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LETTER TO THE EDITOR

Proportion of unaffected sites in a reaction–diffusion process

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Abstract. We consider the probability $P(t)$ that a given site remains unvisited by any of a set of random walkers in d dimensions undergoing the reaction $A+A \to 0$ when they meet. We find that, asymptotically, $P(t) \sim t^{-\theta}$ with a universal exponent $\theta = \frac{1}{2} - O(\epsilon)$ for $d = 2 - \epsilon$, while, for $d > 2$, θ is non-universal and depends on the reaction rate. The analysis, which uses field-theoretic renormalization-group methods, is also applied to the reaction $kA \to 0$ with $k > 2$. In this case, a stretched exponential behaviour is found for all $d \geqslant 1$, except in the case $k = 3$, $d = 1$, where $P(t) \sim e^{-\mathrm{const}(\ln t)^{3/2}}$.

In a recent letter, Derrida *et al* [1] have found new non-trivial and apparently universal exponents associated with the zero-temperature relaxational dynamics of the one-dimensional Ising and Potts models. The occurrence of such exponents is surprising given the trivial nature of the conventional static and dynamic exponents in these models. However, the quantity considered by these authors, namely the probability $P(t)$ that, starting from a random initial configuration, a given site has not been crossed by a domain wall, is not simply related to the usual response functions, and might be expected to show more interesting behaviour. The fact that a simple universal power law $P(t) \sim t^{-\theta}$ is obtained for large t, however, requires some explanation.

In this letter, we provide such an explanation within the context of a generalization of this problem to arbitrary dimensionality d. Since the motion of domain walls for $d > 1$ is very difficult to treat analytically, instead we observe that, in one dimension, the motion and annihilation of Ising domain walls at zero temperature is equivalent to a reaction–diffusion process of point particles A undergoing the irreversible reaction $A + A \to 0$. The study of this problem is readily capable of generalization to arbitrary d, and many of its features have already been elucidated using a number of approaches [2]. In particular, it is found that there is an upper critical dimension $d_c = 2$, above which the mean density $n(t)$ behaves as $1/(\lambda t)$, where λ is the reaction rate, as predicted by a simple rate equation neglecting correlation effects, while for $d < 2$, these effects cannot be ignored and the behaviour is modified to $t^{-d/2}$, with an amplitude independent of λ. Recently, a systematic field-theoretic renormalization-group approach to this problem has been developed [3], which not only yields the exponents but also correlation functions and universal amplitudes within an ϵ-expansion. It is also straightforward to generalize the analysis to the reaction $kA \to 0$. In this case, above the upper critical dimension $d_c(k) = 2/(k-1)$, one finds $n(t) \sim 1/(\lambda t)^{d_c(k)/2}$, while for $d < d_c$, $n(t) \sim t^{-d/2}$ with a universal amplitude.

Within this type of reaction–diffusion problem, then, we ask the following question: from a random initial condition (mean density n_0) at time $t = 0$, what is the late-time dependence of the probability $P(t)$ that a given site has never been visited by a walker? A simple approach to this problem is to note that $P(t) - P(t+\delta t)$ is the probability of finding a walker at the given site (the origin, say), in the time interval $(t, t+\delta t)$, given that the origin has never been visited in the past. This will happen only if a particle happens to lie close to the origin at time t. Thus,

$$-P'(t)\delta t \sim D\delta t P(t)\tilde{n}(t)$$

where D is the diffusion constant and $\tilde{n}(t)$ is the density at a site adjacent to the origin, given that the origin is never visited, that is, with a repulsive potential there.

For $d > 2$, only a finite fraction of particles near the origin has ever visited the origin in the past, so that $\tilde{n}(t) \propto n(t) \sim t^{-d_c(k)/2}$. For $k = 2$, this leads to $P(t) \sim t^{-\text{const}/\lambda}$, i.e. a power law with a *non-universal* exponent, while for $k > 2$, we obtain a stretched exponential behaviour $P(t) \sim e^{-\text{const}\, t^{(k-2)/(k-1)}}$. For $d < 2$, however, almost all particles near the origin have visited it at some time in the past, so that $\tilde{n}(t) \ll n(t)$. When $2 > d > d_c(k)$ (which is possible when $k > 2$), particle correlations may be neglected and we may use the inhomogeneous rate equation

$$\partial n/\partial t = D\nabla^2 n - k\lambda n^k \tag{1}$$

selecting the required events by imposing the condition $n(r = 0, t) = 0$. This problem has the radially symmetric scaling solution $n(r, t) = t^{-d_c(k)/2} f(r/(Dt)^{1/2})$. For $r \ll (Dt)^{1/2}$, the nonlinear term is unimportant (corresponding to the fact that the density is so low that annihilation events rarely occur), and f satisfies Laplace's equation with solution $f \sim (r/(Dt)^{1/2})^\epsilon$, where $\epsilon = 2 - d$. Thus, $\tilde{n}(t) \sim n(t)t^{-\epsilon/2}$ and the stretched exponential becomes $P(t) \sim e^{-\text{const}\, t^{(d-d_c(k))/2}}$. For $d < d_c(k)$, if we assume that $\tilde{n}(t)$ is suppressed relative to the bulk density by this same factor, we find that $\tilde{n}(t) \sim t^{-d/2-\epsilon/2} = t^{-1}$, resulting in a power law $P(t) \sim t^{-\theta}$ consistent with the result of Derrida *et al* [1]. However, to justify this argument and to demonstrate the universality of θ, it is necessary to proceed more systematically.

We first relate $P(t)$ to an appropriate correlation function in the field-theoretic description of the problem. We follow the notation and formalism of [3]. Following Doi [4] and Peliti [5], the master equation for the reaction–diffusion problem is encoded in a Hamiltonian, or Liouvillean, which may be expressed in the 'second-quantized' form

$$H = (D/b^2)\sum_{\text{n.n.}}(a_i^\dagger - a_j^\dagger)(a_i - a_j) - \lambda\sum_i(1 - (a_i^\dagger)^k)a_i^k$$

where the first term is a sum over nearest neighbours and represents a continuous-time random walk on a lattice with spacing b, and the second term represents the annihilation process $kA \to 0$. The time translation operator is e^{-Ht}, which may be written as a path integral by dividing the interval $(0, t)$ into small slices of duration Δt. At each slice, a complete set of coherent states

$$\int e^{-\phi_t^*\phi_t} e^{\phi_t a^\dagger}|0\rangle\langle 0|e^{\phi_t^* a}\, d\phi_t^*\, d\phi_t$$

is inserted (lattice labels are suppressed for clarity). The matrix elements $\langle 0|e^{\phi_{t+\Delta t}^* a} e^{\phi_t a^\dagger}|0\rangle = e^{\phi_{t+\Delta t}^*\phi_t}$ then give rise, when combined with the measure factors $e^{-\phi_t^*\phi_t}$, to the time-derivative piece in the action

$$S = \int (\phi(t)^*\partial_t\phi(t) + D\nabla\phi^* \cdot \nabla\phi + \lambda(\phi^{*k} - 1)\phi^k)\, dt$$

in the limit $\Delta t \to 0$.

In the second quantized formalism, the probability $P(t)$ that a given site, which may be chosen to be the origin $j = 0$, is never visited is simply given by inserting the operator $\delta_{a_0^\dagger a_0,0}$ at each time slice. Thus, at the origin, instead of the matrix element given above, one should compute

$$\langle 0|e^{\phi^*_{t+\Delta t}a}\delta_{a^\dagger a,0}e^{\phi_t a}|0\rangle = 1$$

which means that, to leading order in Δt, the factor from the measure is not cancelled, corresponding to an insertion of $\prod_t e^{-\phi^*_{0,t}\phi_{0,t}}$ in the path integral. In the continuum limit, the lattice fields are rescaled so that $\phi^*\phi \to b^d\phi^*\phi$, so that finally

$$P(t) = \int \mathcal{D}\phi^*\mathcal{D}\phi \exp\left(-h\int \phi^*(0,t)\phi(0,t)\,\mathrm{d}t\right)\exp(-S[\phi^*,\phi])$$

where $h = b^d/\Delta t$.

As explained in [3, 5], in order to compute statistical averages with respect to the action S, it is necessary to evaluate projections onto the state $\langle 0|\prod_j e^{a_j}$. It is then convenient to make the shift $\phi^* = 1 + \bar{\phi}$, so that $\bar{\phi}$ annihilates this state when acting to the left. The required insertion then has two pieces

$$\exp\left(-h\int_0^t \bar{\phi}(0,t')\phi(0,t')\,\mathrm{d}t'\right) \qquad \text{and} \qquad \exp\left(-h\int_0^t \phi(0,t')\,\mathrm{d}t'\right).$$

In the first factor, the time integral can be taken up to infinity, and thus the term $h\int \bar{\phi}(0,t')\phi(0,t')\,\mathrm{d}t'$ may be regarded as a repulsive potential and included in the action S, while the second factor is the piece whose expectation value we now wish to evaluate with respect to this modified action. It is convenient to rewrite this as a cumulant expansion

$$\begin{aligned} P(t) &\sim \left\langle \exp\left(-h\int_0^t \phi(0,t')\,\mathrm{d}t'\right)\right\rangle \\ &= \exp\left(-h\int_0^t \langle\phi(0,t')\rangle\,\mathrm{d}t' + h^2\int_0^t\int_0^{t'} \langle\phi(0,t')\phi(0,t'')\rangle_c\,\mathrm{d}t'\,\mathrm{d}t'' + \cdots\right). \end{aligned} \tag{2}$$

Dimensional analysis then dictates that h has dimension (wave number)$^{2-d}$, so the additional interaction term is *irrelevant* for $d > 2$ and may therefore be neglected in studying the late-time asymptotics. For $d > d_c(k)$, the arguments of [3] show that all loop corrections to the field theory are also irrelevant. The sum of the tree diagrams is then given by the solution to the naive rate equation $\langle\phi(0,t)\rangle \sim 1/(\lambda t)^{d_c(k)/2}$. (In fact the amplitude will be modified in the neighbourhood of the origin, but not the exponent, for $d > 2$.) On substitution into the first term of the cumulant expansion, this then leads to the same result as the earlier naive argument. The higher-order terms in the cumulant expansion all involve at least one more power of λ and, hence, their integrals are down by successive powers of $t^{-(d-d_c(k))/2}$. The appearance of the borderline dimensionality $d = 2$ is simply related to the recurrence property of random walks.

For $d < 2$, however, the h interaction is either marginal or relevant, and it is necessary to perform a full renormalization-group analysis. Fortunately, this is fairly simple since the renormalizations of h and λ do not mix. This is because the renormalization of h may be discussed in terms of its contribution to the propagator $\langle\phi(x,t)\bar{\phi}(x',t')\rangle$, to which λ does not contribute, while, since λ is a bulk coupling, its renormalization cannot be affected by the localized interaction $h\bar{\phi}\phi(0)$. The bulk renormalization of λ is discussed in [3]. Here we use the notation ℓ_R to denote the dimensionless renormalized coupling $\lambda_R\kappa^{-2\epsilon'/d_c(k)}$, where $\epsilon' = d_c(k) - d$. The renormalization of h is then carried out for $\lambda = 0$. Since this is a Gaussian theory, this is simple but non-trivial, due to the localized form of the interaction. The renormalised coupling h_R may be defined in terms of the truncated Fourier–Laplace transform of $\langle\phi(x,t)\bar{\phi}(0,t')\phi(0,t')\bar{\phi}(x'',t'')\rangle$, evaluated at the normalization-point imaginary frequency $s = \kappa^2$. We thus find

$$h_R = h\,(1 + hI_d(\kappa))^{-1}$$

where

$$I_d(\kappa) = \int \frac{1}{s+p^2}\frac{d^d p}{(2\pi)^d}\bigg|_{s=\kappa^2} \equiv B(d)\frac{\kappa^{-\epsilon}}{\epsilon}.$$

The dimensionless coupling $g_R = h_R\kappa^{-\epsilon}$ (where now $\epsilon = 2 - d$) then has the beta function

$$\beta_g(g_R) = -\epsilon g_R + B(d)g_R^2$$

where $B(2) = 1/2\pi$. This is exact to all orders in g_R. In addition to the coupling constant renormalization, however, it is necessary to perform a multiplicative renormalization of $\phi(0,t)$. This may be seen by considering the correlation function $\langle\phi(0,t)\bar{\phi}(p=0,t=0)\rangle$, whose Laplace transform is $s^{-1}(1+hI_d(s^{1/2}))^{-1}$, of which the divergence for $d=2$ cannot be removed by the renormalization of h. We therefore define $\phi_R(0,t) = Z_0\phi(0,t)$ to remove this factor, where $Z_0 = 1 + (B(d)/\epsilon)h\kappa^{-\epsilon}$.

Consider now $C_R^{(1)}(t, g_R, \ell_R, \kappa) = \langle\phi_R(0,t)\rangle$. This satisfies a renormalization-group equation

$$\left(\kappa\frac{\partial}{\partial\kappa} + \beta_g(g_R)\frac{\partial}{\partial g_R} + \beta_\ell(\ell_R)\frac{\partial}{\partial \ell_R} - \gamma_0(g_R)\right)C_R^{(1)} = 0$$

where $\gamma_0 = (\kappa\partial/\partial\kappa)\ln Z_0 = -B(d)g_R$. The solution as $t \to \infty$, for $d < 2$, is

$$C_R^{(1)}(t, g_R, \ell_R, \kappa) \sim (\kappa^2 t)^{-d/2}(\kappa^2 t)^{-\epsilon/2}C_R^{(1)}(\kappa^{-2}, g^*, \tilde{\ell}(t), \kappa) \qquad (3)$$

where $g^* = \epsilon/B(d)$ and $\tilde{\ell}(t)$ is the running coupling ℓ_R. The first prefactor on the right-hand side comes from the canonical scaling dimension of ϕ, the second from the anomalous dimension $\gamma_0(g^*)$.

For $k > 2$, there is a regime where $d_c(k) < d < 2$. In this case, λ is irrelevant and $\tilde{\lambda} \sim t^{\epsilon'/d_c(k)}$, with $\epsilon' < 0$. The correlation function of the right-hand side of equation (3) is then given by the sum of tree diagrams, equivalent to solving inhomogeneous rate equation (1) (with ϕ replacing n) with the boundary condition $\kappa^\epsilon g^*\phi(0) = \lim_{r\to 0} S_d r^{d-1}\partial\phi/\partial r$, which comes from varying with respect to $\bar{\phi}(0)$ and integrating by parts. S_d is the area of a unit d-dimensional sphere and $\tilde{\lambda} = \tilde{\ell}\kappa^\epsilon$. The solution is proportional to $\tilde{\lambda}^{-d_c(k)/2}$, so that $C_R^{(1)}(t) \sim 1/t^{1+\epsilon'/2}$. As before, the higher cumulants are irrelevant for $d > d_c(k)$, so we obtain the stretched exponential result for $P(t)$ given in the summary below. At $d = 2$, the prefactor $(\kappa^2 t)^{-\epsilon/2}$ is replaced by $(\ln(\kappa^2 t))^{-1}$. This results in an extra $(\ln t)^{-1}$ factor in the exponent.

When $d < d_c(k)$, $\tilde{\ell}$ also flows towards a non-trivial fixed point $\ell^* = O(\epsilon')$, so that the correlation function on the right-hand side of equation (3) is asymptotically independent of t. The prefactors combine to give a simple $1/t$ dependence, which integrates to give $\ln t$. The amplitude of this term is given, to leading order in ϵ', by setting $\ell = \ell^*$ in the solution of equation (1), which gives a *universal* amplitude of $O(\epsilon'^{-d_c(k)/2})$. Corrections to this, come from loop corrections to the right-hand side and, more importantly, from the higher-order cumulants, which satisfy similar renormalization-group equations and whose integrals all scale like $\ln t$. However, their amplitudes are suppressed for small ϵ' by powers of $\epsilon'^{(k-2)/(k-1)}$. For $d = d_c(k)$, $\tilde{\ell}(t)$ flows to zero like $(\ln t)^{-1}$, so that $C^{(1)} \sim (1/t)(\ln t)^{1/(k-1)}$, with the higher-order cumulants being suppressed only by powers of $\ln t$.

To summarise the different cases when $k > 2$, we have

$$P(t) = \begin{cases} \exp(-\mathrm{const}\, t^{1-d_c(k)/2}) & d > 2 \\ \exp(-\mathrm{const}\, t^{1-d_c(k)/2}/\ln t) & d = 2 \\ \exp(-\mathrm{const}\, t^{(d-d_c(k))/2}) & 2 > d > d_c(k) \\ \exp(-\mathrm{const}(\ln t)^{k/(k-1)}) & d = d_c(k) \\ t^{-\theta} & d < d_c(k) \text{ with } \theta = O(\epsilon'^{-d_c(k)/2}). \end{cases}$$

Turning now to $k = 2$, the case $d > 2$ has already been discussed. For $d < 2$, the same arguments as for $k > 2$ show that $P(t) \sim t^{-\theta}$, with a universal exponent. However, the dependence on ϵ is now of a different form. To leading order, we may solve the rate equation to calculate the right-hand side of equation (3), setting $\tilde{\ell} = \ell^*$ and $g^* = 0$. (Higher-order terms in g^* are higher order in ϵ.) This means that the amplitude is, to leading order, that of the bulk density [3] $\langle\phi(t)\rangle \sim 1/(4\pi\epsilon)t$. In addition, there is a factor of $hZ_0^{-1} \sim 2\pi\epsilon$ in relating $h\langle\phi(0,t)\rangle$ to $C_R^{(1)}(t)$. Thus, the factors of ϵ cancel and we find

$$\theta = \tfrac{1}{2} + O(\epsilon). \tag{4}$$

The case $d = 2$ is the most interesting, since both h and λ are marginally irrelevant there. In this case, the prefactor behaves as $(4\pi/h)(\ln t)^{-1}$, while $\phi(0,t)$ (to leading order in g_R) behaves as $(1/8\pi)(\ln t/t)$ [3]. Thus, we get a competition between the two running couplings which results in a power behaviour for $P(t)$, with $\theta = \frac{1}{2}$, consistent with its limit as $\epsilon \to 0$. Although equation (4) has the appearance of a conventional mean-field result with $O(\epsilon)$ corrections below $d = d_c = 2$, this is not the case: the value of θ for $d = 2$ comes about by a subtle cancellation of fluctuation effects, and the exponent, for $d > d_c$, is not universal. In addition, for $d = 2$, the corrections to $C^{(1)}(t)$ are suppressed by powers of $\ln t$ only. Thus, the leading corrections to $\ln P(t)$ are proportional to $\int^t (1/t' \ln t')\,\mathrm{d}t' \sim \ln\ln t$. This will give a logarithmic prefactor multiplying the power law $t^{-1/2}$. Unfortunately, the calculation of the exponent of this logarithm requires a two-loop calculation which is more difficult.

In principle, it is possible to compute higher-order terms in the ϵ-expansion (4). However, a similar expansion [3] for the bulk density amplitude does not appear to extrapolate well to $d = 1$. The $O(\epsilon)$ corrections to equation (4), which come from the second cumulant in equation (2), are expected to be negative, consistent with the result of Derrida *et al* [1], who find that $\theta \approx 0.37$ for $d = 1$. It is also straightforward to extend the analysis of the case $k = 2$ to include the reaction $A + A \to A$. If the rate for this second process is λ', the effect is to change the interaction part of the action S to $(2\lambda + \lambda')\bar{\phi}\phi^2 + (\lambda + \lambda')\bar{\phi}^2\phi^2$. This may be brought back to the standard form [3] by rescaling $\phi = \xi\phi'$, $\bar{\phi} = \xi^{-1}\bar{\phi}'$, where $\xi = 2(\lambda+\lambda')/(2\lambda+\lambda')$. The result is that the density amplitude for $d < 2$, and therefore the exponent θ to lowest order, is modified by this factor of ξ [3]. In one dimension, the reaction $A + A \to A$ occurs in the domain wall dynamics of the q-state Potts model with $q \neq 2$, with $\lambda'/\lambda = q - 2$. Thus, to leading order in ϵ, the power is modified to

$$\theta = \frac{q-1}{q} + O(\epsilon)$$

so that, at least to this order, θ increases with q as found for $d = 1$ [1]. The q-dependence is, however, more complicated for the higher-order terms.

After this paper was completed, I was made aware of related work by Krapivsky *et al* [6], in which the problem with $k = 2$, considered above, appears as a limiting case, with a single immobile impurity, of a heterogenous annihilation process. Using the Smoluchowski approximation, these authors obtain results qualitatively similar to those found above.

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