Journal of Statistical Physics, Vol. 95, Nos. 1/2, 1999

Persistence in Reaction-Diffusion Problems: I. Bosons

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Received September 22, 1998

We consider the persistence probability that a site, initially unoccupied, remains unoccupied for a long time t in reaction-diffusion systems. The models considered are bosonic, i.e., multiple occupancy of the sites is allowed and can be exactly diagonalized. The persistence shows a wide variety of time dependences depending on the model, the dimensionality, and even the initial conditions.

KEY WORDS: Reaction-diffusion; persistence.

1. INTRODUCTION

Recently Derrida *et al.*[1, 2, 3] have discussed the persistence probability in reaction-diffusion systems. The persistence probability, $P_o(t)$, is defined as the probability that a given site (the origin), initially unoccupied, is never visited during the time t. In some systems, notably the case of random walkers undergoing the reaction $A + A \to o$, $P_o(t)$ has an interesting power law $t^{-\theta}$ dependence. The exponent $\theta = \frac{3}{8}$ for one-dimensional Ising Glauber dynamics. This problem has been studied by Cardy[4] using renormalization group methods who finds $\theta = \frac{1}{2} - 0(\varepsilon)$ in a related Bose system of random walkers undergoing annihilation in $d = 2 - \varepsilon$ dimensions. In the case $kA \to o$, $k > 2$ a stretched exponential behavior is found in most cases. Some problems related to that considered here are diffusion with random traps (Lubensky[5]), diffusion controlled annihilation (Krapivsky *et al.*[6, 7]) and the studies of persistent spins and the zeros of Gaussian processes by Majumdar *et al.*[8] and Derrida *et al.*[9]

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0022-4715/99/0400-0171$16.00/0

The dynamics of stochastic systems such as reaction-diffusion models is described by a master equation governing the time evolution of the probabilities that the system is in a given micro state. A second quantized formulation is particularly useful to describe the diffusion and creation or annihilation of the particles and the master equation is equivalent to a Schrödinger-like equation[10]

$$\frac{\partial P}{\partial t} = -HP$$

where P is the state vector of the probabilities and H is the Hamiltonian. If multiple occupancy of sites is allowed H is conveniently expressed in terms of boson operators while if sites are restricted to single occupancy Pauli or Fermi operators are more appropriate.

It is not necessary to use the formalism of second quantization and the results of this paper could also be obtained from results on the first passage time in random walks.[11] This latter formulation is used by Derrida *et al.*[1, 2, 3]

The constraint that the site at the origin is never visited can be incorporated into the Hamiltonian by adding an impurity at the origin

$$H = H_o + \mu a_o^+ a_o \tag{1}$$

where H_o is the Hamiltonian of the pure reaction-diffusion system, $a_o^+ a_o$ is the number operator for particles at site o and μ is the impurity potential. The persistence probability is then

$$P_o(t) = \lim_{\mu \to \infty} \langle F| \, e^{-Ht} \, |I\rangle \tag{2}$$

where $\langle F|$ is a complete set of final states and $|I\rangle$ is the initial state. For a large class of initial states P_o is expected to be independent of the initial state for large t. However, this is not always true for all initial states and we will give an example of such a situation where initially the particle is confined to the vicinity of origin (referred to as the short range case). $P_o(t)$ can also depend on the number N of sites in the system depending on the relative magnitudes of t and N. As we are considering diffusion the interesting situation is when $t^{d/2} \ll N$ $(d < 2)$ and $t \ll N$ $(d > 2)$. We have set the diffusion constant to unity.

In this paper we consider a number of exactly solvable bosonic reaction–diffusion problems. In Section 2 as an illustration a simple diffusion problem is treated and the effects of the initial distribution is studied in 3.

Biased diffusion is considered in 4 and a problem where deposition also occurs is studied in 5. In subsequent papers using similar techniques we study Fermi systems including those arising from mappings of kinetic interacting spin models and stochastic interacting particle systems.

2. SIMPLE DIFFUSION

We begin by considering simple diffusing, non-interacting particles on a d-dimensional cubic lattice of N sites. The Hamiltonian is

$$H=\tfrac{1}{2}\sum_{nn}(a_i^+-a_j^+)(a_i-a_j)+\mu a_o^+ a_o \tag{3}$$

We have set the diffusion constant to unity, the sum is over all nearestneighbor pairs and the a_i^+, a_i are pseudo-boson[5] creation and annihilation operators with

$$a^+\,|n\rangle=|n+1\rangle, \qquad a\,|n\rangle=n\,|n-1\rangle, \qquad [a_i, a_j^+]=\delta_{ij} \tag{4}$$

Introducing Fourier transforms

$$a_j=\frac{1}{\sqrt{N}}\sum_k e^{i\vec{k}\cdot\vec{j}}b_k, \qquad a_j^+=\frac{1}{\sqrt{N}}\sum_k e^{i\vec{k}\cdot\vec{j}}b_k^+ \tag{5}$$

in (3) H becomes

$$H=\sum_k \omega_k b_k^+ b_k+\frac{\mu}{N}\sum_{kk'} b_k^+ b_{k'} \tag{6}$$

where $\omega_k=d-\cos k_x\cdots$. It is convenient to introduce even and odd operators

$$B_k=\frac{1}{\sqrt{2}}(b_k+b_{-k}), \qquad B_o=b_o, \qquad A_k=\frac{1}{\sqrt{2}}(b_k+b_{-k}) \tag{7}$$

with similar definitions for the creation operators. The odd operators A do not couple with the impurity and do not enter the problem if we restrict the initial distributions to be symmetric and thus will be omitted. H becomes

$$H=\Sigma'\omega_k B_k^+ B_k+\frac{\mu}{N}(B_o^+ +2^{1/2}\Sigma'_k B_k^+)(B_o+2^{1/2}\Sigma'_k B_k) \tag{8}$$

where the prime means $k > o$. This Hamiltonian is easily diagonalized. The impurity states have energies E_α which are the solutions of

$$\mu g(E_\alpha) = 1, \qquad g(\varepsilon) = \frac{1}{N} \sum_k \frac{1}{\varepsilon - \omega_k} \tag{9}$$

In terms of boson annihilation and creation operators ξ_α, ξ_α^+ for the impurity states

$$B_k^+ = \frac{1}{\sqrt{N}} \sum_\alpha u_k^\alpha \xi_\alpha^+, \qquad B_o^+ = \frac{1}{\sqrt{2N}} \sum_\alpha u_o^\alpha \xi_\alpha^+ \tag{10}$$

with similar results for the annihilation operators. The coefficients

$$u_k^\alpha = \frac{\mu C_\alpha}{E_\alpha - \omega_k}, \qquad \mu^2 C_\alpha^2 = \frac{-2}{g'(E_\alpha)} \tag{11}$$

Using the orthogonality and normalization relations

$$\frac{1}{2N} \sum_k u_k^\alpha u_k^\beta = \delta_{\alpha\beta}, \qquad \frac{1}{N} \sum_\alpha u_k^\alpha u_{k'}^\alpha = \delta_{k,k'} + \delta_{k,-k'} \tag{12}$$

the Hamiltonian takes the simple form

$$H = \sum_\alpha E_\alpha \xi_\alpha^+ \xi_\alpha \tag{13}$$

The probability that the site at the origin is never visited is given by (2). We first consider the case where there is only a single diffusing particle (this is generalized to a finite density of non-interacting diffusing particles below). Then

$$\langle F| = \langle o| \sum_j a_j, \qquad |I\rangle = \frac{1}{N} \sum_j a_j^+ \, |o\rangle \tag{14}$$

where $|o\rangle$ is the vacuum state and we have assumed that initially the particle has equal probability of being on any site. Using (5) and (10) to express the operators in terms of those of the impurity problems the expectation value in (2) is easily evaluated and

$$P_{o1}(t) = \lim_{\mu \to \infty} \frac{1}{2N} \sum_\alpha u_o^{\alpha 2} e^{-E_\alpha t}, \qquad P_{o1}(o) = 1 \tag{15}$$

where the subscript 1 indicates only one particle. It is simpler to evaluate $\dot{P}_{o1}$ and using (11)

$$\dot{P}_{o1}(t) = -\lim_{\mu \to \infty} \frac{1}{2N} \sum_{\alpha} \frac{\mu^2 C_\alpha^2}{E_\alpha} e^{-E_\alpha t} \tag{16}$$

This is conveniently written as a contour integral using the fact that $(g(\varepsilon) - \mu^{-1})^{-1}$ has simple poles at $\varepsilon = E_\alpha$ in the right half plane with residues $1/g'(E_\alpha) = \frac{1}{2}\mu^2 C_\alpha^2$. Then

$$\dot{P}_{o1}(t) = -\lim_{\mu \to \infty} \frac{1}{2\pi i N} \int_{-\sigma - i\infty}^{-\sigma + i\infty} \frac{d\varepsilon e^{-\varepsilon t}}{\varepsilon(g(\varepsilon) - \mu^{-1})} \tag{17}$$

Then letting $\mu \to \infty$ and putting $\xi = iy$ we get

$$\dot{P}_{o1}(t) = -\frac{1}{2\pi i N} \int_{i\sigma - \infty}^{i\sigma + i\infty} \frac{dy}{y g(iy)} e^{-iyt} \tag{18}$$

In the continuum limit in d dimensions

$$g(iy) = \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} \frac{d^d k}{iy - \omega_k} \tag{19}$$

When t is large we require $g(iy)$ for small y and it takes different forms depending on dimensionality.

(a) $d > 2$. The integral in (19) converges when $y = o$ and we can make the small y replacement $g(iy) = -I_d$ where I_d is Watsons integral

$$I_d = \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} \frac{d^d k}{d - \cos k_{x\ldots}} \tag{20}$$

Then

$$\dot{P}_{o1}(t) = -\frac{1}{N I_d}, \qquad P_{o1}(t) = 1 - t/N I_d \tag{21}$$

(b) $d = 2$. Since y is small we use $\omega_k = k^2/2$ in (19) and introduce a cut off k_m which gives $g(iy) = -(1/2\pi) \ln(ik_m^2/2y)$. Substitution in (18) gives

$$\dot{P}_{o1}(t) = -\frac{2\pi}{N \ln t}, \qquad P_{o1}(t) = 1 - \frac{2\pi t}{N \ln t} \tag{22}$$

where we have only kept the leading logarithmic terms.

(c) $d=1$. Again setting $\omega_k = k^2/2$ we find $g(iy) = -e^{i\pi/4}/\sqrt{2y}$ which leads to

$$\dot{P}_{o1}(t) = -\frac{1}{N}\left(\frac{2}{\pi t}\right)^{1/2}, \qquad P_{o1}(t) = 1 - \frac{2}{N}\left(\frac{2t}{\pi}\right)^{1/2} \tag{23}$$

It is clear that these results are only valid when $t^{d/2} < N$ $(d<2)$ and $t<N$ $(d>2)$ as discussed in Section 1.

These results are readily extended to the case where there is initially a finite density ρ of diffusing particles per site. Then

$$\langle F| = \langle 0| \left(\sum_j a_j\right)^{\rho N}, \qquad |I\rangle = C_N \left(\frac{1}{\sqrt{N}} \sum_j a_j^+\right)^{\rho N} |o\rangle \tag{24}$$

where the normalization constant $C_N^{-1} = N^{\rho N/2}\Gamma(1+\rho N)$. It is easily shown that

$$P_{op}(t) = (P_{o1})^{\rho N} \tag{25}$$

where P_{o1} are the above results for a single diffusing particle. Then letting $N \to \infty$ we find

$$\begin{aligned} P_{op} &= e^{-\rho t/Id} && d>2 \\ &= e^{-2\pi\rho t/\ln t} && d=2 \\ &= e^{-2\rho(2t/\pi)^{1/2}} && d=1 \end{aligned} \tag{26}$$

The persistence probability depends on dimensionality and the exponents are the trivial ones expected in random walk problems.

3. EFFECT OF INITIAL DISTRIBUTION

In this section we choose an initial distribution in which all the particles are within a finite distance of the origin. In the previous section initially the particles were distributed uniformly over the whole lattice. Considering a single diffusing particle the final state is as before in (14) and

$$|I\rangle = \sum_j \beta_j a_j^+ |o\rangle, \qquad \sum_j \beta_j = 1, \beta_j = \beta_{-j} \tag{27}$$

The β_j must all be positive. The distribution is symmetric around the origin and normalized. In terms of impurity operators (10)

$$|I\rangle = \frac{1}{\sqrt{2N}} \sum_{k,\,\alpha} u_k^\alpha \hat{\beta}_k \xi_\alpha^+ \, |o\rangle \tag{28}$$

where $\hat{\beta}_k$ is the Fourier transform of β_j. In the $\mu \to \infty$ limit we have $\sum_k u_k^\alpha = o$ and we can replace (28) by

$$|I\rangle = \frac{1}{\sqrt{2N}} \sum_k u_k^\alpha (\hat{\beta}_k - \hat{\beta}_o)\, \xi_\alpha^+ \, |o\rangle \tag{29}$$

When this is substituted in (2) we find

$$P_{o1s}(t) = \frac{1}{2N} \sum_{\alpha,\,k} u_o^\alpha u_k^\alpha (\hat{\beta}_k - \hat{\beta}_o)\, e^{-E_\alpha t} \tag{30}$$

where the subscript s indicates the short range case. As an example we take $\beta_j = (1/2d) \sum_n \delta_{j,\,n}$, where n are all the nearest-neighbor sites to the origin. Then $\hat{\beta}_o - \hat{\beta}_k = \omega_k/d$ and using (11) we can write (30) in the form

$$P_{o1s}(t) = \frac{1}{2d} \sum_\alpha \frac{\mu^2 C_\alpha^2}{E_\alpha} \left(1 - \frac{1}{N} \sum_k \frac{E_\alpha}{E_\alpha - \omega_k}\right) e^{-E_\alpha t} \tag{31}$$

The second term in the bracket is of order μ^{-1} and so we can neglect it. Then

$$P_{o1s}(t) = \frac{1}{2d} \sum_\alpha \frac{\mu^2 C_\alpha^2}{E_\alpha} e^{-E_\alpha t} \tag{32}$$

Comparision with (16) shows that $P_{o1s}(t) = (-N/d)\, \dot{P}_{o1}(t)$ which gives the results

$$\begin{aligned} P_{o1s}(t) &= \frac{1}{dI_d} && d > 2 \\ &= \frac{\pi}{\ln t} && d = 2 \\ &= \left(\frac{2}{\pi t}\right)^{1/2} && d = 1 \end{aligned} \tag{33}$$

For $d>2$ the particle has a probability $1/dI_d$ of reaching the origin in a short time or otherwise diffuses away. $d=2$ is the marginal case and in $d=1$ the persistence probability decays to zero with exponent $\frac{1}{2}$.

4. BIASED DIFFUSIONS

We consider a one-dimensional system in which the hopping rate to the right is greater than that to the left. The Hamiltonian is now

$$H=\sum_k \omega_{kb} b_k^+ b_k + \frac{\mu}{N} \sum_{kk'} b_k^+ b_{k'} \tag{34}$$

where $\omega_{kb}=\omega_k+i\Delta \sin k$. Δ is the anisotropy in the hopping rate and we use the subscript b to distinguish the biased case. The separation into even and odd states no longer occurs but H can still be diagonalized by introducing impurity states with energies E_α which are solutions of

$$\mu g_b(E_\alpha)=1, \qquad g_b(\varepsilon)=\frac{1}{N}\sum_k \frac{1}{\varepsilon-\omega_{kb}} \tag{35}$$

The energies E_α are either real or occur in complex conjugate pairs. In terms of the creation and annihilation operators ξ_α^+, ξ_α for the impurity states.

$$b_k^+ = \frac{1}{\sqrt{N}} \sum_\alpha u_{kb}^\alpha \xi_\alpha^+, \qquad b_k = \frac{1}{\sqrt{N}} \sum_\alpha u_{kb}^\alpha \xi_\alpha \tag{36}$$

Where u_{kb} is given by a generalization of (11) in which ω_k is replaced by ω_{kb}.

Using the orthogonality relations

$$\frac{1}{N}\sum_k u_{kb}^\alpha u_{kb}^\beta = \delta_{\alpha\beta}, \qquad \frac{1}{N}\sum_\alpha u_{kb}^\alpha u_{k'b}^\alpha = \delta_{kk'} \tag{37}$$

the Hamiltonian takes the form

$$H=\sum_\alpha E_\alpha \xi_\alpha^+ \xi_\alpha \tag{38}$$

We choose the same initial and final states as in the unbiased case (14) and find

$$\dot{P}_{o1b}(t) = -\frac{1}{2\pi i N}\int_{i\sigma-\infty}^{i\sigma+\infty} \frac{dy}{y g_b(iy)} e^{-iyt} \tag{39}$$

of exactly the same form as in (18). In this one-dimensional case for small y, $g_b(iy) = -1/\sqrt{\Delta^2 - 2iy}$ and after substitution in (39) and distortion of the contour

$$\dot{P}_{01b}(t) = -\frac{\Delta}{N}\left[1 + \frac{1}{\pi}\int_o^\infty \frac{r^{1/2}\,dr}{1+r}\, e^{-(\Delta^2/2)(1+r)}\right] \tag{40}$$

For $\Delta^2 t < 1$ this reduces to (23) and for $\Delta^2 t > 1$

$$\dot{P}_{01b}(t) = -\frac{\Delta}{N}\left[1 + \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{(\Delta^2 t)^{3/2}}\, e^{-\Delta^2 t/2}\right] \tag{41}$$

The second term is negligible and $P_{01b}(t) = 1 - (\Delta t/N)$. For a finite density of particles

$$P_{o\rho b}(t) = e^{-\Delta \rho t}, \qquad d = 1 \tag{42}$$

and so bias causes an exponential decay rather than the stretched exponential form in (26).

5. DEPOSITION

In this section we consider the effects of deposition of particles, in addition to diffusion, on the persistence. The Hamiltonian of the diffusion-deposition system is

$$H_o = \tfrac{1}{2} \sum_{kk} (a_i^+ - a_j^+)(a_i - a_j) - \varepsilon \sum_i (a_i^{+2} - 1) \tag{43}$$

Pairs of particles are deposited at a rate ε at random on the sites in addition to the diffusion. This can also be regarded as a growth model in which particles are deposited on the sites to form columns with height proportional to the number of particles and particles can hop between neighboring columns.

Beginning with the vacuum state at $t = 0$ the average number of particles per site is $2\varepsilon t$. This model is quadratic in boson operators and the Hamiltonian (43) together with the impurity potential $\mu a_o^+ a_o$ can be diagonalized by generalizing the methods used in Section 2. A Bogoliubov transformation is involved because of the particle creation term in H_o (Eq. (43)). Nevertheless, the impurity state energies and amplitudes can be given in forms allowing the evaluation of the persistence probability via contour integral procedures similar to those used in 2. Choosing the initial state to be the vacuum the persistence probability for large t and $N \to \infty$ is found to be

$$\begin{aligned} P_o(t) &= \exp\left(-\frac{\varepsilon t^2}{I_d}\right) && d > 2 \\ &= \exp\left(\frac{-2\pi\varepsilon t^2}{\ln t}\right) && d = 2 \\ &= \exp\left(-\frac{8}{3}\varepsilon\left(\frac{t^3}{\pi}\right)^{1/2}\right) && d = 1 \end{aligned} \tag{44}$$

As expected the deposition leads to a more rapid decay of the persistence probability $P_o(t) \sim e^{-t^\delta}$ with $\delta = 2$ for $d > 2$ with a log correction for $d = 2$ and $\delta = 3/2$ for $d = 1$. The form is like that without deposition (Eq. (26)) with ρ replaced by εt.

6. CONCLUSIONS

We have studied the persistence probability, $P_o(t)$, in some exactly soluble bosonic reaction-diffusion systems. The time dependence of $P_o(t)$, not surprisingly, shows different behavior depending on the model and the dimensionality. Thus for a simple diffusing system at finite density it is a simple or stretched exponential. If deposition is included it decays more rapidly with time. If initially all the particles are within a short distance of the persistent site a different behavior ensues.

Generalized combinations of processes could be treated by similar procedures. The methods also apply to certain systems with interactions: for example one-dimensional Ising Glauber dynamics with or without bias can be mapped to free fermions. This, and related problems with persistence behavior will be treated elsewhere.

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