Diffusion-limited coalescence and annihilation on a one-dimensional expanding medium

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We consider diffusion-controlled reactions (reactions in which the typical reaction time is short in comparison to the typical time spent by a pair particles before reacting) which take place on a one-dimensional expanding medium. In particular, we consider the irreversible single-species coalescence reaction $A + A \to A$, and the irreversible single-species annihilation reaction $A + A \to \varnothing$.

These reactions have been extensively studied in static media. It is well known that a simple mean-field approach does not work when the mixing of the reactants is impaired by, e.g., the low dimensionality of the medium. A method that is able to cope with this scenario for a one-dimensional medium is the Interparticle Distribution Function (IPDF) method [1]. Here we generalize this method to the case of uniformly expanding media. We discover that the mixing of diffusing particles and the corresponding reaction kinetics are, in some cases, largely modified by the expansion of the medium.

The mathematical complexities induced by the expansion can be reduced to a large extent if one works with comoving coordinates. Let $x = y(0)$ be the coordinate of a fixed point at the initial time $t = 0$. Due to the expansion, this fixed point changes its position, $y(t)$ being its coordinate at time t. If the expansion of the medium is uniform $y(t)$ and x are related by $y(t) = a(t)x$, where $a(t)$ is the scale factor and $a(0) = 1$. The quantity $x = y/a(t)$ is the comoving coordinate associated with the position y at time t.

The interparticle probability density function $p(x,t)$ is defined as the density of probability of finding a gap of size x (in comoving coordinates) between two neighboring particles. Let us define the auxiliary function $q(x,t) = p(x,t)/c(t)$, where $c(t)$ is the number density of particles in comoving space, and let us define the Brownian conformal time $\tau(t)$ as

$$\tau(t) = \int_0^t \frac{ds}{a^2(s)}. \tag{1}$$

It is possible to prove [2] that the auxiliary function $q(x,t)$ satisfies a standard diffusion equation

$$\frac{\partial q}{\partial \tau} = 2D\frac{\partial^2 q}{\partial x^2}, \tag{2}$$

where D is the diffusion constant of the reacting particles. This is a key result because from $q(x,t)$ we can find the survival probability $S(t)$ of a particle, the structure of the system (arrangement of particles), etc. In particular,

$$c(t) = c(0)S(t) = \int_0^\infty q(x,t)dx. \tag{3}$$

In some cases we can get exact solutions from these expressions. For example, for a completely random initial distribution of particles (Poisson distribution) one obtains

$$S(t) = e^{z^2}\text{erfc}(z), \tag{4}$$

with $z = c_0\sqrt{2D\tau(t)}$ for coalescence reactions and $z = 2c_0\sqrt{2D\tau(t)}$ for annihilation reactions. In Fig. 1 we compare, for coalescence reactions, $S(t)$ obtained by means of Eq. (4) with simulation results. The agreement is excellent. It is clear that the behaviour of $S(t)$ depends on $\tau(t)$, or equivalently, on the expansion scale factor $a(t)$. It turns out that $\tau(t \to \infty) = \tau_\infty < \infty$ for some (fast) expansions, e.g., a power-law expansion $a(t) = (1 + t/t_0)^\gamma$ with $\gamma > 1/2$ or an exponential expansion $a(t) = \exp(Ht)$ with $H > 0$. In these cases the survival probability of the reacting particles tends to a finite value at long times, $S(t \to \infty) = S_\infty > 0$, in other words, the expansion is so fast that the reactions stop prematurely and the spatial distribution of particles freezes before reaching the fully self-ordered state. This behavior is similar to the freeze-out behaviour displayed by the early universe in the context of cosmology.

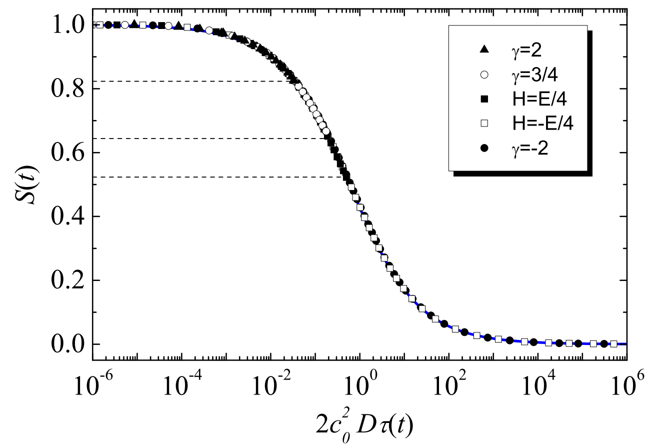

Fig. 1. Survival probability $S(t)$ *vs.* $z^2 = 2c_0^2 D\tau(t)$ for coalescence. The symbols correspond to simulation results for power-law expansions with $t_0 = 1000$ and $\gamma = 2, 3/4, -2$, and exponential expansions with $H = 10^{-4}$ and $H = -10^{-4}$. Dashed lines correspond to the limiting value S_∞ of the survival probability for $\gamma = 2$ ($S_\infty \approx 0.823$), $\gamma = 3/4$ ($S_\infty \approx 0.644$), and $H = 10^{-4}$ ($S_\infty \approx 0.523$). The solid line is the exact solution in Eq. (4).

[1] D. ben-Avraham and S. Havlin, *Diffusion and Reactions in Fractals and Disordered Systems* (Cambridge University Press, Cambridge, 2005).

[2] F. Le Vot, C. Escudero, E. Abad, and S. B. Yuste, Encounter-controlled coalescence and annihilation on a one-dimensional growing domain, arXiv:1804.03213.