mathbf{r}}\},t) + \frac{p(1-q)}{2d}\sum_{\mathbf{l}} P(\mathbf{R}+\mathbf{l},\{\sigma_{\mathbf{r}}\},t) + \frac{pq}{2d}\sum_{\mathbf{l}} P(\mathbf{R}+\mathbf{l},\cdots,-\sigma_{\mathbf{R}+\mathbf{l}},\cdots,t) \quad (1)$$

where $\{\mathbf{l}\}$ represent the $2d$ orthogonal lattice vectors (which have magnitude l). To obtain the magnetization density, we firstly define the marginal averages as

$$\Theta(\mathbf{r}_1,t \mid \mathbf{R}) \equiv \mathrm{Tr}_\sigma\ \sigma_{\mathbf{r}_1}\ P(\mathbf{R},\{\sigma_{\mathbf{r}}\},t)\ . \quad (2)$$

Applying Eq.(2) to Eq.(1), we get

$$\Theta(\mathbf{r},t+\delta t \mid \mathbf{R}) - \Theta(\mathbf{r},t \mid \mathbf{R}) = \frac{p}{2d}\sum_{\mathbf{l}}[\Theta(\mathbf{r},t \mid \mathbf{R}+\mathbf{l}) - \Theta(\mathbf{r},t \mid \mathbf{R})] - \frac{pq}{d}\,\Theta(\mathbf{r},t \mid \mathbf{r})\sum_{\mathbf{l}}\delta_{\mathbf{r},\mathbf{R}+\mathbf{l}}\ . \quad (3)$$

One can see from Eq.(3) that, without the second term on the right-hand side, the results of lattice diffusion are recovered. It's also not too difficult to see that there is a contribution from the second term only if a spin is in the vicinity of BA.

We close this section by mentioning that we can obtain the average value of the spin at the origin [which we shall call the average magnetization density] from $\Theta(\mathbf{r}, t \mid \mathbf{R})$. This is simply given by

$$m_0(t) = \sum_{\mathbf{R}} \Theta(\mathbf{0}, t \mid \mathbf{R}). \tag{4}$$

for all t.

3 Lattice calculation of Average Magnetization Density

Referring to the equation of motion (3) for the marginal average we set $d = 1$, and for convenience we set the hopping probability $p = 1$, giving

$$\Theta(x, R, t + \delta t) = \frac{1}{2}\left[\Theta(x, R + l, t) + \Theta(x, R + l, t)\right] - q\ \Theta(x, x, t)\left[\delta_{x,R-l} + \delta_{x,R+l}\right]. \tag{5}$$

As an initial condition we take the BA to be located at the origin, and all spins to be +1, except the spin at the origin which is taken to be −1. [This convention is useful for $q = 1$ so that all spins have value +1 after one time step. However if $q \ll 1$ it is more convenient to take the spin at the origin to be initially +1 as the chance of it flipping after one time step is small. We stress that these different choices for the initial value of the spin at the origin have no effect on the asymptotic properties of the system, and only serve to smoothen the magnetization density in the immediate vicinity of the origin.] Thus $\Theta(x, R, 0) = \delta_{R,0}(1 - 2\delta_{x,0})$. The solution of (5) may be attained by discrete Fourier and Laplace transform. Defining the former via

$$\tilde{\Theta}(x, k, t) = \sum_{R} \Theta(x, R, t) e^{ikR} \tag{6}$$

and the latter via

$$\hat{\Theta}(x, R, z) = \sum_{n=0}^{\infty} \Theta(x, R, n\delta t)\ z^n\ , \tag{7}$$

it is fairly straightforward to diagonalize Eq.(5) to the form

$$\hat{\tilde{\Theta}}(x, k, z) = (1 - 2\delta_{x,0}) - 2qzf(k)e^{ikr}\frac{\hat{\Theta}(x, x, z)}{1 - zf(k)}\ , \tag{8}$$

where $f(k) = \cos kl$. One may now solve the above equation self-consistently for $\hat{\Theta}(x,x,z)$ by inverting the discrete Fourier transform. One has

$$\hat{\Theta}(x,x,z) = (1-2\delta_{x,0}) \int dk\; e^{-ikr} \frac{D(k,z)}{1+2qz} \int dk\; f(k) D(k,z) \ , \tag{9}$$

where $D(k) = [1-zf(k)]^{-1}$ and the momentum integrals are over the two-dimensional Brillouin zone. The average magnetization density at the origin is calculated by summing $\Theta(0,R,t)$ over R, which is equivalent to the zero Fourier mode $\grave{\Theta}(0,0,t)$. Thus, substituting (9) into (8) we have after some rearrangement

$$\sum_R \hat{\Theta}(0,R,z) = \sigma_0(0)/(1-z) \left[1 + q'(1-z) \int dk\; D(k,z)/1 + q' \int dk\; D(k,z)\right] \ , \tag{10}$$

where $q' \equiv 2q/(1-2q)$. [The function $\int dk\; D(k,z)$ is very well known in the theory of random walks [3], and is the discrete Laplace transform of the probability of a random walker to return to its starting point after n steps.] Finally we must find the inverse Laplace transform of the above equation. For large n we can extract the asymptotic form of the average magnetization by invoking the Tauberian theorem [3]. In this case we need the form of the Laplace transform as $z \to 1$. Using [3]

$$\int dk\; D(k,z) \sim 1/(1-z^2)^{1/2} \ , \tag{11}$$

Substitute into (10). This gives

$$\sum_R \hat{\Theta}(0,R,z) = \frac{\sigma_0(0)}{(1-z)} \left[\frac{1-2q+2q(1-z)(1-z^2)^{-1/2}}{1-2q+2q(1-z^2)^{-1/2}}\right] \ , \tag{12}$$

and we can now rewrite the above equation to arrive at

$$\sum_R \hat{\Theta}(0,R,z) = \sigma_0(0)/(1-z)\,[1 - Aq/1 + Bq] \ , \tag{13}$$

where

$$A = 2\left[1 - \frac{(1-z)^{1/2}}{(1+z)^{1/2}}\right] \ , \tag{14}$$

and

$$B = 2\left[\frac{1}{(1-z^2)^{1/2}} - 1\right] \ , \tag{15}$$

4 Quenched random rate results

4.1 Analytic results

We now consider situations where the coupling rates are symmetric but spatially inhomogeneous. Microscopically, these are modeled by attaching to each lattice position x a quenched random variable $q_x \in (0,1)$ drawn from a uniform distribution $S(\{q_x\})$. The random variable q_x gives the probability of switching in the event that the BA visits the site x. Here we consider the switching rates $q_x \in (0,1)$ which are independent random variables drawn from a uniform distribution.

$$S(\{q_x\}) = (1/q_m)\ \theta(q_m - q)\theta(q)\ , \tag{16}$$

where $q_x \in (0,1)$ From Eq.(13) which is the result of the average performed in the usual way using Laplace transform, we perform an average of this density over the distribution of the random couplings(16). We then have

$$\langle \sum_R \hat{\Theta}(0,R,z)\rangle_S = \frac{\sigma_0(0)}{(1-z)}\frac{1}{q_m}\int_0^{q_m} dq \left[\frac{1-\dot{A}q}{1+Bq}\right]\ , \tag{17}$$

and

$$\langle \sum_R \hat{\Theta}(0,R,z)\rangle_S = \frac{\sigma_0(0)}{(1-z)}\left[\frac{1}{(2q_m)}\frac{\left[1-\left(\frac{1-z}{1+z}\right)^{1/2}\right]}{\left[\left(\frac{1}{1-z^2}\right)^{1/2}-1\right]^2}\log\left[1+2q_m\left(\left(\frac{1}{1-z^2}\right)^{1/2}-1\right)\right]\right] - \frac{\sigma_0(0)}{(1-z)}\left[\frac{\left[\left(\frac{1}{1-z^2}\right)^{1/2}-\left(\frac{1-z}{1+z}\right)^{1/2}\right]}{\left[\left(\frac{1}{1-z^2}\right)^{1/2}-1\right]}\right]\ , \tag{18}$$

. Defining $z = 1-\epsilon$, and letting $\epsilon \to 0$, we get

$$\langle \sum_R \hat{\Theta}(0,R,z)\rangle_S = \frac{\sigma_0(0)}{\epsilon}\left\{\frac{1}{(2q_m)}\left[\sqrt{2}\epsilon(1+O(\sqrt{\epsilon}))\right] \log\left[1+\frac{2q_m}{\sqrt{2\epsilon}}(1+O(\epsilon))\right] - \left[\sqrt{2}\epsilon(1+O(\epsilon))\right]\right\}\ , \tag{19}$$

Taking Inverse Laplace transform and then applying the discrete Tauberian theorem [3], we get

$$\langle \sum_R \Theta(0,R,n)\rangle_S = \sigma_0(0)/2q_m \log n/(2\pi n)^{1/2}[1+O(1/\log n)] \tag{20}$$

4.2 Monte-Carlo simulation result

We have performed Monte Carlo simulations of the discrete model as defined in Sec. II, in order to test the results obtained in the last sections from the lattice calculations.

In the simulations which for we present results, we are concerned with a system with $d = 1$ and where there are symmetric quenched random rates. We have set the hopping rate p of the BA, along with the flipping probability q, to unity. For this infinite one-dimensional chain of sites, the chain length is unimportant, so long as one ensures that the BA has never touched the edges in any of its realizations up to the latest time at which data is extracted. We now monitor and measure the magnetization density. We perform the averaging in batches; namely, we use the same set of quenched rates for a batch of 1000 systems, which are then averaged over their different BA histories. We repeat this for N_b batches (with $N_b \sim 10^3$). Thus we average over different realizations of the quenched rates. We choose the quenched couplings $\{q_{\mathbf{x}}\}$ to be uncorrelated random variables drawn from a uniform distribution in the range $[0, 1]$. In a given run, at each time step the BA is moved left or right with equal probability and the spin it leaves behind is flipped with probability q. Each run starts with the same initial spin configuration; namely all spins up. We average over between 10^6 realizations (or runs) to meet the desired quality of the data. Such simulations required a few days on a DEC Alpha 233 MHz workstation.

In the figure, we show the average magnetization density for the system with quenched rates, and compare it to the same quantity in a "pure" system. We find at first that our results can not be fitted to the theoretical prediction (20). However, a closer analysis revealed that great care must be taken in making the comparison. The point is that one wishes to compare theory and simulation for long times (when the asymptotic form given in (20) becomes valid). However, it turns out that there is a new cross-over time t_f within the numerical simulations, beyond which the theoretical prediction is expected to break down. This cross-over time emerges due to insufficient averaging over batches. In the simulation we average over N_b batches, and thus select N_b couplings from the uniform distribution. This will be a smallest sampling value $q_f \sim 1/N_b$ of the coupling, and thus from this finite sampling of S, we cannot discern if we are really using a uniform distribution with non-zero weight all the way down to $q = 0$, or a distribution with non-zero weight only down to $q = q_f$. In the latter case, one can shown (from either the lattice or continuum theories) that the logarithmic slowing down will vanish after a time $t_f \sim 1/q_f^2$. Thus, in our simulations we can only expect to see the logarithmic slowing down for times much less than $t_f \sim N_b^2$. So, in order to makes this time-window as large as possible it is important to perform as many batch averages as possible, at the expense of averaging over BA histories within a given batch.

From the figure once again we want to emphasize that the average magnetization density from the simulation , and the analytic asymptotic result agree fairly well and the difference may be well fitted against the slow logarithmic corrections. Note, for times longer than those shown on the plot, the data fails to agree with the predicted result due to cross-over into the regime $t \gg t_f$ in which finite sampling effects dominate.

5 Summary and Conclusions

In Sec. II we introduce a disceret version of the model, which consists of a BA flipping spins on a lattice. The model is non-trivial since the value of a given spin depends very sensitively on the path of the BA. We presented a master equation formulation of the model and derived an equation of motion for the marginal average of the magnetization density.

In Sec. III and the first part of Sec. IV, we apply the lattice calculation to study the system with symmetric but inhomogeneous couplings. Thus, the probability for the agent to switch a given element is given by a quenched random variable. We incorporated this new effect into the continuum model by generalizing the constant parameter q to a quenched random field q_m described by a distribution $S[q]$. We investigated the simple case in which S is spatially uncorrelated, with a uniform on-site distribution function. We find that the average magnetization density at the origin decays more slowly than in the homogeneous case, by a factor $\sim \log n$. Finally in Sec. VB we describe the details of our numerical simulations, and presented figure supporting the analytic predictions from the previous sections.

In conclusion, we have solved a model analytically and computer experimentally in which a BA interacts with a bimodal inhomogeneous environment (*i.e.* a medium containing two types of particles, spins, bits, etc.). Our primary application has been an environment composed of bits of data, which the BA steadily corrupts.

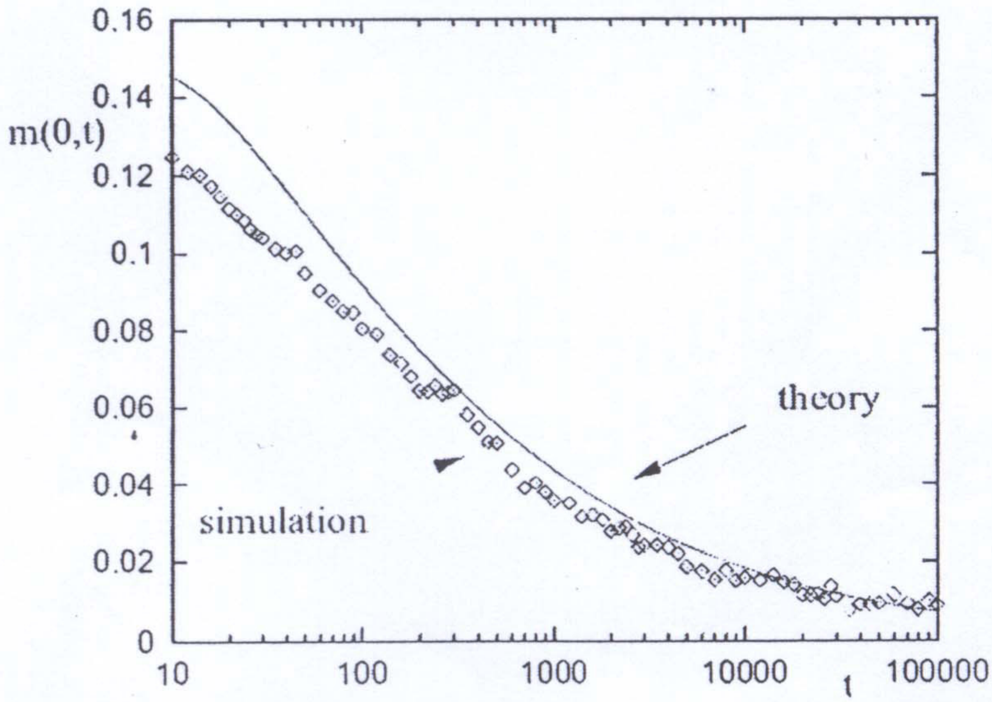

Figure. Plot of the magnetization density at the origin (averaged over both BA histories and the quenched rates) versus time. The solid line is the asymptotic form of the theoretical prediction Eq. 20) with no free parameters.

The model may also be seen to be a very simplified version of other systems. For instance the bistable medium can be taken to be composed of two chemical species A and B (with vanishingly low mobility) and the BA to be a high mobility catalyst, inducing a reversible reaction between A and B (and *vice versa*). Alternatively we can think of the BA as a wandering impurity in an ionic crystal (such as an anion or cation vacancy in $NaCl$) or a semiconductor compound (such as Zn in $GaAs$), which has a small probability of reordering the local bi-atomic structure as it passes through a given unit cell. However, the data corruption process appears to us the most interesting application, as well as being the most potentially relevant. This is especially true given the enormous efforts dedicated to creating memory storage devices of ever-decreasing size. Such miniaturization will lead to new causes of soft error production, amongst which will inevitably be found the Brownian agent.

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