Master de Physique
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Brownian and ballistic annihilation processes

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Abstract

Diffusion-reaction processes can model many interesting situations. They are used for instance to model disease propagation in the same way as chemical reactions: H+S $\to$ 2S (contamination), S $\to$ H (healing), S$\to \emptyset$ (death) with H healthy and S sick. Depending on the reactive particles dynamical properties (ballistic or brownian), on the space dimensionality, *etc*, interesting phenomena are observed.

In 1983 D. Toussaint and F. Wilczek[1] considered a simple situation of 2 reactive Brownian species A, $\overline{\mathrm{A}}$ obeying $\mathrm{A}+\overline{\mathrm{A}} \to \emptyset$. This was meant to be a toy description of the matter-antimatter annihilation that might have occurred in the early cosmological times. They were interested in finding out whether such model could predict a local excess of matter over antimatter. It turned out that this model provides a simple and non trivial example of case where usual chemical kinetics fails to predict the observed situation in low dimensional spaces.

1 Mean-field chemical kinetics

Given two species A, $\overline{\mathrm{A}}$ one introduces the average concentrations $[\mathrm{A}](t)$, $[\overline{\mathrm{A}}](t)$. The bimolecular reaction scheme $\mathrm{A} + \overline{\mathrm{A}} \to \emptyset$ is described by the equations

$$\begin{aligned} \frac{\mathrm{d}[\mathrm{A}]}{\mathrm{d}\,t} &= -k_2[\mathrm{A}][\overline{\mathrm{A}}] \\ \frac{\mathrm{d}[\overline{\mathrm{A}}]}{\mathrm{d}\,t} &= -k_2[\mathrm{A}][\overline{\mathrm{A}}] \end{aligned} \tag{1}$$

Starting with identical concentrations $[\mathrm{A}](0) = [\overline{\mathrm{A}}](0) = n_0$ leads by symmetry to $[\mathrm{A}](t) = [\overline{\mathrm{A}}](t)$ and

$$\frac{\mathrm{d}[\mathrm{A}]}{\mathrm{d}\,t} = -k_2[\mathrm{A}]^2 \tag{2}$$

with solution $[\mathrm{A}](t) = \dfrac{n_0}{1 + n_0 k_2 t} \sim t^{-1}$.

Simulations, or more detailed analysis shows that the asymptotic behaviour $[\mathrm{A}] \sim t^{-\alpha}$ does not correspond to $\alpha = 1$ if the space dimension is equal to 1 or 2, Toussaint & Wilczek (1983). The reason is that the kinetic equations are implicitly associated to a mean-field approximation saying that the local species concentration is everywhere close to the average gross system concentration. This is only true if the space dimension is larger than an **upper critical dimension** d_c. Below d_c strong spatio-temporal correlations leads to anomalous exponents. The current projects aims at playing with this idea of deviation from mean-field kinetic exponent behaviour.

[1]F. Wilczek, Nobel prize in physics 2004 for bringing the concept of asymptotic freedom in quantum chromodynamics

2 Ballistic annihilation in 1-dimension

Definition of the system and particles kinetics

Ballistic trajectories are straight lines in time t-position x representation. Particles in 1d can be ordered according to increasing positions. In the limit of vanishingly small sizes and identical masses, each elastic collision simply correspond to an exchange of label of the lines. Particles ordering cannot be changed by collisions.

To complete the description of the system one enforces some L periodicity to the space coordinates. Positions x and $x + L$ therefore corresponds to the same physical point.

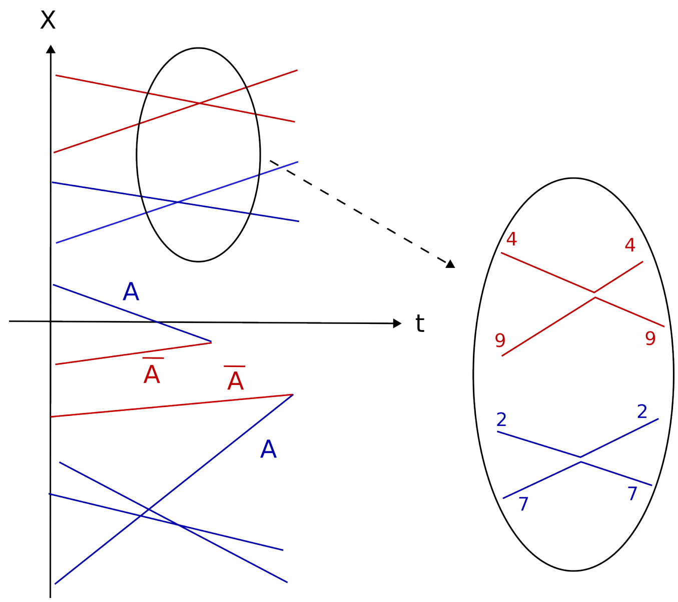

Figure 1: Collisions of ballistic A, $\overline{\text{A}}$ particles. A particles (blue) and $\overline{\text{A}}$ particles (red) move along straight lines in a time t-position x world lines diagram. A and $\overline{\text{A}}$ particles annihilate upon encounter. A-A and $\overline{\text{A}} - \overline{\text{A}}$ collisions simply correspond to an exchange of identities of the line labels.

Algorithm

The idea is to start with ordered or randomly distributed initial particles positions A, $\overline{\text{A}}$ and velocities. Consider for instance equally spaced initial positions, or random uniform initial positions. Velocities can be drawn from well defined values $\{-v_0, 0, +v_0\}$ or from a gaussian Maxwell velocity distributions. Consider situations where the number of A and $\overline{\text{A}}$ are exactly the same, and situations where one exceeds the other.

Compute positions $x_j(i\delta t)$ for a discrete sequence of time values $i\delta t$. It is advised to place particles in well ordered positions, as cyclic order will be maintained as time passes. Think of how to implement periodicity. You can work with "wrapped" coordinates, *i.e.* particles are put back in the interval $[0, L]$ whenever they escape from above or below.

To detect collisions, it is sufficient to consider the two nearest neighbours of any given particle. A collision occurs when the sign of the differences $x_j(t) - x_{j+1}(t)$ and $x_j(t + \delta t) - x_{j+1}(t + \delta t)$ changes. For instance one can compute for every next nearest neighbour pair the product

$$(x_j(t) - x_{j+1}(t))(x_j(t + \delta t) - x_{j+1}(t + \delta t))$$

and check for the occurrence of a negative value (collision).

A collision between A and $\overline{\mathrm{A}}$ will lead to the removal of both particles. A collision between a pair of A or $\overline{\mathrm{A}}$ will lead to an exchange of position and velocity of the pair immediately following the collision.

$$x_j(t+\delta t) \leftrightarrow x_{j+1}(t+\delta t)$$
$$v_j(t+\delta t) \leftrightarrow v_{j+1}(t+\delta t)$$

After testing with a reduced number of particles (one should be able to reproduce Fig.1 with `matplotlib.pyplot`), increase the number to $\sim 10^3$ initial particles. Compute the average concentrations as a function of time. Repeat the simulations to gain statistics and obtain smooth averaged curves.

3 Brownian annihilation in 1-dimension

The idea is similar to the previous situation but Gaussian random increments of positions δx_j will be added to the particles positions (continuous Brownian walks). Alternatively one can also devise a Brownian walk on lattice, where particles move with constant negative or positive increments, see *e.g.* Fig. 2.

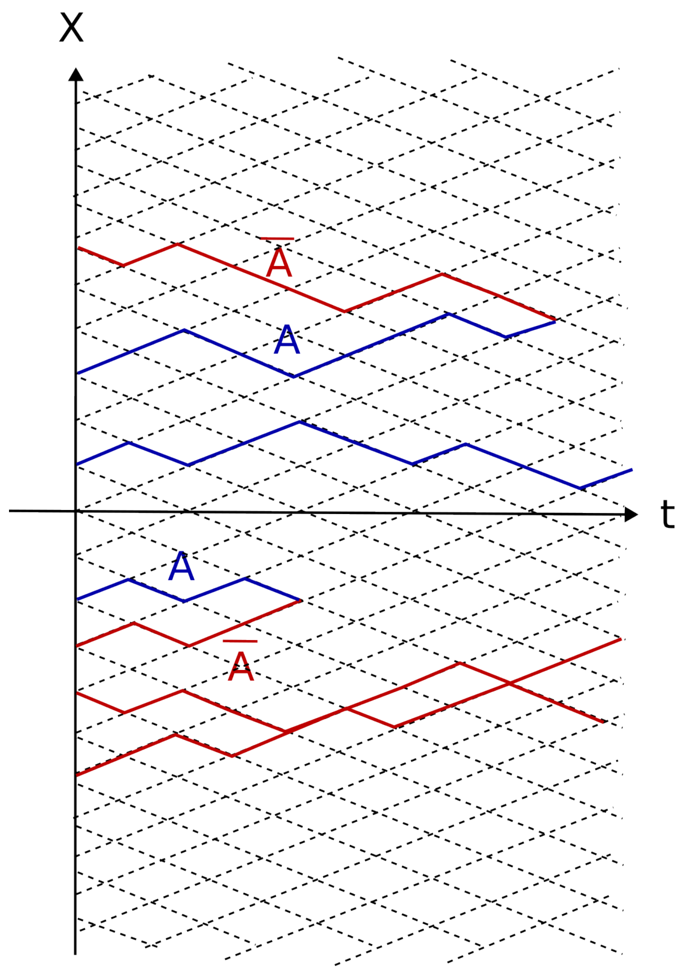

Figure 2: Discrete random walks of A, $\overline{\mathrm{A}}$ particles leading to collisions. Discreteness of the walk facilitates the detection of collisions.

Brownian diffusive random annihilation corresponds to the case studied by Toussaint and Wilczek. Try to compare your exponent with the mean-field prediction t^{-1}. Check on your data if there is evidence of bad mixing and local excess of one of the species with respect to the other. Try to represent your results as in Fig. 1 and 2.

References

Toussaint D., Wilczek F., , Particle–antiparticle annihilation in diffusive motion 1983, The Journal of Chemical Physics, 78, 2642