EXACT RESULTS FOR A THREE-BODY REACTION-DIFFUSION SYSTEM

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ABSTRACT

A system of particles hopping on a line, singly or as merged pairs, and annihilating in groups of three on encounters, is solved exactly for certain symmetrical initial conditions. The functional form of the density is nearly identical to that found in two-body annihilation, and both systems show non-mean-field, $\sim 1/\sqrt{t}$ instead of $\sim 1/t$, decrease of particle density for large times.

Diffusion limited reactions in low dimensions have attracted much theoretical interest [1-11]. Indeed, fluctuation effects are most profound in low dimensions, implying deviations from the mean-field rate-equation behavior. Numerical, analytical, and in few cases exact results have been obtained for two-body reactions $A + A \to$ products, and $A + B \to$ products, in $d = 1$. Particle input and production (fragmentation) have also been allowed for in recent studies [4,8,12].

Exact solutions are available only for the simplest reactions. Specifically, for the two-body annihilation, $A + A \to$ inert, the most detailed exact results have been obtained by methods also used for the Glauber-dynamics Ising models. The particles A are then interfaces on a lattice dual to the Ising spin lattice [5,9,13]; the time evolution is continuous. Exact results for cellular-automata type, simultaneous-update, discrete time dynamics, have also been derived [11]. For reactions $A + A \to A$, possibly with particle input and fragmentation, continuum-limit results have been obtained by various random-walk arguments [7,12], some of which are not limited [7] to $d = 1$.

In this work, exact results will be obtained for a certain three-body reaction scheme to be defined shortly. The method of solution involves consideration of Z_k-symmetric, k-state "spins" on a linear lattice. Multistate, Potts-spin $d = 1$ lattice has been considered [14] as a model of mixed pairwise annihilation and coagulation of interfaces between the fully ordered ($T = 0$) Potts phases; the limit $k = \infty$ was solved by random-walk methods [14]. The approach adopted here is quite different: discrete-time and space cellular-automaton dynamics will be defined, and the case $k = 3$ will be shown to have certain simplified properties allowing an exact solution.

It is convenient to use directly the roots-of-unity complex representation of Z_k, the numbers $\exp(2\pi i n/k)$, with $n = 0, 1, 2, \ldots, k-1$. Our "spin" variables, $\sigma_j(t)$, take on these k distinct values. Here the time t increases in integer steps, $t = 0, 1, 2, \ldots$. The spin variables are at even lattice sites $j = 0, \pm 2, \pm 4, \ldots$, for even times, and at odd lattice sites for odd times. Let

$$\sigma_j(t) = \exp\left[2\pi i n_j(t)/k\right] \tag{1}$$

We identify the reacting-diffusing particles as follows. On a dual lattice, i.e., in the interstice between two neighboring spins at $j-1$ and $j+1$, we calculate the number $\sigma_{j+1}/\sigma_{j-1} = \sigma_{j+1}\sigma^*_{j-1}$, where star denotes complex conjugate. The result is put in the form $\exp(2\pi i N_j/k)$, where $N_j = (n_{j+1} - n_{j-1}, \bmod k)$, is a number in the range $0, \ldots, k-1$. We then identify the number of particles at j (at time t) as $N_j(t)$ thus calculated. Note that the particles occupy the dual lattice sites with even j for odd times, and with odd j for even times t.

Next, we define the reaction-diffusion dynamics. At each time step $t \to t+1$, all the $N_j(t)$ particles at the dual-lattice site j hop *as a group* to the right, to site $j+1$ of the dual lattice, or to the left, to site $j-1$, with equal probability. Thus the resulting number of particles hopping to site m can be in the range $0, \ldots, 2k-2$. More precisely, this number can be 0, N_{m-1}, N_{m+1}, or the sum $N_{m-1} + N_{m+1}$. However, we now add the reaction process of instantaneous annihilation of k particles, at all sites at which there are more than k particles present after hopping. Thus, in those sites m which received $N_{m-1}(t) + N_{m+1}(t)$ particles, we define $N_m(t+1)$ as $(N_{m-1}(t) + N_{m+1}(t), \bmod k)$.

These dynamics can be put in a convenient linear form in terms of the Z_k-symmetric spins,

$$\sigma_j(t+1) = \left[1 - \zeta_j(t+1)\right]\sigma_{j-1}(t) + \zeta_j(t+1)\sigma_{j+1}(t) \tag{2}$$

Here we assigned independent and uncorrelated random variables $\zeta_m(t)$ to each spin at each time step $t > 0$. Stochastic variables $\zeta_m(t)$ take on values 0 or 1 with equal probability. For $k = 2$ this and related linear dynamical rules lead to a factorizable hierarchy of relations for equal-time, p-spin correlation functions [11,15]. The factorization property will also apply for $k > 2$.

Essentially, the p-spin correlation functions at fixed time t can be calculated from relations which only involve $p, (p-1), (p-2), \ldots$-spin correlations, but do not couple to higher-order correlations. The resulting expression are, however, difficult to treat exactly, and all the available results for $k = 2$ have been for 2-spin correlations with symmetric (translationally-invariant) initial conditions. In terms of the spin variables, the simplest tractable initial conditions are fully random ones: spins $\sigma_j(0)$ are uncorrelated at different sites j, and distributed identically at each j, with $\langle \sigma_j(0) \rangle = s$. Here s is a complex number which, for $k = 3$, must be within (or on the boundary of) the triangle defined by 1, $\exp(2\pi i/3)$ and $\exp(4\pi i/3)$ in the complex plane.

The average $\langle \ldots \rangle$ for times $t > 0$ will denote both averaging over the stochastic evolution, i.e., over the choices of the variables $\zeta_m(t)$, and over the distribution of the initial values $\sigma_j(0)$. However, the $s \neq 0$ uncorrelated distribution of the initial spin values implies a subtle correlation in the initial distribution of the reacting-diffusing particles on the dual lattice, as emphasized for $k = 2$ in the Glauber-type approach [9].

Thus, even though our solution can be easily extended to general s, we will put $s = 0$. In fact, we assume that the reacting-diffusing particles are initially distributed as follows for $k = 3$: at each dual-lattice site, one randomly places 0, 1, or 2 particles at time $t = 0$. The average initial density is $\rho(0) = 1$, and such distribution ensures that each spin has equal probability to have the three allowed complex values (for $k = 3$; extension to $k \neq 3$ is trivial).

For times $t > 0$ the particle density will decrease from $\rho(0) = 1$. In fact, the mean-field rate equation prediction for $k = 3$ can be easily derived, and it is $\rho(t) \sim 1/t$ for large times. We now put $k = 3$ and derive the exact expression for $\rho(t)$. The result yields $\rho(t) \sim 1/\sqrt{t}$ for large times, similar to the fluctuation-induced modification of the asymptotic density in the case of the two-body annihilation $A + A \rightarrow$ inert, which corresponds to another solvable case, $k = 2$.

The case $k = 3$ is special due to the property that the density of particles on the dual lattice can be expressed in terms of the 2-spin correlations of the Z_k spins for $k = 3$ (and if fact also for $k = 2$) but not for $k > 3$. Indeed, if $g = \exp(2\pi i\ell/k)$ is one of the k roots of unity constituting the representation of $Z_{k>2}$, then the appropriate phase number, $\ell = 0, 1, \ldots, k-1$, can be calculated as a linear form $a_{(1)} + a_{(2)}g + a_{(3)}g^*$ only for $k = 3$. Indeed, three complex coefficients $a_{(1),(2),(3)}$ are just the right number to be fixed to get the three values $\ell = 0, 1, 2$ properly. For $k > 3$, the expression required would involve higher integer powers of g and g^* and it would no longer be linear. For $k = 3$ the explicit result is

$$\ell = 1 + \frac{1}{\sqrt{3}}\mathrm{Re}\left[(-\sqrt{3} + i)g\right] \tag{3}$$

Recalling our rule of calculating the particle number $N_j(t)$, we conclude that the average particle density at site j (of the dual lattice) at time t is given by

$$\rho(t) = 1 + \frac{1}{\sqrt{3}}\mathrm{Re}\left[(-\sqrt{3} + i)\langle\sigma_{j+1}(t)\sigma^*_{j-1}(t)\rangle\right] \qquad (k = 3) \tag{4}$$

where we omitted the index j for $\rho(t)$ due to translational invariance. Relation (4) applies *only* for $k = 3$ and expresses the particle density in terms of the 2-spin correlation function of the Z_3 spins.

The dual-lattice sites can be empty, singly-occupied, or pair-occupied. Let $\rho_{\mathrm{single}}(t)$ denote the density of those particles which are in single-occupancy sites at time t. The density of particles which are in pairs if then simply $(\rho - \rho_{\mathrm{single}})$. Note that the initial conditions selected earlier correspond to $\rho_{\mathrm{single}}(0) = \frac{1}{3}$. The single-occupancy property of a site is indicated by the value of $\ell(2 - \ell) = 0, 1, 0$, for $\ell = 0, 1, 2$, respectively. This expression can also be written as a linear form in g and g^* (for $k = 3$). As a result we obtain the relation

$$\rho_{\rm single}(t) = \frac{1}{3}\left\{1 - {\rm Re}\left[(1+i\sqrt{3})\langle\sigma_{j+1}(t)\sigma^*_{j-1}(t)\rangle\right]\right\} \qquad (k=3) \tag{5}$$

Let us point out that all the "linearity" properties also apply for $k = 2$. In fact, all calculations are then with real variables: the elements of Z_2 are simply ± 1. The dynamics (2) for the case $k = 2$ describes particles hopping on a dual lattice and annihilating pairwise on encounters, i.e., the cellular-automaton (simultaneous-dynamics) variant of the reaction $A + A \to$ inert; see [11]. Relation (4) is replaced by

$$\rho(t) = \frac{1}{2}\left[1 - \langle\sigma_{j+1}(t)\sigma_{j-1}(t)\rangle\right] \qquad (k=2) \tag{6}$$

Turning back to $k = 3$, we note that the dynamical rules (2) imply

$$\langle\sigma_m(t)\rangle \equiv s = 0 \tag{7}$$

for translationally invariant initial conditions. Since $s = 0$, we can work with the 2-spin correlation function directly (for $s \neq 0$ one has to consider the "connected" part; the expressions are not much more complicated though). Thus, we define

$$G_n(t) = \langle\sigma_j(t)\sigma^*_{j+n}(t)\rangle \tag{8}$$

which does not depend on j due to translational invariance. This correlation function can be considered for $n = 0, 2, 4, \ldots$ only. Indeed, we have $G_{-n}(t) = G^*_n(t)$ generally.

By using (2), one can then derive the discrete-space and time diffusion equation for $G_n(t)$,

$$G_n(t+1) - G_n(t) = \frac{1}{4}\left[G_{n+2}(t) - 2G_n(t) + G_{n-2}(t)\right] \tag{9}$$

which must be solved for $n = 2, 4, \ldots$ and $t = 1, 2, \ldots$, subject to the initial and boundary conditions

$$G_0(t \geq 0) = 1 \qquad \text{and} \qquad G_{n>0}(t = 0) = 0 \tag{10}$$

In writing (10), we used $s = 0$ which implies a certain simplification of the problem. Indeed, by (9) the correlation function $G_n(t)$ is then *real* for these initial conditions. The form of the solution is thus essentially identical to that for $k = 2$. Relations (4), (5), (6) yield, for *real* $k = 3$ correlation function,

$$[\rho(t)]_{k=3} = 2\,[\rho(t)]_{k=2} = 1 - G_2(t) \qquad\qquad (s = 0) \tag{11}$$

$$\rho_{\text{single}}(t) = \frac{1}{3}\rho(t) \qquad\qquad (k = 3, s = 0) \tag{12}$$

The discrete diffusion equation (9) can be analyzed be generating function techniques [11]. The result for the density ($k = 3$) is

$$\rho(t) = \frac{(2t+2)!}{2^{2t+1}\left[(t+1)!\right]^2} \tag{13}$$

This function decreases smoothly from the initial value 1, and in fact provides analytic continuation to all positive times t. The large-time asymptotic form is

$$\rho(t \gg 1) \simeq \frac{2}{\sqrt{\pi t}} \tag{14}$$

The fact that the density for $k = 3$ turns out nearly identical to that for $k = 2$ may at first seem disappointing. However, one must recall that *all* the various exact calculations for model $1d$ reactions, based on the solution methods which involve evaluation of 2-spin correlation functions, always end up with continuous or discrete versions of the diffusion equation, — property shared with the Glauber Ising model in $1d$. Thus, the diversity of the functional forms obtained is limited [16]. The reaction scheme for $k=3$ is quite different from that for $k=2$. Indeed, if we denote particles in singly-occupied sites by A, and the pairs of particles, hopping as one unit, by B, then the reactions in the $k=3$ system are $A+B \to$ inert, $A+A \to B$, $B+B \to A$. Generally, such reaction scheme differs from the $k=2$ reaction, $A+A \to$ inert, both in its mean-field rate equation form and in the time dependence of densities and correlations.

Our results essentially suggest that for symmetric initial conditions (i.e., equal concentrations $\frac{1}{3}$ of species A and B), the densities of the $k=3$ and $k=2$ reaction schemes are proportional, and both are fluctuation-dominated, $\sim 1/\sqrt{t}$, as opposed to the rate-equation prediction, $\sim 1/t$, for large times.

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REFERENCES

1. M. Bramson and D. Griffeath, Ann. Prob. **8**, 183 (1980).
2. D.C. Torney and H.M. McConnell, J. Phys. Chem. **87**, 1941 (1983).
3. K. Kang, P. Meakin, J.H. Oh and S. Redner, J. Phys. A**17**, L665 (1984).
4. T. Liggett, *Interacting Particle Systems* (Springer-Verlag, New York, 1985).
5. Z. Racz, Phys. Rev. Lett. **55**, 1707 (1985).
6. A.A. Lushnikov, Phys. Lett. A**120**, 135 (1987).
7. M. Bramson and J.L. Lebowitz, Phys. Rev. Lett. **61**, 2397 (1988).
8. Review: V. Kuzovkov and E. Kotomin, Rep. Prog. Phys. **51**, 1479 (1988).
9. J.G. Amar and F. Family, Phys. Rev. A**41**, 3258 (1990).
10. L. Braunstein, H.O. Martin, M.D. Grynberg and H.E. Roman, J. Phys. A**25**, L255 (1992).
11. V. Privman, J. Stat. Phys. (1992), in print.
12. D. ben–Avraham, M.A. Burschka and C.R. Doering, J. Stat. Phys. **60**, 695 (1990), and references therein.
13. A.J. Bray, J. Phys. A**23**, L67 (1990).
14. B. Derrida, C. Godrèche and I. Yekutieli, Phys. Rev. A**44**, 6241 (1992).
15. M. Scheucher and H. Spohn, J. Stat. Phys. **53**, 279 (1988), and references therein.
16. Dynamical problems in $1d$ can also be reformulated as eigenvalue problems of certain quantum spin systems. M. Droz, M. Henkel and V. Rittenberg, private communication (1992), have explored this connection, which should allow the use of the Baxter-Yang equation approach to identify new integrable systems without the restriction to special cases such as relations (6) or (4).