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Perturbation theory for the one-dimensional trapping reaction

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Abstract

We consider the survival probability of a particle in the presence of a finite number of diffusing traps in one dimension. Since the general solution for this quantity is not known when the number of traps is greater than two, we devise a perturbation series expansion in the diffusion constant of the particle. We calculate the persistence exponent associated with the particle's survival probability to second order and find that it is characterized by the asymmetry in the number of traps initially positioned on each side of the particle.

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1. Introduction

Our understanding of the nonequilibrium dynamics of many-body systems has been greatly advanced through the study of particle reaction models. Typically, these models involve a number of particles of different species that undergo reactions which lead to a lack of conservation of particle number. Whilst the most obvious physical application is to the kinetics of chemical reactions [1, 2], these models also enjoy mappings to a range of phenomena. These include interfacial growth [3], domain coarsening in magnetic media and fluids [4, 5] and aggregation [6]. Reaction–diffusion systems have also held their own as prototypes for the development of theoretical tools, such as field-theoretic techniques [8], the renormalization group [7] and exact methods in low dimensions [9].

In this work, we consider the dynamics of the $A + B \rightarrow \emptyset$ reaction, i.e. a system comprising two particle species that mutually annihilate (or form an inert product) on contact. This problem was introduced in the seminal paper of Toussaint and Wilczek [10] as a model of monopole–antimonopole annihilation in the early universe. Since then, there have been applications to chemical kinetics and condensed matter physics—see, for example, [11] for a review.

In a reaction system, such as $A + B \to \emptyset$, one is chiefly interested in the concentration of A and B particles after time t given some initial condition. The 'traditional' approach to the problem is to write down differential *rate equations* for the density of each particle species, denoted by $\rho_A(\vec{x}, t)$ and $\rho_B(\vec{x}, t)$ respectively [1]. One has for ρ_A

$$\frac{\partial \rho_A(\vec{x}, t)}{\partial t} = D_A \nabla^2 \rho_A - r\rho_A\rho_B \tag{1}$$

and the same equation for ρ_B if one exchanges the labels A and B. In words, this equation says that both particle species diffuse with diffusion constants D_A and D_B and particles are removed at a rate proportional to the reaction constant r and the joint probability to find an A–B pair at coordinate $\vec{x}$ at time t. Under the assumption that the particles are well mixed at all times, $\rho_{A,B}(\vec{x}, t) = \rho_{A,B}(t)$ and one can neglect the Laplacian in the rate equations. In physics parlance, this is equivalent to making a mean-field approximation which becomes exact in the 'reaction-limited' regime where the reaction rate is slow compared to the diffusion rate. Here, we are interested in the opposite 'diffusion-limited' regime.

The long-time form of ρ_A and ρ_B depends on whether the initial numbers of A and B particles are equal or not. Consider first the case $\rho_A(0) = \rho_B(0)$. Since each reaction event removes both an A and a B particle, their densities remain equal at all times. Then, we have for $\rho(t) = \rho_A(t) = \rho_B(t)$

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -r\rho^2 \tag{2}$$

whose solution at large times is $\rho(t) \sim 1/(rt)$. It turns out that this behaviour holds only in more than four dimensions. Through rigorous bounding arguments [12] and renormalization group analysis [13] it is now well understood that in dimensions $d < 4$ the density decays as $\rho(t) \sim 1/t^{d/4}$. These results serve as a reminder of the importance of density fluctuations and correlations in low dimensions, which were explicitly ignored in the mean-field approach. Also we note that, in this problem, there exists a *dynamical scaling regime* in which the characteristic length-scale in the problem (here the interparticle separation $\ell = \rho^{-1/d}$) is related to a characteristic timescale through a power-law.

When the initial densities of A and B particles are not equal, the situation is somewhat different. Consider an initial condition that has $\rho_A(0) < \rho_B(0)$. Then, as time progresses the $A + B \to \emptyset$ reaction implies that the ratio $\rho_A(t)/\rho_B(t)$ decreases. Eventually, one has a small number of A particles in a sea of B particles whose density remains effectively constant. In the rate-equation formalism (1) we have, under the assumption that particles are well mixed and $\rho_B(t) = \text{const} = \rho_B$, that the density of A particles decays as $\rho_A(t) \sim \mathrm{e}^{-r\rho_B t}$. Again it is known that this result holds only in a space of suitably large dimensionality. In particular, Bramson and Lebowitz [12] used bounding arguments to show that, at long times, the A particles experience a stretched-exponential decay $\rho_A(t) \sim \mathrm{e}^{-\lambda_d t^{d/2}}$ in fewer than two dimensions, and $\rho_A(t) \sim \mathrm{e}^{-\lambda_2 t/\ln t}$ in the critical dimension $d = 2$. Values of the constants λ_d for $d \leqslant 2$ were recently reported by us [14] with the details to be presented elsewhere [15].

Clearly, the special case of a single A particle in the presence of a sea of B particles will be governed by these asymptotics. Then, one can interpret $\rho_A(t)$ as the *survival probability* of the A particle. If the distribution of B particles is homogeneous over all space, and the diffusion constants of the A and B particles are the same, one can also view $\rho_A(t)$ as the fraction of particles that have not met any other particles. Thus the reaction $A + B \to \emptyset$ in the limit of a low density of A particles has been discussed under the guises of *uninfected walkers* [16] in which random walkers infect each other on contact, *diffusion in the presence of traps* [17, 18] in which the B particles are considered as traps for the A particles, and *predator–prey models* [19] in which one asks for the survival of a prey (the A particle) being 'chased' by diffusing predators (the B particles). To avoid confusion, we shall use only the trapping terminology, and in this work we restrict ourselves to the case of a single A particle and a *finite* number of diffusing traps (B particles) in one spatial dimension. When we make no distinction between the particle and the traps, we shall use the generic term *walkers*.

Before we formally introduce our model and review some exactly known results, let us make a few comments about the relationship between the trapping reaction and *persistence* in diffusive systems. Persistence is a property that can be defined for any stochastic dynamical system as it is simply the probability that a random variable does not change sign between time 0 and a time t. In many cases, a persistence probability $Q(t)$ decreases as a power-law in time, $Q(t) \sim t^{-\theta}$ in which θ is a *persistence exponent* (see, e.g., [20] for a review). In the trapping reaction, we can define two distinct persistence properties: (i) a *site* persistence, which measures the probability that a particular point in space (or site on a lattice) has not been crossed by any walker; and (ii) a *walker* persistence, which is the probability that a particular walker (here the A particle) has not yet met another walker. In this terminology, one can make the transition from walker to site persistence by decreasing the particle's diffusion constant to zero. Then the particle is static, and the probability that it survives is equal to the probability that a particular point has not been crossed.

In the following section, we will show that the site persistence probability in the presence of N traps in one dimension is known exactly to decay with an exponent $\theta = N/2$. On the other hand, the more general walker persistence probability, where the particle has a nonzero diffusion constant, is not known exactly. The principal purpose of this paper is to present the full details of a perturbation theory for the walker persistence exponent that was outlined in a previous work [14]. As well as describing the approach in greater detail, we also extend the calculation to second order in (a quantity closely related to) the particle's diffusion constant. We find that the persistence exponent depends on a quantity that characterizes the level of asymmetry between the number of traps initially positioned to each side of the particle.

To close this introductory section, we make a few remarks as to why the case where both the particle and the traps diffuse is considerably more complicated than that in which either species is static (the case of static traps is sometimes referred to as the Donsker–Varadhan problem [17] for which the particle persistence decays as a stretched exponential). When the particle is static, the probability that none of the N independently diffusing traps has crossed a particular point is simply the product of probabilities for each of the traps separately not to have crossed that point. However, any movement of the particle (in the subset of trajectories for which the particle survives) correlates the motion of the traps, and so the probabilities for each of the traps not to have met the particle are no longer independent. To understand this point more clearly, consider a set of walkers on the one-dimensional lattice. When the particle takes a step to the left (say), all the traps to the left hop one site closer to the particle in concert, whereas those to the right all hop one site away. It is this collective motion of the traps in the particle's frame of reference that makes the problem very difficult mathematically, and as far as we are aware, exact expressions for the walker persistence exponent are known only when the number of traps $N \leqslant 2$.

In the following section, we discuss these known results more quantitatively, and make the connection to isotropic diffusion in an N-dimensional 'hyperwedge' geometry. Then, in section 3, we describe how one sets up a perturbation theory using a path-integral approach. A judicious choice of timescale reveals that the natural parameter in the perturbation expansion has a geometric significance in the hyperwedge problem. In section 4 we go on to calculate the coefficients of the first- and second-order terms in the perturbation expansion, before concluding with some discussion and open questions.

2. Model definition and review of known results

The model we consider is defined as follows. At time $t = 0$, a particle is placed at the origin of a one-dimensional space $x_0(0) = 0$. Additionally, a set of mobile traps are placed at positions $x_i(0) = y_i$ with $i = 1, 2, \ldots, N$ such that N is the number of traps. We will at times need to distinguish between those traps initially placed to the left and right of the particle. To this end, we introduce the shorthand $\sigma_i = \mathrm{sgn}(y_i)$ and the quantities N_L and N_R which are the numbers of traps that have $\sigma_i < 0$ and $\sigma_i > 0$ respectively.

The system evolves through the independent diffusion of the particle and traps. We shall take the diffusion constant of the particle to be D' and that of the traps to be D. Then, we can write a Langevin equation

$$\dot{x}_i = \eta_i(t) \tag{3}$$

in which $\eta_i(t)$ is a Gaussian white noise with zero mean and correlator

$$\langle \eta_i(t)\eta_j(t')\rangle = 2D_i\delta_{i,j}\delta(t'-t) \tag{4}$$

where $D_0 = D'$ and $D_i = D$ for $i \neq 0$.

If, at any time, a trap coordinate $x_i(t)$ coincides with the particle coordinate $x_0(t)$, the particle becomes 'trapped'. We seek an expression for the *survival probability* $Q(t)$, i.e. the probability that the particle has not yet fallen into a trap.

It is convenient to work in the particle's frame of reference and so we introduce the relative coordinates $X_i(t) = x_i(t) - x_0(t)$ and their initial values $Y_i = y_i$ since $x_0(0) = 0$. Then the connection to persistence becomes clearer, since $Q(t)$ is the probability that none of the variables X_i has changed sign until a time t. From (3) and (4) we obtain the underlying Langevin equations in the variables X_i. These read

$$\dot{X}_i = \xi_i(t) \tag{5}$$

in which the noise $\xi_i(t)$ has mean zero and correlator

$$\langle \xi_i(t)\xi_j(t')\rangle = 2(D\delta_{i,j} + D')\delta(t'-t) \equiv 2D_{ij}\delta(t'-t). \tag{6}$$

Here we have introduced the matrix $D_{ij} = D\delta_{i,j} + D'$ which expresses the way in which the traps' trajectories are correlated in the frame of reference of a diffusing particle (i.e. when $D' \neq 0$).

In the introduction, we remarked that the survival probability $Q(t)$ can be calculated exactly when $D' = 0$. Although this is a classic result (see, e.g., [21]), we present the details of the calculation here as it will be needed when calculating the coefficients in the perturbation expansion that we construct for general D' in the next section.

We begin by writing down the Fokker–Planck equation for the probability distribution function $G_N(\{X\}, t|\{Y\})$ that holds when $D' = 0$. It reads

$$\frac{\partial}{\partial t} G_N(\{X\}, t|\{Y\}) = D \sum_{i=1}^{N} \frac{\partial^2}{\partial X_i^2} G_N(\{X\}, t|\{Y\}) \tag{7}$$

and is subject to the absorbing boundary condition $G_N = 0$ if any of the X_i are zero (i.e. when a trap meets the stationary particle). Clearly, since the traps diffuse independently, the solution of this equation is just

$$G_N(\{X\}, t|\{Y\}) = \prod_{i=1}^{N} G_1(X_i, t|Y_i) \tag{8}$$

where $G_1(X, t; Y)$ is the probability for a walker starting at Y to be at X and not to have crossed the origin up to time t. For a walker starting at $Y > 0$, this quantity is given by

$$G_1(X, t|Y) = \frac{1}{\sqrt{4\pi Dt}} \left[\exp\left(-\frac{(X-Y)^2}{4Dt} \right) - \exp\left(-\frac{(X+Y)^2}{4Dt} \right) \right] \tag{9}$$

for $X > 0$. We note that this is the correct solution since the two terms on the right-hand side separately obey (7) with $N = 1$ and this particular combination of solutions satisfies the boundary condition $G_1(0, t|Y) = 0$.

To obtain the probability for a walker starting at Y not to have crossed the origin until time t we simply integrate (9) over all $X > 0$ to find

$$Q_1(t|Y) = \operatorname{erf}\left(\frac{Y}{2\sqrt{Dt}} \right). \tag{10}$$

Note that, by symmetry, we must have $Q_1(t|-Y) = Q_1(t|Y)$ so the general result is

$$Q_1(t|Y) = \operatorname{erf}\left(\frac{|Y|}{2\sqrt{Dt}} \right). \tag{11}$$

Finally, using (8) we find that the probability that none of the traps has met the stationary particle is

$$Q_N(t) = \prod_{i=1}^{N} \operatorname{erf}\left(\frac{|Y_i|}{2\sqrt{Dt}} \right) \sim \left(\frac{1}{\pi Dt} \right)^{N/2} \prod_{i=1}^{N} |Y_i| \tag{12}$$

in which we have used the fact that

$$\operatorname{erf} x = \frac{2}{\sqrt{\pi}} \left(z - \frac{z^3}{3} + \cdots \right) \tag{13}$$

to obtain a form for $Q_N(t)$ valid at large times $t \gg |Y|^2_{\max}/D$. This is long enough for *all* the traps to have had ample opportunity to reach the particle. The persistence exponent θ associated with the survival probability $Q(t)$ can be defined formally as

$$\theta = -\lim_{t\to\infty} t \frac{\mathrm{d}}{\mathrm{d}t} \ln Q(t) \tag{14}$$

and so for the case $D' = 0$ we have from (12) that $\theta = N/2$.

It is instructive to consider an approach that has been used (see [19, 22] for a more in-depth overview) to find the persistence exponent θ exactly for the case $N = 2$ and $D' \neq 0$ since it will reveal a connection with the perturbation series that we derive in the next section.

The essence of this approach is to perform a second coordinate transformation that renders the correlated diffusion described by equations (5) and (6) isotropic in the N-dimensional space spanned by the coordinates X_i. To perform this transformation, one considers the diffusion matrix $D_{ij} = D\delta_{i,j} + D'$. The eigenvectors of this matrix indicate the directions in which the N-dimensional diffusion is independent whilst the corresponding eigenvalues give the diffusion constants in those directions. One finds that one of the eigenvectors is $(1, 1, 1, \ldots, 1)$ and has an eigenvalue $D + ND'$. The remaining eigenvectors are degenerate with eigenvalue D and hence form a basis set in the $(N-1)$-dimensional space perpendicular to $(1, 1, 1, \ldots, 1)$. In order to make the diffusion isotropic, one must scale in the $(1, 1, 1, \ldots, 1)$ direction by a factor $(1 + ND'/D)^{-1/2}$.

Whilst this coordinate transformation gives rise to simple, isotropic diffusion in the N-dimensional space, the boundary conditions become more complicated. In the space spanned by the variables X_i, the absorbing boundary is constructed from the set of orthogonal planes that have $X_i = 0$ with $i = 1, 2, \ldots, N$. The coordinate transformation just described rotates these planes so that they are no longer orthogonal. It is a straightforward exercise in linear algebra to determine that the angle between two planes i and j in the transformed coordinate system is $\Theta_{ij} = \arccos(-\sigma_i\sigma_j\alpha_N)$ in which the parameter α_N takes the form

$$\alpha_N = \frac{D'}{D + (N-1)D'}. \tag{15}$$

Hence two planes that correspond to traps that start on opposite sides of the particle close up whereas two planes that correspond to traps starting on the same side of the particle open out.

To determine the persistence exponent θ given by equation (14) it is necessary to solve the diffusion equation in an N-dimensional wedge geometry. As far as we know, results are available only for the case of a two-dimensional wedge [22, 23]. Then, the particle's survival probability decays with the exponent

$$\theta = \frac{\pi}{2\Theta_{12}}. \tag{16}$$

For the case where both traps initially surround the particle, we have $\sigma_1\sigma_2 = -1$ and so

$$\theta = \frac{\pi}{2\arccos\alpha_2}. \tag{17}$$

Similarly when both traps are initially positioned to one side of the particle, we have $\sigma_1\sigma_2 = 1$ and thus

$$\theta = \frac{\pi}{2(\pi - \arccos\alpha_2)} \tag{18}$$

since $\arccos(-x) = \pi - \arccos(x)$.

Although this approach has thus far proved intractable for $N > 2$, we have spent some time outlining it because, in the perturbation theory that we construct below, it turns out that the natural expansion parameter is the quantity α_N introduced above. Note that $\alpha_N = 0$ corresponds to the case where the particle is static and the N-dimensional hyperwedge is in fact a corner of an N-dimensional hypercube. Thus the expansion for small α_N derived below using an alternative path-integral approach gives results for diffusion in a geometry perturbed from an N-dimensional hypercube.

3. Perturbation expansion via a path-integral approach

The starting point in the derivation of a perturbation expansion for the persistence exponent θ is to note that the statistical weight of a particular set of trajectories $\vec{X}(t) = [X_1(t), X_2(t), \ldots, X_N(t)]$ governed by equations (5) and (6) can be written in the form $\mathrm{e}^{-S[\vec{X}]}$. In this expression, $S[\vec{X}]$ is an 'action' functional defined as

$$S[\vec{X}] = \frac{1}{4}\sum_{i,j=1}^{N}[D^{-1}]_{ij}\int_0^t \mathrm{d}t'\,\dot{X}_i(t')\dot{X}_j(t') \tag{19}$$

in which D^{-1} is the inverse of the matrix D in equation (6). It is straightforward to show that

$$[D^{-1}]_{ij} = \frac{1}{D}\left(\delta_{ij} - \frac{D'}{D+ND'}\right). \tag{20}$$

It is helpful at this stage to introduce a rescaled time variable

$$\tau = \frac{D+ND'}{D+(N-1)D'}Dt \tag{21}$$

such that the action becomes

$$S[\vec{X}] = S_0 - \frac{D'}{D + (N-1)D'} S_1 = S_0 - \alpha_N S_1 \tag{22}$$

in which the diagonal part S_0 and off-diagonal part S_1 of the action are given by

$$S_0[\vec{X}] = \frac{1}{4} \sum_i \int_0^\tau \mathrm{d}\tau' [\dot{X}_i(\tau')]^2 \tag{23}$$

$$S_1[\vec{X}] = \frac{1}{4} \sum_{i \neq j} \int_0^\tau \mathrm{d}\tau' \dot{X}_i(\tau') \dot{X}_j(\tau') \tag{24}$$

where now a dot denotes differentiation to the rescaled time variable τ. Note that when $\alpha_N = 0$ the action $S[\vec{X}] = S_0[\vec{X}]$ which gives the statistical weight for N walkers executing *independent* diffusive motion with diffusion constant unity. We will treat the off-diagonal part (that describes the correlations between the walkers) as a perturbation with the quantity α_N given by equation (15) as the expansion parameter, as advertised.

To this end, observe that out of all possible trajectories $\vec{X}(\tau)$, only a subset corresponds to the particle surviving until time τ. These trajectories are defined through the persistence condition that $\operatorname{sgn} X(\tau') = \operatorname{sgn} X(0)$ for $0 < \tau' \leqslant \tau$. We shall use the symbol $\int_R \mathcal{D}\vec{X}(\tau)$ to denote integration over this restricted set of surviving trajectories. Then, the probability that the particle survives is

$$Q(\tau) = \frac{\int_R \mathcal{D}\vec{X}(\tau) \exp(-S[\vec{X}])}{\int \mathcal{D}\vec{X}(\tau) \exp(-S[\vec{X}])} \tag{25}$$

in which the integral of the weights over the restricted trajectories is normalized by the integral over all possible trajectories.

Now, note that the survival probability $Q_N(\tau)$ of a stationary particle in the presence of N traps diffusing independently with diffusion constant unity is given by the path-integral expression

$$Q_N(\tau) = \frac{\int_R \mathcal{D}\vec{X}(\tau) \exp(-S_0[\vec{X}])}{\int \mathcal{D}\vec{X}(\tau) \exp(-S_0[\vec{X}])}. \tag{26}$$

Combining this with (25) we find that

$$\begin{aligned} Q(\tau) &= Q_N(\tau) \frac{\int_R \mathcal{D}\vec{X}(\tau) \exp(-S[\vec{X}])}{\int_R \mathcal{D}\vec{X}(\tau) \exp(-S_0[\vec{X}])} \frac{\int \mathcal{D}\vec{X}(\tau) \exp(-S_0[\vec{X}])}{\int \mathcal{D}\vec{X}(\tau) \exp(-S[\vec{X}])} \\ &= Q_N(\tau) \frac{\langle \mathrm{e}^{\alpha_N S_1[\vec{X}]} \rangle_R}{\langle \mathrm{e}^{\alpha_N S_1[\vec{X}]} \rangle_U} \end{aligned} \tag{27}$$

in which the notation $\langle \cdot \rangle$ indicates an average over paths weighted by $\mathrm{e}^{-S_0[\vec{X}]}$ and the subscripts R and U denote the restricted and unrestricted ensembles of paths. (Recall that paths that cross the origin are excluded from the former).

To obtain a perturbative expression for the persistence exponent θ we make use of (14) and (27) to find, in the rescaled time variable τ,

$$\begin{aligned} \theta &= -\lim_{\tau \to \infty} \tau \frac{\mathrm{d}}{\mathrm{d}\tau} \ln Q(\tau) \\ &= -\lim_{\tau \to \infty} \tau \frac{\mathrm{d}}{\mathrm{d}\tau} (\ln Q_N(\tau) + \ln \langle \mathrm{e}^{\alpha_N S_1[\vec{X}]} \rangle_R - \ln \langle \mathrm{e}^{\alpha_N S_1[\vec{X}]} \rangle_U). \end{aligned} \tag{28}$$

The asymptotic form of $Q_N(\tau)$ is known from equation (12). To compute the averages of $S_1[\vec{X}]$ perturbatively, we make use of the fact that $\ln\langle e^{\lambda x}\rangle$ defines the generating function of the cumulants of x. Specifically,

$$\ln\langle e^{\lambda x}\rangle = \lambda\langle x\rangle + \frac{\lambda^2}{2}(\langle x^2\rangle - \langle x\rangle^2) + O(\lambda^3). \tag{29}$$

Putting all this together, we find that θ has a series expansion

$$\theta = \frac{N}{2} - \lim_{\tau\to\infty} \tau\frac{d}{d\tau}\left[\alpha_N(\langle S_1\rangle_R - \langle S_1\rangle_U) + \frac{\alpha_N^2}{2}\left(\langle S_1^2\rangle_R - \langle S_1\rangle_R^2 - \langle S_1^2\rangle_U + \langle S_1\rangle_U^2\right)\right] \tag{30}$$

to second order in the parameter α_N defined in equation (15). Of course, one could go to higher order by including more terms from the cumulant expansion (29).

4. Walker persistence exponent to second order

As a first step in computing the mean and variance of S_1 in the two ensembles, we shall determine the structure of these quantities. For either the restricted or the unrestricted average, we have

$$\langle S_1\rangle = \frac{1}{4}\sum_{i,j}{}' \int_0^\tau d\tau' \langle \dot{X}_i(\tau')\dot{X}_j(\tau')\rangle \tag{31}$$

in which the notation $\sum'$ means the sum over combinations of the indices such that each index is different. (Note that all permutations of a set of distinct indices are included in this sum.) Since we are averaging over ensembles of trajectories of *independently* diffusing traps, and the indices i and j are always different, we have

$$\langle S_1\rangle = \frac{1}{4}\sum_{i,j}{}' \int_0^\tau d\tau' \langle \dot{X}_i(\tau')\rangle\langle\dot{X}_j(\tau')\rangle. \tag{32}$$

Hence to calculate the mean of S_1 we must find the mean velocity of a random walk with diffusion constant unity in each of the ensembles.

For the variance of S_1 we have

$$\begin{aligned}\langle S_1^2\rangle - \langle S_1\rangle^2 = \frac{1}{16}\sum_{i,j}{}'\sum_{k,\ell}{}' \int_0^\tau d\tau_1 \int_0^\tau d\tau_2 (\langle \dot{X}_i(\tau_1)\dot{X}_j(\tau_1)\dot{X}_k(\tau_2)\dot{X}_\ell(\tau_2)\rangle \\ - \langle \dot{X}_i(\tau_1)\dot{X}_j(\tau_1)\rangle\langle\dot{X}_k(\tau_2)\dot{X}_\ell(\tau_2)\rangle).\end{aligned} \tag{33}$$

The terms in the double summation can be divided into three groups. In the first, all four indices are different, and two averages factorize to cancel. A second set of terms has two indices the same, the other two different (there are four ways this property can be satisfied). Finally, there are two ways to arrange for the indices to comprise two pairs the same. Thus the variance can be written as

$$\begin{aligned}\langle S_1^2\rangle - \langle S_1\rangle^2 = \frac{1}{16}\int_0^\tau d\tau_1 \int_0^\tau d\tau_2 \Bigg[4\sum_{i,j,k}{}' \left(\langle \dot{X}_i(\tau_1)\dot{X}_i(\tau_2)\rangle - \langle\dot{X}_i(\tau_1)\rangle\langle\dot{X}_i(\tau_2)\rangle\right) \\ \times\langle\dot{X}_j(\tau_1)\rangle\langle\dot{X}_k(\tau_2)\rangle + 2\sum_{i,j}{}' \left(\langle \dot{X}_i(\tau_1)\dot{X}_i(\tau_2)\rangle\langle\dot{X}_j(\tau_1)\dot{X}_j(\tau_2)\rangle\right. \\ \left. - \langle\dot{X}_i(\tau_1)\rangle\langle\dot{X}_i(\tau_2)\rangle\langle\dot{X}_j(\tau_1)\rangle\langle\dot{X}_j(\tau_2)\rangle\right)\Bigg]\end{aligned} \tag{34}$$

which reveals that we must calculate not just the mean velocity $\langle \dot{X}_i(\tau')\rangle$ but also the velocity correlation function $\langle \dot{X}_i(\tau_1)\dot{X}_i(\tau_2)\rangle$ over the two ensembles.

The unrestricted averages are easily found. Since each of the walkers performs diffusion with a diffusion constant of unity in the rescaled time τ, we have $\dot{X}_i(\tau') = \eta_i(\tau')$ where $\eta_i(\tau')$ is a Gaussian white noise with zero mean and a correlator $\langle \eta_i(\tau_1)\eta_i(\tau_2)\rangle = 2\delta(\tau_2-\tau_1)$. Hence

$$\langle \dot{X}_i(\tau')\rangle_U = 0 \quad \text{and} \quad \langle \dot{X}_i(\tau_1)\dot{X}_i(\tau_2)\rangle_U = 2\delta(\tau_2-\tau_1). \tag{35}$$

The restricted averages involve more work, since we must calculate the mean velocity of a walker at time τ' *given* that it survives until a later time τ; similarly, we must include the fact that the walker survives until a specified time τ in the calculation of the velocity correlation function. Before getting into the details, therefore, let us propose their general form and the implications of such a form in context of expression (30). On dimensional grounds, we suggest that

$$\langle \dot{X}_i(\tau')\rangle_R = \frac{1}{\sqrt{\tau'}} F_i(\tau_0/\tau', \tau'/t) \tag{36}$$

$$\langle \dot{X}_i(\tau_1)\dot{X}_i(\tau_2)\rangle_R = 2\left[\delta(\tau_2-\tau_1) + \frac{1}{\tau_+} G_i(\tau_0/\tau_-, \tau_-/\tau_+, \tau_+/\tau)\right] \tag{37}$$

in which τ_0 is some early timescale in the problem and τ_- (τ_+) are the smaller (respectively larger) of τ_1 and τ_2. Guided by (35), and confirmed by explicit calculation to be presented below, we have included a delta-function contribution in the two-time correlation function.

The upshot of this is that all the integrals in (32) and (34) reduce to one of two forms. These are

$$\int_0^\tau \frac{\mathrm{d}\tau'}{\tau'} f(\tau_0/\tau', \tau'/\tau) \tag{38}$$

$$\int_0^\tau \frac{\mathrm{d}\tau_+}{\tau_+^2} \int_0^{\tau_+} \mathrm{d}\tau_- g(\tau_0/\tau_-, \tau_-/\tau_+, \tau_+/\tau) \tag{39}$$

in which the functions f and g are various combinations of the velocity and velocity-correlation functions. It is not the values of these integrals that we are interested in, but the limit that appears in the perturbation expansion (30). It is straightforward to show that

$$\lim_{\tau\to\infty} \tau \frac{\mathrm{d}}{\mathrm{d}\tau} \int_0^\tau \frac{\mathrm{d}\tau'}{\tau'} f(\tau_0/\tau', \tau'/\tau) = f(0,0) \tag{40}$$

$$\lim_{\tau\to\infty} \tau \frac{\mathrm{d}}{\mathrm{d}\tau} \int_0^\tau \frac{\mathrm{d}\tau_+}{\tau_+^2} \int_0^{\tau_+} \mathrm{d}\tau_- g(\tau_0/\tau_-, \tau_-/\tau_+, \tau_+/\tau) = \int_0^1 \mathrm{d}u\, g(0,u,0). \tag{41}$$

The fact that zeros appear in the arguments of the functions f and g implies that when calculating $\langle \dot{X}_i(\tau')\rangle_R$ and $\langle \dot{X}_i(\tau_1)\dot{X}_i(\tau_2)\rangle_R$ we need only determine their forms in the regime $\tau_0 \ll \tau', \tau_1, \tau_2 \ll \tau$ to obtain the expansion (30).

We now indicate how to calculate these quantities. First, note that $\langle \dot{X}_i(\tau')\rangle_R = \frac{\mathrm{d}}{\mathrm{d}\tau'}\langle X_i(\tau')\rangle_R$. This reduces the problem to the calculation of the mean position of a walker at time τ' taking into account that it does not cross the origin (survives) until at least a time τ. For the case where a walker's initial position $Y_i > 0$, this quantity can be expressed as

$$\langle X_i(\tau')\rangle_R = \int_0^\infty \mathrm{d}X_i\, X_i \frac{P_1(\tau; X_i, \tau'|Y_i)}{Q_1(\tau|Y_i)} \tag{42}$$

in which $P_1(\tau; X_i, \tau'|Y_i)$ is the probability that a single walker visits X_i at time τ' and does not visit the origin at any time $0 \leqslant \tau' \leqslant \tau$. In order to average X_i with respect to this distribution, it has been normalized through the factor $Q_1(\tau|Y_i)$, which is the probability the walker survives until time τ and is given by equation (11).

Since the diffusion process is Markovian, we can perform the factorization $P_1(\tau; X_1, \tau'|Y_i) = Q_1(\tau - \tau'|X_i)G_1(X_i, \tau'|Y_i)$, where we recall that $G_1(X_i, \tau'|Y_i)$ is the probability that a walker is at X_i at time τ' given that it started at Y_i and whose form is given by equation (9). Inserting the explicit expressions for $Q_1(\tau|Y)$ and $G_1(X, \tau|Y)$ into (42) we find

$$\langle X_i(\tau')\rangle_R = \int_0^\infty \mathrm{d}X_i X_i \frac{\mathrm{erf}\left(\frac{X_i}{2\sqrt{\tau-\tau'}}\right)\left[\exp\left(-\frac{(X_i-Y_i)^2}{4\tau'}\right) - \exp\left(-\frac{(X_i+Y_i)^2}{4\tau'}\right)\right]}{\sqrt{4\pi\tau'}\,\mathrm{erf}\left(\frac{Y_i}{2\sqrt{\tau}}\right)}. \tag{43}$$

Now we can use the fact that when calculating the exponent θ using (30) it is sufficient to know $\langle X_i(\tau')\rangle_R$ in the regime $\tau_0 \ll \tau' \ll \tau$. We take $\tau_0 = Y_i^2$ (recalling that the rescaled time variable has units of length squared) and on expanding the integrand in the previous expression, we find

$$\langle X_i(\tau')\rangle_R = \frac{1}{2\sqrt{\pi}(\tau')^{3/2}} \int_0^\infty \mathrm{d}X_i X_i^3 \exp\left(-\frac{X_i^2}{4\tau'}\right) = 4\sqrt{\frac{\tau'}{\pi}} \tag{44}$$

in this regime. Finally, we differentiate to obtain

$$\langle \dot{X}_i(\tau')\rangle_R = \frac{2}{\sqrt{\pi\tau'}} \tag{45}$$

when $\tau_0 \ll \tau' \ll \tau$ and $Y_i > 0$. Since we are working at times much larger than $\tau_0 = Y_i^2$, the dependence on the magnitude of Y_i has dropped out of this expression. However, the sign of the average velocity clearly changes if we consider a walker with initial position $Y_i < 0$. Hence the correct limiting form of the function $F_i(\tau_0/\tau', \tau'/\tau)$ in equation (36) is

$$F_i(0,0) = \frac{2\sigma_i}{\sqrt{\pi}} \tag{46}$$

in which $\sigma_i = \mathrm{sgn}(Y_i)$.

The two-point velocity correlation function $\langle \dot{X}_i(\tau_1)\dot{X}_i(\tau_2)\rangle_R$ is obtained in a similar way. We defer the details of the calculation to the appendix, quoting here only the result over the required range $\tau_0 \ll \tau_1, \tau_2 \ll \tau$ which is

$$\langle \dot{X}_i(\tau_1)\dot{X}_i(\tau_2)\rangle_R = 2\left[\delta(\tau_2 - \tau_1) + \frac{2}{\pi\tau_+}\sqrt{\frac{\tau_+ - \tau_-}{\tau_-}}\right]. \tag{47}$$

Recall that $\tau_- = \min\{\tau_1, \tau_2\}$ and $\tau_+ = \max\{\tau_1, \tau_2\}$. Note that this expression is in agreement with the proposal (37), and reveals the limiting form of the function G to be

$$G_i(0, \tau_-/\tau_+, 0) = \frac{2}{\pi}\sqrt{\frac{\tau_+}{\tau_-} - 1}. \tag{48}$$

Once again, the dependence of this quantity on the walker's initial position Y_i has dropped out; furthermore, the two-point correlation function is independent of the sign of Y_i, so we can drop the subscript i on G.

We now consider the first-order term in (30). We have

$$\begin{aligned}\langle S_1\rangle_R - \langle S_1\rangle_U &= \frac{1}{4}\sum_{i,j}{}' \int_0^\tau \mathrm{d}\tau' \langle \dot{X}_i(\tau')\rangle_R \langle \dot{X}_j(\tau')\rangle_R \\ &= \frac{1}{4}\sum_{i,j}{}' \int_0^\tau \frac{\mathrm{d}\tau'}{\tau'} F_i(\tau_0/\tau', \tau'/t) F_j(\tau_0/\tau', \tau'/t).\end{aligned} \tag{49}$$

The unrestricted averages have disappeared from the right-hand side of this expression because $\langle \dot{X}_i \rangle_U = 0$. Now, using equation (40), we find that the limiting form of this expression required in the expansion (30) reads

$$\lim_{\tau\to\infty} \tau \frac{\mathrm{d}}{\mathrm{d}\tau} (\langle S_1 \rangle_R - \langle S_1 \rangle_U) = \frac{1}{4} {\sum_{i,j}}' F_i(0,0) F_j(0,0) = \frac{1}{\pi} {\sum_{i,j}}' \sigma_i \sigma_j. \tag{50}$$

To perform the remaining summation, we note that $\sigma_i \sigma_j$ is equal to +1 if walkers i, j both start on the same side of the origin, and is equal to -1 if they start on opposite sides of the origin. If there are N_L (N_R) walkers initially to the left (right), there are $N_L(N_L - 1) + N_R(N_R - 1)$ positive terms in the summation and $2N_L N_R$ negative terms. Thus one finds that the coefficient of α_N in (30) is

$$\lim_{\tau\to\infty} \tau \frac{\mathrm{d}}{\mathrm{d}\tau} (\langle S_1 \rangle_R - \langle S_1 \rangle_U) = \frac{1}{\pi} (\Delta^2 - N) \tag{51}$$

in which $\Delta = N_L - N_R$.

Let us now turn to the second-order term in (30). From (34) we have the general form

$$\frac{1}{2} \left(\langle S_1^2 \rangle_R - \langle S_1 \rangle_R^2 - \langle S_1^2 \rangle_U + \langle S_1 \rangle_U^2 \right) = \frac{1}{32} \int_0^\tau \mathrm{d}\tau_1 \int_0^\tau \mathrm{d}\tau_2 \left[4 {\sum_{i,j,k}}' A_{ijk}(\tau_0/\tau_1, \tau_1, \tau_2, \tau_2/\tau) + 2 {\sum_{i,j}}' B_{ij}(\tau_0/\tau_1, \tau_1, \tau_2, \tau_2/\tau) \right]. \tag{52}$$

In the regime $\tau_0 \ll \tau_1, \tau_2 \ll t$ we have from (35), (45) and (47)

$$A_{ijk}(0, \tau_-, \tau_+, 0) = \frac{8\sigma_j \sigma_k}{\pi^2} \left[\frac{\pi \delta(\tau_2 - \tau_1)}{\tau_2} + \frac{2}{\tau_+^2} \frac{\tau_+}{\tau_-} \left(\sqrt{1 - \frac{\tau_-}{\tau_+}} - 1 \right) \right] \tag{53}$$

$$B_{ij}(0, \tau_-, \tau_+, 0) = -\frac{16}{\pi^2 \tau_+^2}. \tag{54}$$

As with the first-order term, we calculate the limit in (30) by making use of the results (40) and (41). This procedure yields the result

$$\lim_{\tau\to\infty} \tau \frac{\mathrm{d}}{\mathrm{d}\tau} \frac{1}{2} \left(\langle S_1^2 \rangle_R - \langle S_1 \rangle_R^2 - \langle S_1^2 \rangle_U + \langle S_1 \rangle_U^2 \right) = \frac{1}{\pi^2} \left[\left(\pi + 4 \int_0^1 \mathrm{d}u \frac{\sqrt{1-u} - 1}{u} \right) {\sum_{i,j,k}}' \sigma_j \sigma_k - 2 {\sum_{i,j}}' \int_0^1 \mathrm{d}u \right]. \tag{55}$$

To obtain the final expression for the expansion (30) we use the fact that

$$\int_0^1 \mathrm{d}u \frac{\sqrt{1-u} - 1}{u} = 2(\ln 2 - 1). \tag{56}$$

Also, we must consider the possible ways of choosing three traps labelled i, j, k from a set of N traps comprising a number N_L with $\sigma = -1$ and N_R with $\sigma = 1$. These considerations lead us to

$${\sum_{i,j,k}}' \sigma_j \sigma_k = (N - 2)(\Delta^2 - N). \tag{57}$$

Similarly, the number of terms in the sum $\sum_{i,j}'$ is just $N(N-1)$ which finally allows us to write down an expression for the exponent θ which constitutes the main result of this paper. It reads

$$\theta = \frac{N}{2} + \frac{1}{\pi}(N-\Delta^2)\alpha_N + \frac{1}{\pi^2}[(N-2)(N-\Delta^2)(\pi - 8(1-\ln 2)) + 2N(N-1)]\,\alpha_N^2 + \mathrm{O}\big(\alpha_N^3\big). \tag{58}$$

As a check of this formula, we consider the exactly solvable cases of $N = 1$ and $N = 2$. When $N = 1$, one can simply transform to a frame in which the particle is stationary. Then, its survival probability is given by equation (11) with D replaced by $D + D'$ which implies a persistence exponent of $\theta = \frac{1}{2}$. Since $\Delta^2 = 1$ when $N = 1$, we find that the perturbative expression for θ (58) also gives the exact result $\theta = \frac{1}{2}$.

When $N = 2$, there are two possible arrangements of the walkers. Either they surround the particle, in which case $\Delta = 0$ and the exact exponent is given by equation (17), or they are both on one side of the particle, which has $\Delta = \pm 2$ and θ is given by equation (18). Expanding these exact expressions as series in α_2 one finds

$$\theta = 1 \pm \frac{2}{\pi}\alpha_2 + \frac{4}{\pi^2}\alpha_2^2 + \cdots \tag{59}$$

where the plus sign is taken for the case $\Delta = 0$ and the minus sign for $\Delta = \pm 2$. Thus to second order in α_2 we find agreement between the perturbation series (58) and the exactly known results.

5. Discussion and conclusion

In this work, we have studied the survival probability of a diffusing particle in the presence of a finite number of mobile traps. In the absence of a complete exact solution for the problem, we have devised a method for calculating the persistence exponent θ (defined by equation (14)) valid when the particle's diffusion constant is small. In order to calculate the coefficients in the expansion, it is necessary to find velocity correlation functions for a random walker in the presence of an absorbing boundary. In this paper, we calculated the exponent θ to second order, culminating in expression (58). We stress that, in principle, one could go to higher order, although the amount of work required to obtain n-time velocity correlation functions is likely to increase rapidly with n.

We wish to make a few remarks about our result (58). First, as we have already noted, the expansion parameter α_N defined by equation (15) has an interpretation in the context of the (hyper)wedge geometry that has been previously used to obtain results for this problem. Although the connection appears at first sight intriguing, it is probably no coincidence since in the two approaches the parameter arises through a rescaling that gives rise to uncorrelated diffusion of the traps with diffusion constant unity. However we do see that a system with perturbed equations of motion (treated using the path-integral approach) can be related to one with the original equations of motion but perturbed boundaries (i.e. the hyperwedge geometry).

Secondly, we find that the expansion to second order (58) depends on two parameters: the total number of traps in the system N and the square difference Δ^2 in the number of traps initially placed on either side of the particle. The origin of this observation lies in the fact that at sufficiently large times the initial position of a particular trap is unimportant. Of course, the number of traps initially positioned to each side of the particle plays an important role, and enters into the perturbation expansion through summations in which some terms are positive and some negative depending on the initial arrangement of the traps. We would expect, therefore, the combination $N - \Delta^2$ to appear in higher order terms in the expansion.

We also note from the expansion (58) that when the asymmetry is small, i.e. $\Delta^2 < N$, the exponent θ is an increasing function of the particle's diffusion constant D' at fixed trap diffusion constant D. Hence, in this near-symmetric situation, the particle is more likely to survive longer if it is at rest than if it is slowly diffusing. Of course, we do not know if θ continues to increase for large D' since we only have the first two terms in the perturbation expansion. However, our intuition suggests that this be the case.

The case of large asymmetry, $\Delta^2 > N$ is more subtle since one of the terms in the coefficient of α_N^2 is always positive. We learn a little by defining the critical asymmetry Δ_c at fixed N and α_N to be that for which the persistence exponent $\theta = \frac{N}{2}$. Then for $\Delta > \Delta_c$ one has a regime in which the particle's survival probability is not (locally) maximized by remaining still. One can understand this phenomenon from the extreme case of all traps being on one side of the particle ($\Delta = \pm N$). Then, there is some probability for the particle to diffuse into the region which is devoid of traps, thereby increasing its survival probability. By rearranging the expansion (58) one finds for small α_N that

$$\Delta_c^2 = N + \frac{2N(N-1)}{\pi}\alpha_N + \mathrm{O}\big(\alpha_N^2\big). \tag{60}$$

Of course, it is again difficult to make any statements for large α_N given only the first two terms of the perturbation series.

The final comment we wish to make about the form of (58) is that, although the quantity α_N seems to be the natural expansion parameter in the problem, the presence of a nontrivial coefficient in the second-order term is not suggestive of there being a simple, closed expression valid for all values of the parameters N, Δ, D and D'. Nevertheless, one might find that the marginal case $N = \Delta^2$ is in some way much easier to understand.

To conclude, we consider how one might treat the trapping reaction in higher dimensions. In a forthcoming work [15], we extend the methods introduced in [14] for the case of an infinite sea of traps to dimensions greater than one. It would be interesting to see if the perturbation theory described in this work could be applied to higher dimensions to treat the case of a finite number of traps.

A generalization of the problem studied here in which there are p families of walkers (with n_j walkers with diffusion constant D_j in family j) has very recently been introduced [24] and was studied perturbatively in dimension $d = 2 - \epsilon$. The quantity considered in that work is the probability that no two walkers from different families have met up to time t. This quantity was found to depend only on the numbers n_j and ratios of diffusion constants. Clearly, the case $p = 2$ with $n_1 = 1$ and $n_2 = N$ corresponds to our system so there is an apparent conflict with our result which depends separately on the number of traps initially to the left and right and not just the total number. We suspect that this is due to the fact that the initial ordering of walkers is important in one dimension. For example, our model can equally well be described as a three-family system with $n_1 = 1$, $n_2 = N_L$ and $n_3 = N_R$ since, in one dimension, the traps to the left can never meet the traps to the right without annihilating the particle. An interesting open question raised in [24] is whether allowing for a finite reaction rate in which walkers from different families can cross with nonzero probability would bring the one-dimensional system in line with the higher dimensional problem.

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Appendix. Two-point velocity function for surviving walks

In this appendix, we outline the derivation of the correlation function $\langle \dot{X}(\tau_1)\dot{X}(\tau_2)\rangle_R$ as given by equation (47). Recall that this is the two-point velocity correlation function for a single random walker that has a diffusion constant D_0 and does not cross the origin at any time $0 \leqslant \tau' \leqslant \tau$, where $\tau > \tau_1, \tau_2$. We shall assume, with no loss of generality, that the walker's initial position $Y > 0$ and that $\tau_1 < \tau_2$.

The starting point is to consider the probability $P_1(\tau; X_1, \tau_1; X_2, \tau_2|Y)$ for the walker to be at X_1 at time τ_1, X_2 at time τ_2 and to survive until time t given that it started at Y. Then,

$$\begin{aligned}\langle X(\tau_1)X(\tau_2)\rangle_R &= \int_0^\infty \mathrm{d}X_1 \int_0^\infty \mathrm{d}X_2 X_1 X_2 \frac{P_1(\tau; X_1, \tau_1; X_2, \tau_2|Y)}{Q_1(\tau|Y)} \\ &= \int_0^\infty \mathrm{d}X_1 \int_0^\infty \mathrm{d}X_2 X_1 X_2 \frac{Q_1(\tau-\tau_2|X_2)G_1(X_2, \tau_2-\tau_1|X_1)G_1(X_1, \tau_1|Y)}{Q_1(\tau|Y)}\end{aligned} \tag{A.1}$$

in which the Markovian property of the diffusion process has been used to write the joint probability distribution function $P_1(\tau; X_1, \tau_1; X_2, \tau_2|Y)$ in terms of the functions $G_1(X, \tau|Y)$ and $Q_1(\tau|Y)$ defined through equations (9) and (11). Note that it was also necessary to normalize the distribution according to the probability that a walker starting at Y survives a time τ.

Assuming that $\tau_0 = Y^2 \ll \tau_1, \tau_2 \ll \tau$, we can expand both the numerator and denominator in (A.1) to first order in $Y/\sqrt{\tau_1}$ and $X_2/\sqrt{\tau}$ to find

$$\begin{aligned}\langle X(\tau_1)X(\tau_2)\rangle_R &= \frac{1}{4\pi\tau_1\sqrt{\tau_1(\tau_2-\tau_1)}} \int_0^\infty \mathrm{d}X_1 \int_0^\infty \mathrm{d}X_2 X_1^2 X_2^2 \exp\left(-\frac{X_1^2}{4\tau_1}\right) \\ &\quad \times \left[\exp\left(-\frac{(X_2-X_1)^2}{4(\tau_2-\tau_1)}\right) - \exp\left(-\frac{(X_2+X_1)^2}{4(\tau_2-\tau_1)}\right)\right].\end{aligned} \tag{A.2}$$

This integral can be evaluated without recourse to further approximations. First one integrates over X_2, which yields

$$\begin{aligned}\langle X(\tau_1)X(\tau_2)\rangle_R &= \frac{1}{2\sqrt{\pi}\tau_1^{3/2}} \int_0^\infty \mathrm{d}X_1 X_1^2 \exp\left(-\frac{X_1^2}{4\tau_1}\right) \left[\left(X_1^2 + 2(\tau_2-\tau_1)\right)\right. \\ &\quad \left. \times \operatorname{erf}\left(\frac{X_1}{\sqrt{4(\tau_2-\tau_1)}}\right) + \sqrt{\frac{4(\tau_2-\tau_1)}{\pi}} X_1 \exp\left(-\frac{X_1^2}{4(\tau_2-\tau_1)}\right)\right].\end{aligned} \tag{A.3}$$

To perform the remaining integration, it is helpful to make a change of variable $X_1 = 2\sqrt{\tau_2-\tau_1}u$ which leads to

$$\langle X(\tau_1)X(\tau_2)\rangle_R = \frac{16(\tau_2-\tau_1)^{5/2}}{\sqrt{\pi}\tau_1^{3/2}} \int_0^\infty \mathrm{d}u \left[\frac{1}{\sqrt{\pi}} u^3 \,\mathrm{e}^{-\alpha u^2} + \frac{1}{2} u^2 \,\mathrm{e}^{-\beta u^2} \operatorname{erf} u + u^4 \,\mathrm{e}^{-\beta u^2}\right] \tag{A.4}$$

in which $\alpha = \tau_2/\tau_1$ and $\beta = (\tau_2-\tau_1)/\tau_1$. Then, using

$$\int_0^\infty \mathrm{d}u\, u^3 \,\mathrm{e}^{-\alpha u^2} = \frac{1}{2\alpha^2} \tag{A.5}$$

$$\int_0^\infty \mathrm{d}u\, u^{2n} \,\mathrm{e}^{-\beta u^2} \operatorname{erf} u = \left(-\frac{\mathrm{d}}{\mathrm{d}\beta}\right)^n \int_0^\infty \mathrm{d}u \,\mathrm{e}^{-\beta u^2} \operatorname{erf} u = \left(-\frac{\mathrm{d}}{\mathrm{d}\beta}\right)^n \frac{\arctan(1/\sqrt{\beta})}{\sqrt{\pi\beta}} \tag{A.6}$$

we obtain, after a lot of manipulation,

$$\langle X(\tau_1)X(\tau_2)\rangle_R = \frac{4\tau_1}{\pi}\left[\left(2+\frac{\tau_2}{\tau_1}\right)\arctan\sqrt{\frac{\tau_1}{\tau_2-\tau_1}}+3\sqrt{\frac{\tau_2-\tau_1}{\tau_1}}\right]. \tag{A.7}$$

To find the velocity correlation function $\langle \dot{X}(\tau_1)\dot{X}(\tau_2)\rangle_R$ we differentiate with respect to τ_1 and τ_2. We find

$$\frac{\partial}{\partial\tau_2}\langle X(\tau_1)X(\tau_2)\rangle_R = \frac{4}{\pi}\begin{cases}\arctan\sqrt{\frac{\tau_1}{\tau_2-\tau_1}}+\frac{\sqrt{\tau_1(\tau_2-\tau_1)}}{\tau_2} & \tau_1 < \tau_2\\ 2\arctan\sqrt{\frac{\tau_2}{\tau_1-\tau_2}}+2\sqrt{\frac{\tau_1-\tau_2}{\tau_2}} & \tau_1 > \tau_2.\end{cases} \tag{A.8}$$

For $\tau_1 < \tau_2$ one has

$$\langle \dot{X}(\tau_1)\dot{X}(\tau_2)\rangle_R = \frac{4}{\pi\tau_2}\sqrt{\frac{\tau_2-\tau_1}{\tau_1}} \tag{A.9}$$

and the same expression with $\tau_1 \leftrightarrow \tau_2$ when $\tau_1 > \tau_2$. At $\tau_1 = \tau_2$, however, there is a jump in (A.8) of height 2 which implies that

$$\langle \dot{X}(\tau_1)\dot{X}(\tau_2)\rangle_R = 2\left[\delta(\tau_2-\tau_1)+\frac{2}{\pi\tau_+}\sqrt{\frac{\tau_+-\tau_-}{\tau_-}}\right]. \tag{A.10}$$

Thus we conclude our derivation of (47).

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