Exact solution of homogeneous ballistic annihilation with a general reaction probability

2000 J. Phys. A: Math. Gen. 33 2365

(http://iopscience.iop.org/0305-4470/33/12/304)

J. Phys. A: Math. Gen. **33** (2000) 2365–2372. Printed in the UK PII: S0305-4470(00)09615-3

Exact solution of homogeneous ballistic annihilation with a general reaction probability

Y Kafri

Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 76100, Israel

Received 16 November 1999

Abstract. The homogeneous single-species $A + A \xrightarrow{p} 0$ reaction with ballistic reactants and a binary-velocity distribution is solved in the case of equal initial densities of particles with positive and negative velocities. Previous studies have considered the model when the pair reaction probability, p, is one. Here the long-time behaviour of the density decay is solved exactly in one dimension for general p. It is shown that, in contrast to recent numerical studies, the decay of the density at long times is a universal quantity independent of the reaction probability.

1. Introduction

The dynamics of reacting particles is a characteristic example of systems far from equilibrium. They appear in a broad spectrum of phenomena ranging from chemical reactions to exciton dynamics. Often, the precise mechanism of the reaction does not affect the macroscopic behaviour, which is dictated by a small number of parameters. Typically these are the number of reacting species and the type of motion these species perform. Many simple reaction processes have been studied extensively and found to exhibit a variety of interesting phenomena such as spontaneous symmetry breaking [1] and pattern formation [2].

One reaction which has received considerable attention is the single-species annihilation reaction $A + A \xrightarrow{p} 0$, with p a reaction probability or rate. When the mean free path of the reactants is much less than the inter-reactant distance it is appropriate to model the particles as diffusive. This case has been studied extensively [3–8]. It was found that in two dimensions and below the late-time decay of the density as a function of time is different from the one predicted by a mean-field approximation. Moreover, the decay of the density is a universal quantity which depends only on the diffusion constant and is independent of the reaction rate p.

When the mean free path of the reactants is much larger than the inter-reactant distance it is appropriate to model the motion of the particles as ballistic. By ballistic motion it is meant that particles move deterministically with constant velocity between collisions. Most of the studies of such processes have been performed on one-dimensional models where particles always react upon contact. This implies that once an initial condition is chosen, the complete time evolution of the system is known: the only source of noise arises from the initial particle distribution. The simplest of these models, which has inspired much work, was introduced by Elskens and Frish [9] and independently by Krug and Spohn [10]. The model is a homogeneous binary-velocity model which exhibits an exponential decay of the density to its asymptotic value when the initial densities of particles with positive and negative velocities are unequal.

0305-4470/00/122365+08$30.00

However, a more interesting behaviour is found when these initial densities are equal. In this case the decay of the density at long times was found to have the (non-mean-field) algebraic decay $\varrho \sim t^{-1/2}$. Other initial-velocity distributions have also been studied [11–16].

In contrast to these models, the study of one-dimensional ballistic systems with general reaction probability $p \neq 1$ is much less explored. However, recently a particular form of initial conditions appropriate for studying reaction fronts was solved exactly [17] for general reaction probability. The solution demonstrates a universal behaviour at late times with respect to the reaction probability p.

In this context, the problem of the homogeneous binary-velocity model with a general reaction probability has been long-standing. In this paper the model is solved exactly in one dimension for the general reaction probability $p > 0$ when the densities of particles with positive and negative velocities are *equal*. The general reaction probability introduces stochasticity into the time evolution of the system in addition to the noise originating from the initial-velocity distribution.

Recent numerical studies [18, 19] have indicated that at long times the density decays as $\varrho \sim t^{-\alpha}$ where α varies between 0.5 and 0.77, depending on the reaction probability. Here it is shown that this is an artifact of the numerics which have not reached the asymptotic behaviour. In fact, for any non-zero reaction probability the density decays at late times as $\varrho \sim A/t^{1/2}$, where A is a universal amplitude independent of the reaction probability p. The dependence on p enters only in terms of $\mathrm{O}(t^{-3/2})$.

The paper is organized as follows: in section 2, the model is defined and known results are reviewed. In section 3 the calculation strategy for the density decay is introduced and then carried out in sections 4. Finally, section 5 concludes with a discussion of the results.

2. The model

The model comprises an infinite line upon which particles are placed at time $t = 0$ such that their positions have a Poissonian distribution with density ϱ_0. Each particle is assigned, with equal probability, a velocity $+c$ (right moving) or $-c$ (left moving), which determines the trajectories the particles follow until reacting. When two particles meet, either a mutual annihilation occurs with probability $p = 1 - q$, or the particles pass through each other with probability q. Alternatively, the particles can be thought of as bouncing elastically off each other with probability q or annihilating with probability p. Note that in this model both the initial-velocity distribution and the reaction probability act as sources of noise, whereas in the $p = 1$ case solved in [9] only the former acts as a source of noise.

The mean-field equations of the model have already been considered in [9], and are given by

$$\partial_t \varrho_R^{MF} = \partial_t \varrho_L^{MF} = -pc\varrho_R^{MF} \varrho_L^{MF} \tag{1}$$

where ϱ_L^{MF} and ϱ_R^{MF} are the densities of left- and right-moving particles, respectively. In the long-time limit these equation give

$$\varrho_R^{MF} = \varrho_L^{MF} \sim \frac{1}{pct} \tag{2}$$

predicting that the density decay is a function of the reaction probability and the particle velocity but independent of the initial density. However, this prediction is wrong and the exact solution with $p = 1$ [9] at long times yields the density decay

$$\varrho = \frac{1}{(\pi \varrho_0 ct)^{1/2}} + \mathrm{O}(t^{-3/2}). \tag{3}$$

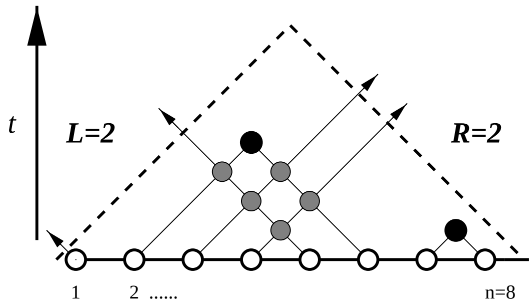

Figure 1. An example of a specific event in which $P_n(R, L) = P_8(2, 2)$. A black filled circle represents two particles which have reacted while a grey filled circle represents particles which have not reacted.

The difference between the mean-field solution and the exact behaviour is due to the fact that the former ignores the fluctuations due to the initial particle distribution. The correct density decay can be understood from the following qualitative argument. Consider the density fluctuations in a domain of length ℓ. The typical fluctuations in the difference of the number of left- and right-moving particles inside the domain is $\propto \ell^{1/2}$. After a time $\propto \ell$ only the residual fluctuation will remain, so that the density ϱ will be $\propto \ell^{-1/2}$. Re-expressing ℓ as a function of t one obtains the correct density-decay exponent $\varrho \propto t^{-1/2}$.

In the following the model is solved exactly in the long-time limit for general $0 < p \leqslant 1$. It will be shown that at long times the decay of the density is surprisingly given by equation (3). This implies that both the exponent characterizing the decay of the density and the amplitude are universal quantities *independent* of the reaction probability p. The dependence of the density decay on p enters only as corrections of $\mathrm{O}(t^{-3/2})$. This universality can be understood in the framework of the simple argument given above: due to the ballistic motion of the particles, at long times their paths intersect so many times that the effective reaction probability becomes one.

3. Calculation strategy

Let $P_n(R, L)$ be the probability that after a group of n particles (denoted by particle 1 to n according to their position along the line) have interacted with each other, R are moving in the positive (right) direction and L are moving in the negative (left) direction. An example of such a specific event where $R = L = 2$ is given in figure 1. Note that $P_n(R, L)$ only takes into account reactions within the specific n particles under consideration and that $R + L \leqslant n$. To obtain the density we first construct recursion relations for the probability $P_n(R, L)$. As will be shown the recursion relations do not have to be solved explicitly in order to obtain the final solution.

Next, consider a particle which at time $t = 0$ is the closest particle to the left of particle 1 and assume that this particle is right moving. Averaging over initial-velocity distributions and the possible reactions of particles $1, 2 \ldots, n$, the probability of this particle to survive after having a chance to interact with the n particles is given by

$$\mathcal{P}(n) = \sum_{L=0}^{n} q^L \sum_{R=0}^{n-L} P_n(R, L) \tag{4}$$

where the factor q^L is assigned when L particles are moving left. Using the recursion relations

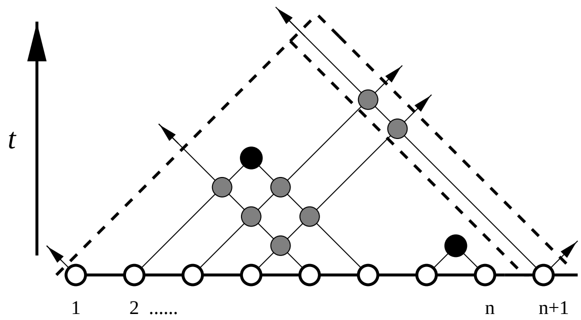

Figure 2. A graphical illustration of the construction of the recursion relations for $P_n(R, L)$. Here the first and second terms of equation (6) are illustrated.

for $P_n(R, L)$ one can evaluate this quantity exactly in the long-time limit using methods which will be described later.

To obtain the decay of the density consider the average number of particles, m_t, with which a given particle collides with up to time t. Due to the ballistic motion of the particles t is given by $r_t/2c$, where r_t is the average distance from the particle and the last (average) particle it meets at time t. Also, for large m_t this distance is given by m_t/ϱ_0 as a consequence of the central limit theorem applied to the initial Poissonian distribution, so that $m_t = 2c\varrho_0 t$. The density at time t is then given by

$$\varrho(t) = \mathcal{P}(2c\varrho_0 t) \tag{5}$$

where that fact that the probability of a right-moving particle to survive, $\mathcal{P}(m_t)$, at time t is equal to that of a left-moving particle by symmetry was used†.

In the following the recursion relations for $P_n(R, L)$ will be used with equations (4) and (5) to obtain the decay of the density at late times. It will be shown that the late-time decay of the density is independent of p and is given by

$$\varrho = \frac{1}{(\pi\varrho_0 ct)^{1/2}} + \mathrm{O}(t^{-3/2}). \tag{6}$$

The quantities which determine the late-time behaviour are the initial density and the particle velocity. Both the exponent characterizing the decay and the amplitude are independent of the reaction probability.

4. Calculation of the density

To construct recursion relations for $P_n(R, L)$ consider a group of $n + 1$ particles and a group of n particles. Using figure 2 one can write

$$P_{n+1}(R, L) = \tfrac{1}{2}q^R P_n(R, L-1) + \tfrac{1}{2}P_n(R-1, L) + \tfrac{1}{2}(1 - q^{R+1})P_n(R+1, L). \tag{7}$$

On the right-hand side the first term is the probability that the particle labelled $n + 1$ is left moving and has not interacted with any of the right-moving particles, the second term is the probability that the particle is right moving and the last term is the probability that it is left moving and has interacted with one of the right-moving particles. The boundary conditions are given by the $n = 0$ group of particles $P_0(R, L) = \delta_{R,0}\delta_{L,0}$.

† This is strictly true only when $\mathcal{P}(n)$ is a power law (see [9]).

The next calculation steps rely heavily on methods which have recently been introduced to obtain exact results for the partially asymmetric exclusion process [20, 21]. These involve q-numbers and q-deformed Hermite polynomials [22–24] and an in depth account of the methods can be found in [20, 21]. In what follows a list of definition and identities which are needed for the calculation will be presented where appropriate.

A q-shifted factorial is defined for $|q| < 1$ through

$$(a; q)_n = \prod_{k=0}^{n-1}(1 - aq^k). \tag{8}$$

The $n \to \infty$ limit of this product is written as $(a; q)_\infty$ and converges when $|q| < 1$ for all $a \in \mathbb{C}$. Since products of q-shifted factorials appear often it is common to introduce the notation

$$\begin{aligned}(a_1, a_2, \ldots, a_k; q)_n &= (a_1; q)_n(a_2; q)_n \ldots (a_k; q)_n \\ (a_1, a_2, \ldots, a_k; q)_\infty &= (a_1; q)_\infty(a_2; q)_\infty \ldots (a_k; q)_\infty.\end{aligned} \tag{9}$$

A q-deformed binomial (often called a Gaussian polynomial) is defined through

$$\binom{n}{m}_q = \frac{(q; q)_n}{(q; q)_m(q; q)_{n-m}} \tag{10}$$

and in the limit $q \to 1$ gives the binomial $\binom{n}{m}$.

With these definitions the recursion relation for $P_n(R, L)$ may be brought into a symmetric form in R and L by introducing

$$P_n(R, L) = (\tfrac{1}{2})^n \binom{R + L}{L}_q T_n(R + L) \tag{11}$$

where $T_n(s)$ satisfies the recursion relation

$$\begin{aligned}T_{n+1}(s) &= T_n(s - 1) + (1 - q^{s+1})T_n(s + 1) \\ T_0(s) &= \delta_{s,0}.\end{aligned} \tag{12}$$

To obtain the density we consider $\mathcal{P}(n)$ at even n. The case of odd n is similar and will not be discussed here. Since particles react in pairs, even n implies that $R + L$ is also even. Using this with equations (4) and (11) one has

$$\begin{aligned}\mathcal{P}(n) &= (\tfrac{1}{2})^n \sum_{L=0}^{n} q^L \sum_{R=0}^{n-L} \binom{R + L}{L}_q T_n(R + L) \\ &= (\tfrac{1}{2})^n \sum_{k=0,1,\ldots}^{n/2} T_n(n - 2k) \sum_{i=0}^{n-2k} \binom{n - 2k}{i}_q q^i\end{aligned} \tag{13}$$

where in the last step the terms were rearranged in groups with the same $T(n - 2k)$.

To proceed note the relation

$$(b + b^\dagger)^n = \sum_{k=0,1,\ldots}^{n/2} T_n(n - 2k) \sum_{i=0}^{n-2k} \binom{n - 2k}{i}_q (b^\dagger)^i (b)^{n-k-i} \tag{14}$$

which was obtained by Derrida and Mallick [25] in the context of the partially asymmetric exclusion process. Here $T_n(s)$ satisfies the recursion relation equation (12) and b and $b^\dagger$ are q-deformed harmonic oscillator operators which satisfy

$$bb^\dagger - qb^\dagger b = 1 - q. \tag{15}$$

When acting on an orthonormal Hilbert 'energy' basis $|n\rangle$, $n = 0, 1, \ldots,$ they give

$$b^\dagger|n\rangle = \sqrt{1-q^{n+1}}|n+1\rangle \qquad (16)$$
$$b|n\rangle = \sqrt{1-q^{n}}|n-1\rangle.$$

The coherent state of the operators b and $b^\dagger$ (often referred to as q-coherent states) is given by

$$|w\rangle\rangle = \sum_{k=0}^{\infty} \frac{w^k}{\sqrt{(q;q)_n}}|n\rangle \qquad (17)$$

and satisfies

$$b|w\rangle\rangle = w|w\rangle\rangle \qquad \langle\langle w|b^\dagger = w\langle\langle w|. \qquad (18)$$

Using the above relations one can easily show that

$$\mathcal{P}(n) = \frac{\langle\langle q|(b+b^\dagger)^n|1\rangle\rangle}{2^n\langle\langle q|1\rangle\rangle}. \qquad (19)$$

Note that when $q = 1$, so that no interactions occur, b and $b^\dagger$ commute and the expression reduces to the expected $\mathcal{P}(n) = 1$. To calculate this an analogue of the harmonic oscillator real space representation is used. For our purposes it is sufficient to note that this basis, denoted by $|P(\cos\theta)\rangle$, satisfies

$$(b^\dagger + b)|P(\cos\theta)\rangle = 2\cos\theta|P(\cos\theta)\rangle \qquad (20)$$

where $\theta \in [0, \pi]$ and that the projection of this basis on the q-coherent state is given by

$$\langle\langle w|P(\cos\theta)\rangle = \frac{1}{(w\mathrm{e}^{\mathrm{i}\theta}, w\mathrm{e}^{-\mathrm{i}\theta}; q)_\infty}. \qquad (21)$$

The completeness relation of the basis is given by

$$1 = \int_0^\pi |P(\cos\theta)\rangle\nu(\cos\theta)\langle P(\cos\theta)| \qquad (22)$$

where the weighting function $\nu(\cos\theta)$ is

$$\nu(\cos\theta) = \frac{(q, \mathrm{e}^{2\mathrm{i}\theta}, \mathrm{e}^{-2\mathrm{i}\theta}; q)_\infty}{2\pi}. \qquad (23)$$

Using these equation (19) can be rewritten as

$$\mathcal{P}(n) = \int_0^\pi \frac{\langle\langle q|P(\cos\theta)\rangle\nu(\cos\theta)(2\cos\theta)^n\langle P(\cos\theta)|1\rangle\rangle}{2^n\langle\langle q|1\rangle\rangle}\,\mathrm{d}\theta \qquad (24)$$

which after doubling the range of integration of θ from 0 to 2π and using equation (21) gives

$$\mathcal{P}(n) = \frac{1}{2^n}\frac{1}{4\pi\mathrm{i}\langle\langle q|1\rangle\rangle}\oint\frac{\mathrm{d}z}{z}\frac{(q, z^2, z^{-2}; q)_\infty}{(z, z^{-1}; q)_\infty(qz, qz^{-1}; q)_\infty}\left(z+\frac{1}{z}\right)^n. \qquad (25)$$

Here the substitution $z = \mathrm{e}^{\mathrm{i}\theta}$ was made.

Finally, to obtain the asymptotic behaviour the method of steepest decent is used [26]. Noting that [22]

$$\langle\langle q|1\rangle\rangle = \sum_{n=0}^{\infty}\frac{q^n}{(q;q)_n} = \frac{1}{(q;q)_\infty} \qquad (26)$$

the final result is given by

$$\mathcal{P}(n) = \sqrt{\frac{2}{\pi n}} + \mathrm{O}(n^{-3/2}). \qquad (27)$$

Using (5) the exact density decay at long times is then

$$\varrho(t) = \frac{1}{(\pi\varrho_0 ct)^{1/2}} + \mathrm{O}(t^{-3/2}). \qquad (28)$$

A more lengthy calculation which will not be presented here shows that the amplitude of $t^{-3/2}$ is not universal due to an explicit dependence on q.

5. Discussion

In this paper the single species $A + A \xrightarrow{p} 0$ reaction model with a binary-velocity distribution was solved exactly, for general reaction probability p, when the densities of right- and left-moving particles are equal. It was shown that the density decay is a universal quantity which is independent of the reaction probability, p, at long times. In the language of the renormalization group this means that the noise introduced by the reaction probability is irrelevant. An intuitive explanation of this result was given. Based on this it is expected that this universality would also be found in the recently studied case of ballistic reactions near an impenetrable boundary [27].

One of the unresolved issues for ballistic reactants is that of dimensions larger than one where very little is known. Another interesting question is the effect of noise induced by quenched disorder on the density decay. Such systems have been recently considered in single-species reactions when the dynamics of the reactants are diffusive [28,29] and interesting effects on the density decay were found.

Acknowledgments

I would like to thank David Mukamel and Magnus J E Richardson for many useful comments and critical reading of the manuscript. I have also benefited from discussion with Martin Evans and am especially grateful to Richard A Blythe for pointing out [25] and introducing me to the methods of calculation.

References

[1] Bramson M and Lebowitz J L 1991 *J. Stat. Phys.* **62** 297
Bramson M and Lebowitz J L 1991 *J. Stat. Phys.* **65** 941
[2] Chopard B, Droz M, Magnin J, Rácz Z and Zrinyi M 1999 *J. Phys. Chem.* A **103** 1432
[3] Toussaint D and Wilczek F 1983 *J. Chem. Phys.* **78**
[4] Peliti L 1986 *J. Phys. A: Math. Gen.* **19** L365
[5] Spouge J L 1988 *Phys. Rev. Lett.* **60** 871
[6] Lushnikov A A 1986 *Sov. Phys.–JETP* **64** 811
[7] Lushnikov A A 1987 *Phys. Lett.* **120** 135
[8] Lee B P 1994 *J. Phys. A: Math. Gen.* **27** 2633
[9] Elskens Y and Frisch H L 1985 *Phys. Rev.* A **31** 3812
[10] Krug J and Sphon H 1988 *Phys. Rev.* A **38** 4271
[11] Privman V (ed) 1997 *Nonequilibrium Statistical Mechanics in One Dimension* (Cambridge: Cambridge University Press)
[12] Droz M, Rey P A, Frachebourg L and Piasecki J 1995 *Phys. Rev.* E **51** 5541
[13] Droz M, Rey P A, Frachebourg L and Piasecki J 1995 *Phys. Rev. Lett.* **75** 160
[14] Krapivsky P L, Redner S and Leyvraz F 1995 *Phys. Rev.* E **51** 3977
[15] Piasecki J, Rey P A and Droz M 1996 *Physica* A **229** 515
[16] Rey P A, Droz M and Piasecki J 1999 *Phys. Rev.* E **59** 126
[17] Richardson M J E 1997 *J. Stat. Phys.* **89** 777
[18] Sheu W S 1996 *J. Phys. Chem.* **100** 17 446
[19] Sheu W S and Chen H Y 1998 *J. Chem. Phys.* **108** 8394
[20] Blythe R A, Evans M R, Colaiori F and Essler F H L 2000 *J. Phys. A: Math. Gen.* **33** 2313 (this issue)
[21] Sasamoto T 1999 *J. Phys. A: Math. Gen.* **32** 7109
[22] Gasper G and Rahman M 1990 *Basic Hypergeometric Series* (Cambridge: Cambridge University Press)
[23] Macfarlane A J 1989 *J. Phys. A: Math. Gen.* **22** 4581
[24] Atakishiyev N M and Feinsliver P 1996 *J. Phys. A: Math. Gen.* **29** 1659
[25] Derrida B and Mallick K 1997 *J. Phys. A: Math. Gen.* **30** 1031

[26] See for example Bender C M and Orszag S A 1978 *Advanced Mathematical Methods For Scientists and Engineers* (New York: McGraw-Hill)

[27] Kafri Y and Richardson M J E 1999 *J. Phys. A: Math. Gen.* **32** 3253
Richardson M J E and Kafri Y 1999 *Phys. Rev.* E **59** R4725

[28] Richardson M J E and Cardy J 1999 *J. Phys. A: Math. Gen.* **32** 4035

[29] Park J M and Deem M W 1998 *Phys. Rev.* E **57** 3618
Chung W J and Deem M W 1999 *Physica* A **265** 486