Stochastic dynamics in a two-level model of disorder: comparison of mean-field and exact solutions

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Abstract. Stochastic dynamics in the presence of quenched disorder (e.g., diffusion in a random medium) is generally treated in a suitable mean-field or effective medium approximation. While numerical simulations may help determine the accuracy of such approximations in specific models, there are relatively few instances in which analytic solutions are possible, to enable a precise comparison to be made with the mean-field results. We consider in this paper a simple but general model of quenched disorder in which a system variable x jumps stochastically between two values x_a and x_b . However, in each level there occurs with a certain probability a branch (or internal) state into which the system may fall, and from which a jump to the other level is possible only after a return to the original (or 'active') state. Four different configurations of the states of the system are thus possible, and the transitions between the states are governed by Markovian transition probabilities. The moments of x and its autocorrelation function are computed in each case, and then configuration-averaged over the four realizations. This represents the exact solution. Next. a mean-field theory of the dynamics is developed: this turns out to involve an effective waiting-time density at each of the two levels that is non-exponential in time, so that the mean-field dynamics is a non-Markovian alternating renewal process. The moments and autocorrelation of x are again computed, and compared with the exact solutions. The extent of the differences at both short and long times is elucidated, and a numerical comparison is presented for the case of maximal disorder.

Keywords. Stochastic dynamics; disorder; mean-field approximation; correlation function.

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1. Introduction and description of the model

Many different physical systems evolve in time according to stochastic dynamics, very often in the presence of frozen, spatial disorder caused by random inhomogeneities. Diffusion in a random environment (or a random walk) is a generic problem of this type, and there exists a considerable literature on the subject (Haus and Kehr 1987; Havlin and Ben-Avraham 1987; Bouchaud and Georges 1990). The dynamics of spin glasses and similar disordered systems (Bouchaud et al 1987; Natterman and Villain 1988) is another major example of this class of problems.

The most common method of tackling such problems may be broadly termed a mean-field or effective medium approach. The details of this approach depend on the particular situation under consideration, but the central idea is as follows: the final configuration-averaging of physical quantities over the different realizations of the disordered system is approximated by an averaging performed at an earlier stage in the calculations. This generally amounts to replacing the original problem involving quenched disorder by a counterpart without such disorder, but one involving effective

parameters (such as coupling strengths, relaxation rates, etc.) that must be determined self-consistently.

While the mean-field approximation (MFA) used in the sense just described is ubiquitous, there are relatively few instances in which its accuracy can be checked directly against an exact solution: the latter are hard to come by, owing to the difficulty of performing exact configuration-averaging after the usual thermal averaging over annealed variables. Numerical simulation must therefore be resorted to, in order to judge the precision of the MFA. Now, the MFA (and suitable extensions of it) may be used to compute both static quantities (such as the equilibrium moments of some variable) as well as dynamic ones (such as time correlation functions). The accuracy of the latter in the MFA is even more difficult to estimate than that of the static averages, in the absence of reliable information on precisely how the MFA distorts the exact dynamical time scales (such as the relaxation rates) of the problem.

In view of these considerations, it is of interest to analyze a simple model of disorder in which both an exact configuration averaging as well as an MFA can be carried out, for static as well as time-dependent moments. This is the purpose of this paper. The model we consider is a two-level system; it is well-known that such systems can be tailored to model a surprisingly large variety of physical situations in statistical and chemical physics, resonance spectroscopy, etc. We shall use the language of the random walk in continuous time of a classical particle, although the origin of the inter-level transitions may be quantum mechanical: we shall be concerned solely with the resulting stochastic dynamics in terms of given transition probabilities. It will be apparent that the formalism to be discussed can be modified in a straightforward manner to apply to diverse situations in reaction rate theory, molecular relaxation, two-layer dispersion phenomena, etc.

The system we consider has two possible levels, in which some physical quantity x takes on values x_a and x_b respectively. The stochastic variable x(t) jumps between x_a and x_b at random instants of time. If there are unique states a and b in which $x = x_a$ and $x = x_b$ respectively, and the waiting time density in each state is an exponential function of time, $\lambda \exp(-\lambda t)$, then x(t) is simply the well-known dichotomic Markov process (or telegraph process) (Barucha-Reid 1960). However, we are interested in introducing and evaluating the effects of quenched disorder on static and time-dependent averages. Accordingly, we suppose that there can be an additional internal state α (respectively, β) in some realizations of the system to which a transition can occur from the state a (respectively b). (One may call the internal states α and β branches, or passive/quiescent/immobile states, in contrast to the principal/active/ mobile states a and b, the terminology depending on the system being modelled). In other words, there is a probability σ (0 < σ < 1) that the branch α (or β) is present, and a probability $(1-\sigma)$ that it is not. The parameter σ is a measure of the quenched randomness in the possible configurations of the states of the system. In this simple model, there are just four configurations, labelled A, B, C and D, as depicted in figure 1. Denoting the a priori probability of the occurrence of the realization R (R = A, B, C or D) by π_R , we have

$$\pi_{A} = (1 - \sigma)^{2}, \quad \pi_{B} = \pi_{C} = \sigma(1 - \sigma), \quad \pi_{D} = \sigma^{2}.$$
 (1)

We assume that the variable x has the same value x_a (respectively, x_b) in the principal state a and branch state α (respectively, in b and β): we want to analyze the effects of possible internal transitions between a and α , and similarly between b and β ,

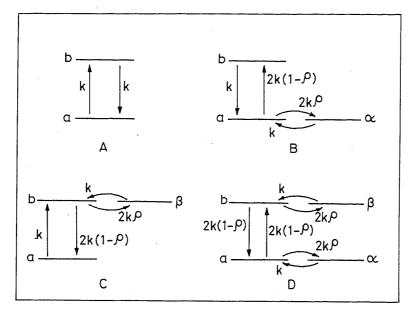


Figure 1. The states in the four configurations A, B, C and D of the system, and the rates for transitions between them.

intermixed with the $a \leftrightarrow b$ transitions that cause changes in the value of the observable x, configuration-averaged over the realizations A, B, C and D of the system. We note (see figure 1) that direct transitions from the branch state α to b (or β), or from β to a (or α), do not occur in the model. The system has to pass from α (respectively, β) to the principal state a (respectively, b) before jumping to the other principal state b (respectively, a).

The dynamics in each of the realizations is that of a random walk on a (very short) linear chain (of just 2 sites in A, 3 sites in B and C, and 4 in D). We may, in the simplest instance, assume the random walk to the Markovian, with a basic transition rate k.* This is the transition rate for jumps out of every initial state for which only a single final state is accessible: namely, $a \rightarrow b$ and $b \rightarrow a$ in A; $a \rightarrow a$ and $a \rightarrow a$ in B; $a \rightarrow b$ and $a \rightarrow a$ in C; and $a \rightarrow a$ and $a \rightarrow a$ and $a \rightarrow a$ in D. On the other hand, the total jump rate out of an initial state for which neighbouring final states exist on both sides is $a \rightarrow a$ and $a \rightarrow a$ in realization B; $a \rightarrow a$ in C; and both $a \rightarrow a$ in D.

At this stage we can widen the scope of applicability of our model by incorporating a possible asymmetry between the branch states α and β , on the one hand, and the principal states a and b, on the other, as follows. Let $\rho(0 < \rho < 1)$ denote the a priori probability of a transition from a to its branch α (respectively, from b to β), while $(1-\rho)$ is the a priori probability of a transition to the other principal state b (respectively, a). The $a \rightarrow \alpha$ and $a \rightarrow b$ transition rates in realization a are then a and $a \rightarrow b$ transition rates in realizations a and a are then a and a and a and a and a are then a and a and a are then a and a and a and a are then a and a are then a and a are then a and a and a are then a are then a and a are then a are then a and a are then a and a are then a and a are then a are then a and a are then a are then a are then a and a are then a

^{*} This assumption can be relaxed, and the underlying dynamics can itself be made non-Markovian, but this is not the purpose of the present paper.

concerned. The parameters ρ and σ represent, respectively, the effects of asymmetry (in the sense just described) and disorder.

In the next section, we solve the simple random walk problem on each realization, and carry out the exact configuration averaging for the equilibrium moments of x and for its autocorrelation function. In \S 3, we develop the MFA appropriate to the model at hand, and compute the same quantities in the MFA. We then compare the results of the MFA with the exact solutions, and comment on the differences between the two.

2. Exact solution

2.1 The probability distributions

In each realization of the system, the random walk between the states is a stationary Markov process with transition rates as shown in figure 1. Let $P_R(i,t|j)$ be the conditional probability (in realization R) of being in the state i at time t, given the initial state j at t=0. (Here i,j run over the states occurring in R.) Let $\tilde{P}_R(i,u|j)$ be the Laplace transform of $P_R(i,t|j)$, and let $P_R(u,j)$, $\delta(j)$ denote column vectors with elements

$$[\mathbf{P}_{R}(u,j)]_{i} = \tilde{P}_{R}(i,u|j), \quad [\delta(j)]_{i} = \delta_{ij}. \tag{2}$$

Then the master equation for P_R reads

$$(u - W_R)\mathbf{P}_R = \mathbf{\delta},\tag{3}$$

where the off-diagonal elements of the transition matrix W_R in each realization are the transition rates shown in figure 1. (W_{ij} is the $i \rightarrow j$ transition rate.) The diagonal elements are given by $W_{jj} = -\sum_{i \neq j} W_{ij}$. The solution to (3) is given by

$$\mathbf{P}_{R} = G_{R} \delta, \tag{4}$$

where

$$G_R = (u - W_R)^{-1}. (5)$$

In other words, the column vector $\mathbf{P}_R(u,j)$ is just the jth column of the resolvent matrix G_R . The latter is given, for each of the realizations, in Appendix A. We note the following salient features of the solution.

There is an obvious symmetry between realizations B and C. The latter is obtained from the former by the substitutions $\alpha \to \beta$, $a \to b$, $b \to a$. In realization D, all expressions are invariant under the simultaneous interchanges $a \leftrightarrow b$, $\alpha \leftrightarrow \beta$.

The equilibrium or stationary distribution in each realization is simply the residue at u=0 of \tilde{P}_R , and can be read off from G_R (or obtained directly from figure 1, using detailed balance). We get

$$P_{A}^{st}(a) = P_{A}^{st}(b) = 1/2;$$

$$P_{B}^{st}(\alpha) = P_{C}^{st}(\beta) = 2\rho/3,$$

$$P_{B}^{st}(a) = P_{C}^{st}(b) = 1/3,$$

$$P_{B}^{st}(b) = P_{C}^{st}(a) = 2(1-\rho)/3;$$

$$P_{D}^{st}(\alpha) = P_{D}^{st}(\beta) = \rho/(1+2\rho),$$

$$P_{D}^{st}(a) = P_{D}^{st}(b) = 1/2(1+2\rho).$$
(6)

The relaxation rates (the rates at which the $\{P_R(i,t|j)\}$ tend to the stationary distributions $\{P_R^{st}(i)\}$, i.e., the eigenvalues of $-W_R$) are as follows: 2k in A: k and 3k in B and C: and k $(1+2\rho)$, k $(5/2-\rho+r)$, $k(5/2-\rho-r)$ in D, where

$$r = (9/4 - \rho + \rho^2)^{1/2}. (7)$$

2.2 Equilibrium moments and variance

The moments of the physical observable x in a given realization are defined by

$$\langle x^n(t)\rangle_R = \sum_{i,j} x_i^n P_R(i,t|j) P_R^{\text{st}}(j). \tag{8}$$

As the stochastic process is a stationary one, these moments are actually time-independent (as may be verified by explicit calculation), and (8) reduces to

$$\langle x^n \rangle_R = \sum_i x_i^n P_R^{\text{st}}(i). \tag{9}$$

We find

$$\langle x^{n} \rangle_{A} = \langle x^{n} \rangle_{D} = (1/2)(x_{a}^{n} + x_{b}^{n}),$$

$$\langle x^{n} \rangle_{B} = (1/3)[(1 + 2\rho)x_{a}^{n} + 2(1 - \rho)x_{b}^{n}],$$

$$\langle x^{n} \rangle_{C} = (1/3)[2(1 - \rho)x_{a}^{n} + (1 + 2\rho)x_{b}^{n}].$$
(10)

The exact configuration-averaged moments are defined by

$$\langle \langle x^n \rangle \rangle = \sum_R \pi_R \langle x^n \rangle_R.$$
 (11)

Using (1) for the π_R , we get at once

$$\langle\!\langle x^n \rangle\!\rangle = (1/2)(x_a^n + x_b^n),$$
 (12)

a not unexpected result. On the other hand, the variance of x involves squaring the mean in each R and then averaging over R with the weights π_R , and we may anticipate a deviation from the value $(x_a - x_b)^2/4$ which we would expect at first sight. We find, defining $\langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$ as usual,

$$\langle (\Delta x)^2 \rangle_{\mathbf{A}} = \langle (\Delta x)^2 \rangle_{\mathbf{D}} = (1/4)(x_a - x_b)^2, \tag{13}$$

but

$$\langle (\Delta x)^2 \rangle_{\rm B} = \langle (\Delta x)^2 \rangle_{\rm C}$$

= $(2/9)(x_a - x_b)^2 (1 - \rho)(1 + 2\rho)$. (14)

Hence the exact configuration-averaged variance of x is

$$\langle \langle (\Delta x)^2 \rangle \rangle = \sum_{R} \pi_R \langle (\Delta x)^2 \rangle_R$$

= $(1/4)(x_a - x_b)^2 [1 - (2/9)\sigma(1 - \sigma)(1 - 4\rho)^2].$ (15)

The factor in square brackets in (15) will turn out to be the measure of the deviation of the MFA from the exact solution.

2.3 Correlation function

The exact expression for the autocorrelation function of x is

$$C(t) = \sum_{R} \pi_R C_R(t), \tag{16}$$

where

$$C_{R}(t) = \langle x(0)x(t)\rangle_{R}$$

$$= \sum_{i,j} (x_{i} - \langle x\rangle_{R})(x_{j} - \langle x\rangle_{R})P_{R}(i,t|j)P_{R}^{st}(j).$$
(17)

The expressions obtained for $C_R(t)$ (R = A, B, C, D) are recorded in Appendix A. Using these, we obtain the result

$$C(t) = (1/4)(x_a - x_b)^2 \left[(1 - \sigma)^2 \exp(-2kt) + (16/9)\sigma(1 - \sigma) \right.$$

$$\times (1 - \rho)(3\rho \exp(-kt) + (1 - \rho)\exp(-3kt)) + \sigma^2 \exp(-(5/2 - \rho)kt)$$

$$\times \left(\cosh(rkt) + \frac{(8\rho - 2\rho^2 - 3/2)}{r(1 + 2\rho)} \sinh(rkt) \right) \right], \tag{18}$$

where $r = (9/4 - \rho + \rho^2)^{1/2}$ as defined in (7). We note that $C(0) = \langle (\Delta x)^2 \rangle$, and that $C(t) \to 0$ when $t \to \infty$, as required.

In the unbiased case (i.e., for $\rho = 1/2$), (18) simplifies to

$$C(t) = (1/4)(x_a - x_b)^2 [(1 - \sigma)^2 \exp(-2kt) + (4/3)\sigma(1 - \sigma)$$

$$\times (\exp(-kt) + (1/3)\exp(-3kt)) + \sigma^2 \exp(-2kt)(\cosh\sqrt{2kt} + (1/\sqrt{2})\sinh\sqrt{2kt})].$$
(19)

3. Mean-field approximation and comparison with exact solution

3.1 Effective waiting-time density

The mean-field approximation (MFA) in problems of this sort consists of deriving an effective, configuration-averaged waiting-time density (Cox 1962) for a transition from one site to another (here, from the level x_a to the level x_b , and vice versa). This WTD is common to all the sites (levels), as it is already configuration-averaged. Translation invariance (here, symmetry between x_a and x_b) is thus implicit in the MFA right from the start, whereas in the exact solution it is restored only after the final configuration-averaging. Our aim is to develop an MFA that is as accurate as possible: In the present instance, this objective makes it more involved than the exact solution itself, but this will not, of course, be the case in more realistic cases of disorder. The effort we expend in developing the MFA in what follows should be regarded in this light.

Let us consider the WTD for a jump in the value of x from x_a to x_b in each of the realizations. (The same WTD would apply to a jump from x_b to x_a , as explained above.) This WTD is a conditional probability density: Given that the value $x = x_a$ has just been attained at t = 0, it is the probability density for the next change to the

value x_b to occur in the interval (t, t+dt). In realizations A and C (in which the branch α is absent), this WTD is simply the exponential corresponding to the total rate k of transitions out of the state a, namely,

$$\phi(t) = k \exp(-kt). \tag{20}$$

$$\chi(t) = 2k \exp(-2kt) \tag{21}$$

for the totality of transitions out of the state a. Since ρ and $(1-\rho)$ are the respective bias factors for $a \to \alpha$ and $a \to b$ transitions, the WTD for a jump from a to α (without going to a) is $\rho \chi(t)$, while that for a jump from a to a (without going to a) is a0. Now, the first passage from a1 to a2 can occur after an arbitrary number of excursions from a3 to a4 and back to a6. Therefore the density a5 given by the renewal type equation

$$\phi_{ab}(t) = (1 - \rho)\chi(t) + \int_0^t dt_2 \int_0^{t_2} dt_1 [\rho \chi(t_1) \phi(t_2 - t_1) \phi_{ab}(t - t_2)].$$
 (22)

The first term on the right represents a direct jump from a to b without an excursion to α . The second term includes all possible excursions $a \to \alpha \to a$ before the transition to b, the factor $\phi(t_2 - t_1)$ being the propagator for the return from α to a. As the factors in the renewal equation are in convolution, we use the Laplace transforms $\widetilde{\phi}$, $\widetilde{\chi}$, $\widetilde{\phi}_{ab}$ etc., where

$$\widetilde{\phi}(u) = \int_0^\infty \mathrm{d}t \, \phi(t) \exp(-ut). \tag{23}$$

Equation (22) then yields

$$\tilde{\phi}_{ab} = (1 - \rho)\tilde{\chi}/(1 - \rho\tilde{\phi}\tilde{\chi}). \tag{24}$$

Inserting the expressions $\tilde{\phi}(u) = k(u+k)^{-1}$ and $\tilde{\chi}(u) = 2k(u+2k)^{-1}$ in (24) and inverting the transform, we find

$$\phi_{ab}(t) = 2k(1-\rho)\exp(-3kt/2) \left[\cosh\left(\frac{kt}{2}(1+8\rho)^{1/2}\right) - (1+8\rho)^{-1/2}\sinh\left(\frac{kt}{2}(1+8\rho)^{1/2}\right) \right].$$
 (25)

This is the WTD for a jump from x_a to x_b (or vice versa) when there is a branch state at the initial level.

The effective WTD for a jump from x_a to x_b (or vice versa) is obtained by configuration averaging the WTD's obtained above. This is the mean field approximation in the problem at hand. Since σ is the probability that a branch state is present at the initial level, we get for the effective WTD $\psi(t)$ in the MFA the expression

$$\psi(t) = (1 - \sigma)\phi(t) + \sigma\phi_{ab}(t) \tag{26}$$

where ϕ and ϕ_{ab} are given by (20) and (25) respectively. For ready reference, we note that the transform of ψ is given in terms of $\tilde{\phi}$ and $\tilde{\chi}$ by the expression

$$\widetilde{\psi} = (1 - \sigma)\widetilde{\phi} + \frac{\sigma(1 - \rho)\widetilde{\chi}}{(1 - \rho\widetilde{\phi}\widetilde{\chi})}.$$
(27)

This will be used in the calculations to follow. We note that, at u=0, $\tilde{\phi}=\tilde{\chi}=\tilde{\psi}=1$, so that all these WTD's are properly normalized.

We shall need also the first waiting time density (Cox 1962) (FWTD) $\psi_1(t)$ for a change in the value of x: given that the value of x is found to be x_a (or x_b) at some arbitrary origin of time t = 0, $\psi_1(t)dt$ is the probability that the first (i.e., next) change in the value of x occurs in (t, t + dt). $[(\psi(t)dt)$, on the other hand, is the probability that the next change in the value of x occurs in (t, t + dt), given that a change has just occurred at t = 0. It is evident that at very long times the averages to be computed will not be sensitive to the precise form of ψ_1 . As far as this asymptotic regime is concerned, we could in fact take $\psi_1(t)$ to be $\psi(t)$ itself (a procedure that would be rigorously correct only for a purely exponential density, which $\psi(t)$ is not.) However, we are interested in developing an MFA that describes the actual dynamics as accurately as possible. (See also the remarks at the end of § 3.4.) With this aim in mind, we deduce an expression for ψ_1 as follows.

When there is no branch state α present, the WTD to jump from x_a to x_b is just $\phi(t) = k \exp(-kt)$, as we have seen already. This is an exponential density, and the corresponding FWTD is therefore $\phi(t)$ itself*. When the branch α is present, let the FWTD for a jump from x_a to x_b be denoted by $\Phi(t)$. Then the configuration-averaged FWTD that we must use in the MFA is given, in a manner analogous to (26), by

$$\psi_1(t) = (1 - \sigma)\phi(t) + \sigma\Phi(t). \tag{28}$$

To find $\Phi(t)$ we argue as follows. If we find that $x = x_a$ at the arbitrary instant of time t = 0, the system could actually be either in state a or in the branch state α , with probabilities in the ratio

$$P_{\mathrm{B}}^{\mathrm{st}}(a)/P_{\mathrm{B}}^{\mathrm{st}}(\alpha) = P_{\mathrm{D}}^{\mathrm{st}}(a)/P_{\mathrm{D}}^{\mathrm{st}}(\alpha) = 1/(2\rho), \tag{29}$$

from (6). Now, if the system is in state a, the WTD to jump to b is $\phi_{ab}(t)$, already found in (25). This is also the first waiting time density (FWTD) from an arbitrary

^{*}This is a well-known result (see, e.g., Cox 1962; Cox and Miller 1965). A renewal process with an exponential WTD is one in which the transition probability density is a constant (λ , say); in any interval of time dt, the probability of a transition is λdt . Successive events are uncorrelated, which is why the FWTD turns out to be the WTD itself in this case.

origin of time t=0 to go from the initial state a to the state b, because any transition out of the state a is governed by the exponential density $\chi(t)$ (in other words, the underlying dynamics is Markovian.) If the system happens to be in the state α at t=0, the WTD to go from α to b is the first passage time density to go from α to b, which we denote by $\phi_{\alpha b}(t)$. Again this is also the FWTD for going from α to b from an arbitrary origin of time t=0, because any transition out of α is governed by the exponential density $\phi(t)$. Since the only possible direct transition from α is to the state a, and this transition is governed by the density $\phi(t)$, we see that the first passage time density from α to b is given by the convolution

$$\phi_{ab}(t) = \int_0^t dt_1 \, \phi(t_1) \, \phi_{ab}(t - t_1). \tag{30}$$

(We recall that $\phi_{ab}(t)$ is the first passage time density to go from a to b in the presence of the branch state α .) Hence the transform of ϕ_{ab} is given by

$$\widetilde{\phi}_{ab} = \widetilde{\phi}\,\widetilde{\phi}_{ab},\tag{31}$$

where $\tilde{\phi}_{ab}$ is given by (24). Putting together the foregoing, the transform of $\Phi(t)$ is given by

$$\tilde{\Phi} = r_a \tilde{\phi}_{ab} + r_\alpha \tilde{\phi}_{\alpha b},\tag{32}$$

where the weight factors r_a and r_α satisfy $r_a + r_\alpha = 1$, $r_a/r_\alpha = 1/(2\rho)$. Hence

$$\widetilde{\Phi} = \frac{(1-\rho)(1+2\rho\widetilde{\phi})\widetilde{\chi}}{(1+2\rho)(1-\rho\widetilde{\phi}\widetilde{\chi})}.$$
(33)

Using the expressions for $\tilde{\phi}$ and $\tilde{\chi}$ and inverting the transform, we find

$$\Phi(t) = \frac{2k(1-\rho)}{(1+2\rho)} \exp(-3kt/2) \left[\cosh\left(\frac{kt}{2}(1+8\rho)^{1/2}\right) + \frac{(4\rho-1)}{(1+8\rho)^{1/2}} \sinh\left(\frac{kt}{2}(1+8\rho)^{1/2}\right) \right].$$
(34)

Finally, $\psi_1(t)$, the FWTD sought, is given by the weighted sum of $\phi(t)$ and $\Phi(t)$, as in (28). We note that $\tilde{\psi}_1(0)$ is also equal to unity, so that $\psi_1(t)$ is a normalized density.

It is of interest to look at the mean times (first moments) corresponding to the different normalized densities obtained above. Writing

$$T_{\phi} = \int_{0}^{\infty} t\phi(t)dt = -\tilde{\phi}'(0). \tag{35}$$

etc., we find (since $kT_{\phi} = 1$ and $kT_{\chi} = 1/2$)

$$kT_{\psi} = 1 + \frac{\sigma(4\rho - 1)}{2(1 - \rho)} \tag{36}$$

and

$$kT_{\psi_1} = 1 + \frac{\sigma(4\rho^2 + 6\rho - 1)}{2(1 + 2\rho)(1 - \rho)}. (37)$$

3.2 Transition probability

The MFA thus amounts to treating x(t) as a dichotomic process that jumps between the value x_a and x_b with a (non-exponential) waiting time density $\psi(t)$. There is no question of individual realizations of the system any longer, as the averaging over configurations has been done already in computing $\psi(t)$. It is worth noting that the original Markovian dynamics is replaced in the MFA by a non-Markovian process, as $\psi(t)$ is not an exponential density.

In the simple model under consideration, we have merely to find the probability that $x = x_b$ at time t, given that $x = x_a$ at t = 0. Let us denote this probability by $\mathbb{P}(x_b, t | x_a)$. Then (since the same WTD governs both $x_a \to x_b$ and $x_b \to x_a$ transitions),

$$\mathbb{P}(x_a, t|x_b) = \mathbb{P}(x_b, t|x_a),\tag{38}$$

and

$$\mathbb{P}(x_a, t|x_a) = 1 - \mathbb{P}(x_b, t|x_a) = \mathbb{P}(x_b, t|x_b). \tag{39}$$

A straightforward enumeration procedure yields, for the transform of \mathbb{P} , the expression (see Appendix B)

$$\widetilde{\mathbb{P}}(x_b, u | x_a) = \widetilde{\mathbb{P}}(x_a, u | x_b) = \widetilde{\psi}_1(u) / [u(1 + \widetilde{\psi}(u))], \tag{40}$$

where $\psi_1(t)$ is the first waiting time density as defined in §3.1 (see eq. (28)). From (39), we have also

$$\widetilde{\mathbb{P}}(x_a, u|x_a) = \widetilde{\mathbb{P}}(x_b, u|x_b) = u^{-1} - \widetilde{\mathbb{P}}(x_a, u|x_b). \tag{41}$$

3.3 Moments and the correlation function in the MFA

As the mean waiting time T_{ψ} is the same when $x = x_a$ or when $x = x_b$, and the stochastic process is a stationary one, it follows trivially that

$$\langle x^n \rangle_{\mathrm{MF}} = (1/2)(x_a^n + x_b^n), \tag{42}$$

and hence

$$\langle (\Delta x)^2 \rangle_{\rm MF} = (1/4)(x_a - x_b)^2.$$
 (43)

(Here $\langle \cdot \rangle_{MF}$ stands for the corresponding average evaluated in the MFA.) The autocorrelation function of x is given by

$$C_{\mathrm{MF}}(t) = (1/2) \sum (x_i - \langle x \rangle_{\mathrm{MF}}) (x_j - \langle x \rangle_{\mathrm{MF}}) \mathbb{P}(x_i, t | x_j)$$
(44)

where x_i, x_j run over the values x_a and x_b , and the factor 1/2 comes from $\mathbb{P}^{st}(x_j)$. Using the results of § 3.2, (44) simplifies to

$$C_{\rm MF}(t) = (1/4)(x_a - x_b)^2 [1 - 2\mathbb{P}(x_b, t | x_a)]. \tag{45}$$

Since $\mathbb{P}(x_b, 0|x_a) = 0$, it is evident that $C_{MF}(0) = \langle (\Delta x)^2 \rangle_{MF}$, as required. The Laplace transform of (45) gives

$$\tilde{C}_{\rm MF}(u) = \frac{(x_a - x_b)^2}{4u} \left[1 - \frac{2\tilde{\psi}_1}{1 + \tilde{\psi}} \right]. \tag{46}$$

Since $\widetilde{\psi}_1(0) = 1$ and $\widetilde{\psi}(0) = 1$, we see that $\widetilde{C}_{MF}(u)$ has no pole at u = 0, and that $C_{MF}(t)$

does tend to zero at $t \to \infty$. The explicit expression for $\tilde{C}_{MF}(u)$ as a function of u is a bit lengthy, and is recorded in Appendix B, (B.3)-(B.5). It is the ratio of a quadratic in u and a cubic in u.

3.4 Comparison of the MFA and the exact solution

As 'translational invariance' (in the present case, the symmetry between the levels x_a and x_b) is restored by configuration averaging, one expects the static moments $\langle x^n \rangle_{\rm MF}$ to agree with the exact expressions $\langle x^n \rangle$. Equations (12) and (42) bear this out.

The variance of x is, however, another matter. This involves the square of the mean, and therefore the result depends on whether the configuration averaging is done before or after the mean is squared. The exact answer, given by (15), differs from that in the MFA, (43). We note that this remains so even if the mean value of x is zero, i.e., even if $x_a + x_b = 0$. (In other words, the discrepancy cannot be removed by merely changing the reference level of x.) We find

$$\langle \langle (\Delta x^2) \rangle / \langle (\Delta x)^2 \rangle_{MF} = 1 - (2/9)\sigma(1 - \sigma)(1 - 4\rho)^2.$$
 (47)

The MFA therefore overestimates the variance. For a given value of the randomness parameter σ , the discrepancy decreases as the asymmetry parameter ρ increases from 0 to 1/4 (at which point the difference vanishes), and then increases again as ρ increases from 1/4 to 1. Figure 2(a) illustrates this for the maximally disordered case, $\sigma=1/2$. When $\rho=1/2$ (the symmetric or unbiased case), the ratio in (47) is 17/18, so that the MFA overestimates the true variance by 1/17, or by about 6%. The same figure obtains also in the case $\rho \to 0$, even though one might naively expect the discrepancy to vanish as the bias factor for a transition from the state a to the branch state α (or from b to β) tends to zero. The reason, of course, is that the value $\sigma=1/2$ implies that the configuration of states is 'asymmetric' (i.e., either B or C) in 50% of the

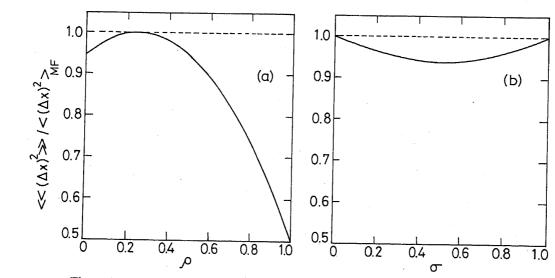


Figure 2. The ratio of the exact configuration-averaged variance of x to the variance in the mean-field approximation, (a) as a function of the asymmetry or bias parameter ρ , for $\sigma = 1/2$; (b) as a function of the randomness parameter σ , for $\rho = 1/2$.

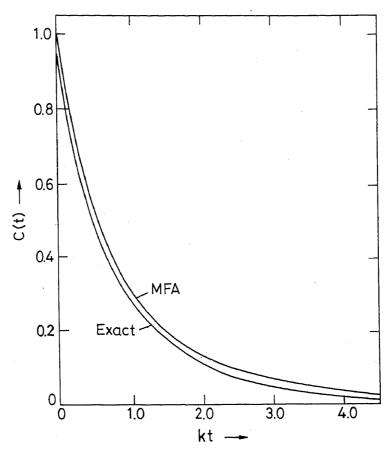


Figure 3. The correlation function of x, in units of $(1/4)(x_a - x_b)^2$, as a function of time, in the case $\sigma = 1/2$, $\rho = 1/2$.

realizations; and even at $\rho = 0$, $P_B^{st}(a) \neq P_B^{st}(b)$ (and similarly for realization C). As $\rho \to 1$, the discrepancy given by (47) increases: the MFA can then overestimate the true variance by as much as 100%, in the case of maximal disorder ($\sigma = 1/2$). (See also the comment following (A.14) in Appendix A.)

For a fixed value of the asymmetry parameter ρ , the difference between the exact variance and the MFA result is largest for $\sigma = 1/2$, as expected. This is illustrated in figure 2(b), drawn for $\rho = 1/2$ (no bias present). The ratio in (47) is again 17/18 at $\sigma = 1/2$, so that the error is about 6% at its largest.*

The variance is just the t=0 limit of the correlation function C(t). In order to get a quantitative estimate of the difference between $C_{\rm MF}(t)$ and the exact correlation C(t), we have plotted these functions in figure 3 in the symmetric ($\rho=1/2$), maximally disordered ($\sigma=1/2$) case. From (19), we find that C(t) is given in this case by

$$C(t) = (1/4)(x_a - x_b)^2 [(1/3)\exp(-kt) + (1/4)\exp(-2kt)(1 + \cosh(\sqrt{2}kt)) + (1/\sqrt{2})\sinh(\sqrt{2}kt)) + 1/9\exp(-3kt)],$$
(48)

^{*} Clearly, higher order cumulants calculated in the MFA would also deviate from the exact configuration-averaged values, for a reason essentially similar to that in the case of the variance.

which is a superposition of five exponentials: we have

$$C(t) = (1/4)(x_a - x_b)^2 [0.2134 \exp(-0.5858 kt) + 0.3333 \exp(-kt) + 0.25 \exp(-2kt) + 0.1111 \exp(-3kt) + 0.0366 \exp(-3.4142 kt)].$$
(49)

On the other hand, $C_{\rm MF}(t)$ is a superposition of three exponentials, given in this case $(\rho = 1/2, \sigma = 1/2)$ by (see Appendix B)

$$C_{\rm MF}(t) \simeq (1/4)(x_a - x_b)^2 \left[0.2411 \exp\left(-0.4486 kt\right) + 0.5769 \exp\left(-1.4268 kt\right) + 0.1820 \exp\left(-3.1246 kt\right) \right]. \tag{50}$$

The behaviour of C(t) at long times is controlled by the smallest relaxation rate. In the particular model under consideration, this occurs in realization D, which can be regarded as a linear chain of four sites (ordered α , a, b, β , with transition rates as in figure 1). The (exact) value of the smallest relaxation rate is

$$\lambda_{\min} = [5/2 - \rho - (9/4 - \rho + \rho^2)^{1/2}]k,\tag{51}$$

which is less than k. In the symmetric case $\rho = 1/2$, this becomes $\lambda_{\min} = (2 - \sqrt{2})k \simeq 0.5858k$. In contrast, the smallest relaxation rate predicted by the MFA (for the values $\rho = 1/2$, $\sigma = 1/2$ of the parameters ρ and σ) is about 0.4486k, a relative error of about 23%, but this is compensated for by the differences in the coefficients weighting the exponentials in the two cases. It is evident from figure 3 that the MFA is a rather good approximation to the exact solution even in the maximally disordered case $(\sigma = 1/2)$.

The relaxation rates as predicted by the MFA are given by the negatives of the zeroes of the cubic d(u) ((B.5), Appendix B.) We note that these rates are dependent on both ρ and σ in the MFA, owing to the occurrence of σ in the effective WTD $\psi(t)$, whereas the exact rates are of course independent of the randomness parameter σ . We may examine further how this spurious dependence affects the long-time behaviour of $C_{\rm MF}(t)$. As $\rho \to 1$, we see that $\lambda_{\rm min} \to 0$, which is to be expected. (The smallness of the $a \to b$ and $b \to a$ transition rates as $\rho \to 1$ leads to very slow relaxation.) We find

$$\lambda_{\min} \simeq (4/3)k(1-\rho) \tag{52}$$

correct to first order in $(1 - \rho)$. In the MFA, too, the smallest relaxation rate tends to zero as $\rho \to 1$, but we find (see Appendix B, Eq. B.7)

$$(\lambda_{\min})_{MF} \simeq (4/3)k(1-\rho)(2-\sigma)^{-1}$$
 (53)

to first order in $(1 - \rho)$. ((52) and (53) agree at $\sigma = 1$.) At the other extreme, as $\rho \to 0$, we find that λ_{\min} approaches k (from below), according to

$$\lambda_{\min} \approx k - (2/3)k\rho + 0(\rho^2). \tag{54}$$

In the MFA, we find (from Appendix B, Eq. (B.8))

$$(\lambda_{\min})_{\rm MF} \simeq k - 2k\rho + 0(\rho^2) \tag{55}$$

for all σ except the limiting value $\sigma = 1$. (In the limiting case $\sigma = 1$, the MFA coincides with the exact solution, as discussed below. Hence $(\lambda_{\min})_{MF}$ behaves as in (54) when $\sigma = 1$ and $\rho \to 0$.)

What are the main qualitative differences between the exact solution and the MFA in a problem of this kind? We have, first, the differences in the expressions for the cumulants (as exemplified by the variance) owing to the premature configuration-averaging performed in the MFA. The second feature is the spurious dependence of the dynamics (i.e., the relaxation rates) on the parameter σ characterizing the disorder, again arising for essentially the same reason. A third feature, related to the second, is the introduction of non-Markovian effects into what is essentially a Markovian random walk on a set of sites with quenched 'spatial' disorder. We have already discussed the first two aspects in the foregoing.

The third aspect arises in the MFA because the effective waiting-time density (in the present problem, $\psi(t)$ is not a simple exponential function of time, implying that successive transitions governed by the WTD are temporally correlated in a non-Markovian manner. The origin of this effect lies in the 'bunching up' of more than one state of the original Markov chain into a single 'level'. In the model under consideration, the two states a and α (respectively, b and β) are bunched together in the MFA into a 'level' in which $x = x_a$ (respectively, $x = x_b$), and then we speak of transition probabilities $\mathbb{P}(x_a, t|x_b)$, etc., from one level to another. It is evident that similar comments apply to more complicated situations, such as diffusion on a random comb (White and Barma 1984; Havlin et al 1987; Goldhirsch and Noskowicz 1987; Balakrishnan and Van den Broeck 1990). In the latter case, we have an arbitrary number of 'branch' states connected to each 'principal' state (or site on the backbone of the comb), with a prescribed number distribution. All these states are bunched together in the MFA to compute the effective WTD at each backbone site for inter-site transitions. It is this 'projection' of states that is responsible for the non-Markovian effects in the MFA.

Finally, it is worth noting that the MFA we have developed can be checked, in some sense, by the following consistency test. (In particular, we have in mind the correctness of our expressions for the effective WTD ψ and the effective FWTD ψ_1). In the absence of the (quenched) disorder, we should expect the MFA to coincide with the exact calculation, as there is no configuration-averaging involved. The disorder disappears in the limits $\sigma = 0$ (no branch sites at all) and $\sigma = 1$ (branch sites present with probability one.) The limit $\sigma = 0$ is a trivial one – only the two-state configuration A survives. It is easily verified (see Appendix B, (B.9) and (B.10)) that the MFA, too, reduces to this solution when $\sigma = 0$. At the other extreme, when $\sigma = 1$, only the realization D survives. Thus

$$[C(t)]_{\sigma=1} = C_{\mathbf{D}}(t) \tag{56}$$

where $C_D(t)$ is given explicitly in (A.11). On setting $\sigma = 1$ in the MFA (see Appendix B, (B.11) and (B.12)), we find that

$$[C_{\rm MF}(t)]_{\sigma=1} = C_{\rm D}(t)$$
 (57)

showing that the mean field solution matches the exact solution in the limit $\sigma = 1$ as well.

In conclusion, the mean field approximation we have developed for the problem under consideration reduces to the exact solution in the absence of disorder, as it

should; further, it is a rather good approximation to the exact solution even when the disorder is maximal, as may be seen at a glance from the behaviour of the correlation function in figure 3.

Acknowledgement

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Appendix A

In realization A, the indices i, j run over the two values a and b. The resolvent $G_A = (u - W_A)^{-1}$ is the 2 × 2 matrix

$$G_{\mathbf{A}} = \Delta_{\mathbf{A}}^{-1} \begin{pmatrix} u+k & k \\ k & u+k \end{pmatrix}, \quad \Delta_{\mathbf{A}} = u(u+2k).$$
 (A1)

The correlation function is given by (17), and in this case it is simply

$$C_A(t) = (1/4)(x_a - x_b)^2 \exp(-2kt).$$
 (A2)

In realization B, i and j run over the values α , a and b, in that order. The resolvent matrix is found to be

$$G_{\rm B} = \Delta_{\rm B}^{-1} \begin{pmatrix} u^2 + 3uk + 2k^2\rho & 2k\rho(u+k) & 2k^2\rho \\ k(u+k) & (u+k)^2 & k(u+k) \\ 2k^2(1-\rho) & 2k(1-\rho)(u+k) & u^2 + 3uk + 2k^2(1-\rho) \end{pmatrix}$$
(A3)

where

$$\Delta_{\mathbf{B}} = u(u+k)(u+3k). \tag{A4}$$

After a bit of algebra, (17) yields in this case

$$C_{\rm B}(t) = (2/9)(x_a - x_b)^2 (1 - \rho) [3\rho \exp(-kt) + (1 - \rho)\exp(-3kt)]. \tag{A5}$$

Realization C is obtained from B by the replacements $a \to b$, $b \to a$, $\alpha \to \beta$. The indices i, j now run over the values a, b and β , in that order. The resolvent matrix $G_{\rm C}$ is therefore obtained from $G_{\rm B}$ by reflecting each element of the latter about the centre of the matrix. ($\Delta_{\rm C}$ is evidently equal to $\Delta_{\rm B}$.) Moreover, the correlation function $C_{\rm B}(t)$ is symmetric under the interchange $x_a \leftrightarrow x_b$, so that it remains unchanged in realization C, i.e.,

$$C_{C}(t) = C_{B}(t). \tag{A6}$$

(We note that going from B to C does not involve replacing the asymmetry parameter ρ by $1 - \rho$.)

In realization D, i and j run over α , a, b and β , in that order. The resolvent is given by

$$G_{\mathbf{D}} = \Delta_{\mathbf{D}}^{-1} g \tag{A7}$$

where

$$\Delta_{\rm D} = u(u + (1 + 2\rho)k)(u^2 + (5 - 2\rho)uk + 4k^2(1 - \rho)),\tag{A8}$$

and the (4×4) matrix g has the following elements (using the symmetry properties of the configuration D):

$$g_{11} = g_{44} = u^3 + 5u^2k + 2(2 + 3\rho - 2\rho^2)uk^2 + 4k^3\rho(1 - \rho),$$

$$g_{12} = g_{43} = 2k\rho(u^2 + 3uk + 2k^2(1 - \rho))$$

$$g_{13} = g_{42} = 4k^2\rho(1 - \rho)(u + k),$$

$$g_{14} = g_{41} = 4k^3\rho(1 - \rho),$$

$$g_{21} = g_{34} = k(u^2 + 3uk + 2k^2(1 - \rho)),$$

$$g_{22} = g_{33} = (u + k)(u^2 + 3uk + 2k^2(1 - \rho)),$$

$$g_{23} = g_{32} = 2k(1 - \rho)(u + k)^2,$$

$$g_{24} = g_{31} = 2k^2(1 - \rho)(u + k).$$
(A9)

After some algebra, we obtain the following expression for the transform of the correlation function in realization D:

$$\widetilde{C}_{D}(u) = (1/4)(x_a - x_b)^2 \left[\frac{(1 + 2\rho)u + k(1 + 12\rho - 4\rho^2)}{(1 + 2\rho)\{u^2 + (5 - 2\rho)uk + 4k^2(1 - \rho)\}} \right].$$
 (A10)

We note that the factor $(u + (1 + 2\rho)k)$ in Δ_D gets cancelled out, so that there is no contribution to $C_D(t)$ from the relaxation rate $k(1 + 2\rho)$. Inverting the transform in (A10), we get

$$C_{D}(t) = (1/4)(x_{a} - x_{b})^{2} \exp\left[-(5/2 - \rho)kt\right]$$

$$\times \left[\cosh(rkt) + \frac{(8\rho - 2\rho^{2} - 3/2)}{r(1 + 2\rho)}\sinh(rkt)\right],$$
(A11)

where

$$r = (9/4 - \rho + \rho^2)^{1/2}. (A12)$$

As a simple check, we consider the limiting cases $\rho = 0$ and $\rho = 1$. We find, first,

$$\lim_{a \to 0} C_{\rm D}(t) = (1/4)(x_a - x_b)^2 \exp(-4kt). \tag{A13}$$

This is precisely what one should expect: $P^{st}(\alpha) = P^{st}(\beta) = 0$ in this case, and the rates for the transitions $a \to b$ and $b \to a$ are equal, each given by 2k. This is similar to the situation in realization A, except that k is replaced by 2k. Similarly, we find that

$$\lim_{\rho \to 1} C_{\rm D}(t) = (1/4)(x_a - x_b)^2, \tag{A14}$$

with no t-dependence at all. But when $\rho=1$, the $a\to b$ and $b\to a$ rates vanish, so that the configuration is essentially split into two disjoint pieces (α,a) and (b,β) with no time evolution of the value of x possible. Hence $C_{\mathbf{D}}(t)$ remains unaltered from its initial (equilibrium) value $C_{\mathbf{D}}(0)$ in this limiting case.

Combining (A2), (A5), (A6) and (A11), we get eq. (18) for C(t).

Appendix B

In the MFA, x(t) is a dichotomic process with an effective waiting time density $\psi(t)$ in each of the levels x_a , x_b . Contributions to the transition probability $\mathbb{P}(x_b, t|x_a)$ must necessarily involve an odd number (2l+1) of jumps $x_a \to x_b \to x_a \to \cdots \to x_b$, and the corresponding probabilities are in convolution. Hence

$$\widetilde{\mathbb{P}}(x_b, u | x_a) = \sum_{l=0}^{\infty} \widetilde{\psi}_1(\widetilde{\psi})^{2l} (1 - \widetilde{\psi}) / u, \tag{B1}$$

where $\psi_1(t)$ is the FWTD (the WTD for the first jump from an arbitrary origin of time), and the final factor $(1 - \tilde{\psi})/u$ is the transform of the holding time distribution corresponding to the WTD $\psi(t)$: this factor takes care of the requirement that no more than (2l+1) jumps occur in the time interval t. Therefore

$$\widetilde{\mathbb{P}}(x_b, u|x_a) = \widetilde{\psi}_1/[u(1+\widetilde{\psi})],\tag{B2}$$

which is (40).

To find $\tilde{C}_{MF}(u)$ from (46), we use (27), (28) and (33). Substituting the expressions $\tilde{\phi} = k(u+k)^{-1}$ and $\tilde{\chi} = 2k(u+2k)^{-1}$ in these, and simplifying, one obtains

$$\tilde{C}_{MF}(u) = (1/4)(x_a - x_b)^2 (n(u)/d(u)),$$
(B3)

where

$$n(u) = (1 + 2\rho)u^{2} + (3 - \sigma + 6\rho + 8\sigma\rho - 4\sigma\rho^{2})uk + (2 - \sigma + 2\rho + 10\sigma\rho - 4\rho^{2})k^{2},$$
(B4)

and

$$d(u) = (1 + 2\rho)[u^3 + (5 + \sigma - 2\sigma\rho)u^2k + (8 - 2\rho + \sigma - 4\sigma\rho)uk^2 + 4(1 - \rho)k^3].$$
(B5)

 $C_{\rm MF}(t)$ decays to zero from the value $(x_a-x_b)^2/4$ at t=0 via a superposition of three exponentials, the rates being given by the negatives of the roots of d(u)=0. (This cubic equation has three real, negative roots in the physical range of the parameters σ and ρ .) In the special case $\rho=1/2$, $\sigma=1/2$, we get

$$\widetilde{C}_{\rm MF}(u) = (1/4)(x_a - x_b)^2 \left[\frac{2u^2 + 7uk + 4k^2}{2u^3 + 10u^2k + 13uk^2 + 4k^3} \right]. \tag{B6}$$

The roots of the denominator are -0.4486k, -1.4268k and -3.1246k. Using these to invert the transform, we obtain (50) for $C_{\rm MF}(t)$.

The long-time behaviour of $C_{\rm MF}(t)$ is controlled by the zero of d(u) with the smallest magnitude, as discussed in the text. As $\rho \to 1$, this root approaches 0. Calling this root $-(\lambda_{\rm min})_{\rm MF}$, we find

$$(\lambda_{\min})_{MF} = (4/3)k(1-\rho)(2-\sigma)^{-1} + \alpha((1-\rho)^2).$$
(B7)

Again, as $\rho \to 0$, this root approaches -k. We now find

$$(\lambda_{\min})_{MF} = k(1 - 2\rho) + \alpha(\rho^2), \tag{B8}$$

provided $\sigma \neq 1$. (The case $\sigma = 1$ is dealt with below.)

We need the limiting cases of the MFA corresponding to the values $\sigma = 0$ and $\sigma = 1$ for the discussion at the end of § 3.4. Setting $\sigma = 0$ in (27) and (30) we obtain

$$[\psi(t)]_{\sigma=0} = [\psi_1(t)]_{\sigma=0} = \phi(t),$$
 (B9)

(as expected.) Equations (B3)-(B5) yield

$$[C_{\rm MF}(t)]_{\sigma=0} = (1/4)(x_a - x_b)^2 \exp(-2kt), \tag{B10}$$

which is the same as $C_A(t)$ (eq. (A2)), as required.

Setting $\sigma = 1$ in (26) and (28), we get

$$[\psi(t)]_{\sigma=1} = \phi_{ab}(t), \quad [\psi_1(t)]_{\sigma=1} = \Phi(t).$$
 (B11)

Here $\phi_{ab}(t)$ and $\Phi(t)$ are the densities given by (25) and (34). Further, (B3)–(B5) give after simplification (a factor (u+k) cancels out between n(u) and d(u))

$$[\tilde{C}_{MF}(u)]_{\sigma=1} = (1/4)(x_a - x_b)^2$$

$$\times \left[\frac{(1+2\rho)u + k(1+12\rho - 4\rho^2)}{(1+2\rho)\{u^2 + (5-2\rho)uk + 4k^2(1-\rho)\}} \right].$$
 (B12)

But this is precisely $\tilde{C}_D(u)$, given by (A10). The MFA thus coincides with the exact solution in the limiting cases of vanishing disorder ($\sigma = 0$ and $\sigma = 1$).

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