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Scaling in ballistic annihilation kinetics*

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Abstract

We investigate the decay dynamics of the ballistic annihilation process, where particles following ballistic trajectories annihilate at each collision. In the framework of a Boltzmann equation, a Gaussian assumption for the velocity distribution is used to obtain analytical predictions for the decay exponents of the density and kinetic energy. In dimensions 1 and 2, these predictions are shown to be in good agreement with the complementary results of Monte Carlo and molecular dynamics simulations.

1. Introduction

Compared to their counterparts with diffusive transport, systems of reacting particles with ballistic transport have received relatively little attention, despite the relevance of such deterministic motion to the modelling of coarsening and growth processes [1, 2]. In this contribution, we consider one of the simplest possible dynamics with ballistic motion and pairwise annihilation of colliding particles ($A + A \to \emptyset$). This model has been introduced and solved for its one-dimensional version by Elskens and Frisch [3], in the situation of a symmetric binary initial distribution of velocities. Using combinatorial analysis, they showed that the density of particles decreases in the long-time limit according to a power law $t^{-\xi}$ with $\xi = 1/2$ [4][1]. Later, a method permitting one to solve the evolution equations, in 1D, with an arbitrary but discrete initial velocity distribution was put forward [5,6] and successfully applied to the case of symmetric three-velocity distributions. However, no solution has been obtained for continuous initial velocity distributions, where the decay exponents have been computed numerically in 1D [7–9]. These studies showed that the exponent ξ characterizing the algebraic decay of the density could depend on the velocity distribution. Recently, in the framework

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[1] Similar results have been obtained independently by Krug and Spohn; see [1]. Moreover, a more general class of stochastic annihilation and coalescence models (reducing to the ballistic annihilation process in some limit) have been introduced and solved in one dimension; see [4].

of the molecular chaos factorization, Krapivsky and Sire [9] proposed bounds for the decay exponent, and obtained an analytic expression for ξ in the limit of large dimensionality.

In this work, we investigate the decay dynamics of the ballistic annihilation process, in arbitrary dimension. In the framework of the Boltzmann equation, we obtain analytically accurate expressions for the decay exponents. These predictions that seem to be lacking in the literature are then tested against direct simulation Monte Carlo (DSMC) simulations providing the numerical solution of the Boltzmann equation, and further confronted with molecular dynamics simulations where the exact equations of motion are integrated, thereby providing an assessment of the validity of Boltzmann's molecular chaos assumption.

2. Scaling and kinetic theory

The system considered consists of identical spheres (radius σ) in dimension d with initial velocity distribution $f(\boldsymbol{v}, t = 0)$ and random initial positions, with the constraint that no overlap between the particles is allowed at $t = 0$. The particles undergo free flight motion, and whenever a pair meet, the two colliding partners instantaneously annihilate each other and are removed from the system. At a given time t, we denote by $\bar{v}$ the typical (rms) time-dependent velocity, and the relevant length scale controlling the ballistic dynamics is the mean free path $\ell \propto 1/(n\sigma^{d-1})$ where $n(t)$ is the number density. On dimensional grounds, we obtain that the collision frequency $\omega(t) \equiv \bar{v}/\ell$ scales like the inverse time: $\omega \propto 1/t$. A formally exact rate equation for the density can be written as $\dot{n} = -\omega n$ which yields an algebraic time dependence for $n(t)$. The same holds for the typical velocity, and we therefore introduce two exponents ξ and γ for the long-time decay: $n(t) \propto t^{-\xi}$ and $\bar{v} \propto t^{-\gamma}$. ξ and γ are *a priori* unknown but related through $\omega \propto 1/t$, which imposes $\xi + \gamma = 1$ (this scaling relation has already been obtained in [6, 7, 9]). Before considering a kinetic theory for the annihilation process, it is instructive to push further the above scaling arguments. We define the kinetic temperature T as the variance of the velocity distribution

$$T(t) = \frac{1}{n(t)} \int v^2 f(\boldsymbol{v}, t)\, \mathrm{d}\boldsymbol{v} = \langle v^2 \rangle \tag{1}$$

while the total density reads $n(t) = \int f(\boldsymbol{v}, t)\, \mathrm{d}\boldsymbol{v}$. Assuming the coarse-grained density and velocity fields homogeneous, we get

$$\frac{\mathrm{d}n}{\mathrm{d}t} = -\omega(t) n \tag{2}$$

$$\frac{\mathrm{d}(nT)}{\mathrm{d}t} = -\omega(t) n T_{\mathrm{coll}} = -\alpha \omega(t) n T \tag{3}$$

where the second line states that the instantaneous average total kinetic energy of a colliding pair, T_{coll}, is lost at each collision event. Unlike T, obtained by averaging v^2 over all particles in the system at a given time, T_{coll} that quantifies the energy dissipation corresponds to an average restricted to particles at contact (and thus in pre-collision configurations; the relation between α and collisional averages of the two-body distribution function will be specified below—see equation (13)—but for the sake of the argument, it is not necessary to be more specific here). In the asymptotic regime, the ratio T_{coll}/T goes to a constant denoted as α in equation (3). Combining equations (2) and (3), we obtain

$$\frac{\mathrm{d}\log n}{\mathrm{d}\log(nT)} = \alpha \tag{4}$$

which can be supplemented with the scaling relations $T \propto \bar{v}^2 \propto t^{2\gamma}$ and $\xi + \gamma = 1$ to relate α to the decay exponents ξ and γ:

$$\xi = \frac{2}{1+\alpha} \qquad \text{and} \qquad \gamma = \frac{\alpha - 1}{\alpha + 1}. \tag{5}$$

We expect the typical colliding partners to be 'hotter' than the mean particle, so $\alpha > 1$, implying $\xi < 1$ and $\gamma > 0$. The above argument explains the failure of the naive mean-field picture where collisional correlations are discarded and the decay rate of the density is written as $\dot{n} \propto -n^2$, corresponding to $\xi = 1$ and $\alpha = 1$. As we shall see below, $\alpha \neq 1$ except in the limit of infinite dimension[2].

In order to get an analytical prediction for α, we resort to the framework of the Boltzmann equation considered in [7, 9], where the two-body distribution function at contact that bears the dynamical information (the particles only interact at contact) is factorized according to the molecular chaos hypothesis [10]:

$$f^{(2)}(\boldsymbol{v}_1, \boldsymbol{v}_2, |\boldsymbol{r}_{12}| = \sigma, t) = f(\boldsymbol{v}_1, t) f(\boldsymbol{v}_2, t). \tag{6}$$

The corresponding Boltzmann equation accounts for the collisional correlations missed by the naive mean-field theory, and can be written as

$$\frac{\partial f(\boldsymbol{v}, t)}{\partial t} = -f(\boldsymbol{v}, t) \int \mathrm{d}\boldsymbol{w}\, |\boldsymbol{v} - \boldsymbol{w}| f(\boldsymbol{w}, t). \tag{7}$$

It is straightforward to obtain that if the initial distribution $f(\boldsymbol{v}, t = 0) \propto v^\mu$ around the velocity origin, the subsequent dynamics preserves this property and $f(\boldsymbol{v}, t > 0) \propto v^\mu$ for $v \to 0$. Previous works [7–9] have shown the influence of the parameter μ ($\mu > -d$) on the decay kinetics (ξ changes with μ).

In the long-time limit, the velocity distribution approaches a scaling form:

$$f(\boldsymbol{v}, t) = \frac{n(t)}{\langle v^2 \rangle^{d/2}} \varphi(\boldsymbol{c}) \tag{8}$$

where we have introduced the rescaled velocity

$$\boldsymbol{c} = \frac{\boldsymbol{v}}{\sqrt{\langle v^2 \rangle(t)}} \tag{9}$$

so $\int \varphi \, \mathrm{d}\boldsymbol{c} = 1$ and $\int c^2 \varphi \, \mathrm{d}\boldsymbol{c} = 1$. Inserting (8) into (7) and remembering (5) yields an equation for the scaling function:

$$\langle c_{12} \rangle \left[1 + \left(\frac{1-\alpha}{2} \right) \left(\mathrm{d} + c_1 \frac{\mathrm{d}}{\mathrm{d}c_1} \right) \right] \varphi(c_1) = \varphi(c_1) \int \mathrm{d}\boldsymbol{c}_2 \, c_{12} \varphi(c_2) \tag{10}$$

where the rescaled collision frequency reads

$$\langle c_{12} \rangle \equiv \langle |\boldsymbol{c}_1 - \boldsymbol{c}_2| \rangle = \int \mathrm{d}\boldsymbol{c}_1 \, \mathrm{d}\boldsymbol{c}_2 \, |\boldsymbol{c}_1 - \boldsymbol{c}_2| \varphi(c_1) \varphi(c_2). \tag{11}$$

Multiplying equation (10) by c_1^p and integrating over $\boldsymbol{c}_1$ gives a hierarchy of relations between α and moments of φ:

$$\alpha = 1 + \frac{2}{p} \left(\frac{\langle c_{12} c_1^p \rangle}{\langle c_{12} \rangle \langle c_1^p \rangle} - 1 \right) \tag{12}$$

[2] It is however possible to find initial distributions for which $\alpha = 1$: by construction, if all the particles have initially the same kinetic energy ($f(\boldsymbol{v}, t = 0) \propto \delta(v - v_0)$), $T_{\mathrm{coll}} = T$ and therefore $\xi = 1$ while γ vanishes. Unlike the above situation, we restrict consideration in this study to initial distributions that are populated near the origin of velocities, so that generically $\alpha \neq 1$.

where $\langle(\cdots)\rangle \equiv \int(\cdots)\varphi(c_1)\varphi(c_2)\,\mathrm{d}\boldsymbol{c}_1\,\mathrm{d}\boldsymbol{c}_2$. In the special case $p = 2$, we recover the definition of α through the kinetic energy dissipation, as expressed by equation (3):

$$\alpha = \frac{T_{\mathrm{coll}}}{T} = \frac{\langle c_1^2\rangle_{\mathrm{coll}}}{\langle c_1^2\rangle} = \frac{\langle c_{12}c_1^2\rangle}{\langle c_{12}\rangle\langle c_1^2\rangle}. \tag{13}$$

It is possible to obtain a set of approximations for α, computing the averages appearing in equation (12) assuming a Gaussian form for φ. Given that the high-velocity tail of φ is overpopulated with respect to the Gaussian distribution (from equation (10), $\varphi(\boldsymbol{c}) \propto c^{-1-d+1/\gamma}\exp(-Ac)$ for large velocities, as already pointed out in [7, 9]), we expect such an approximation to be all the more reliable as expressed in terms of moments of order as low as possible. It is then noteworthy that taking the limit of vanishing velocity of the rescaled Boltzmann equation (10) allows one to relate α to moments of order 1, unlike equation (12):

$$\alpha = 1 + \frac{2}{\mu + d}\left(1 - \frac{\langle c_1\rangle}{\langle c_{12}\rangle}\right). \tag{14}$$

In the subsequent analysis, we concentrate on the much-studied case $\mu = 0$ [7–9], for which the Gaussian assumption for φ leads to accurate expressions for α. This ansatz can be considered as the zeroth-order expansion of the exact distribution in a well chosen basis of Sonine functions [11, 12], and we denote as α_0 the corresponding estimate for α, which is easily computed from equation (14):

$$\alpha_0 = 1 + \frac{2}{d}\left(1 - \frac{\sqrt{2}}{2}\right) \qquad \Longleftrightarrow \qquad \xi_0 = \frac{2d}{2(d+1) - \sqrt{2}}. \tag{15}$$

Within Boltzmann kinetic theory, the exact large-d behaviour of α and ξ has been obtained in [9] up to order $1/d$. It is interesting to note that expressions (15) match the exact one up to this order. In the opposite limit $d = 1$, the same authors obtained numerically $\xi \simeq 0.769(5)$, whereas we obtain $\xi_0 \simeq 0.773(5)$ from (15): the agreement is good, of the order of 0.5%. It can in principle be improved by the explicit inclusion of non-Gaussian corrections [12]. In the next section, simulations of the situation $d > 1$ will be performed.

3. Numerical simulations

Two complementary numerical approaches have been implemented:

- The direct simulation Monte Carlo (DSMC) method, where a Markov chain is generated with the same probabilities of transition as the Boltzmann equation under study [13]. This method explicitly relies on the molecular chaos factorization and provides the 'exact' time-dependent solution of the Boltzmann equation.
- Molecular dynamics simulations (see [14]), where the exact dynamics is simulated, in a finite system with periodic boundary conditions. This method is more CPU-time consuming than the previous one, and finite-size effects hinder a precise determination of the scaling exponents: the decay of the particle density implies a concomitant increase of the mean free path as t^{ξ}, which eventually becomes of the order of the simulation box size. The initial particle number needs to be large so that on the one hand the system is able to reach the asymptotic regime before suffering from finite-size pollution, and on the other hand the shape of the velocity distribution can be obtained at large times with the required accuracy. In practice, systems with $N = 5 \times 10^4$–5×10^5 particles have been considered.

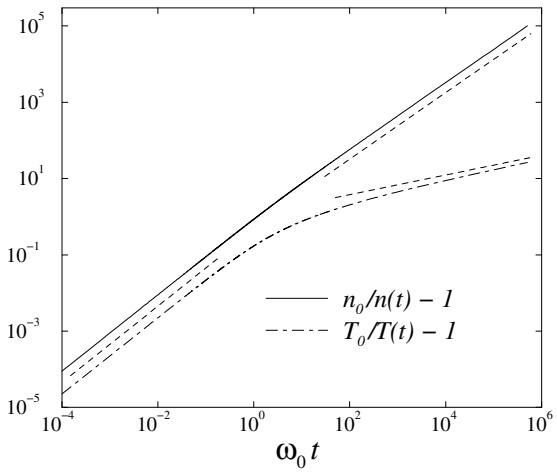

Figure 1. Evolution of the rescaled inverse density and inverse temperature with time, in dimension 2. ω_0 is the collision frequency in the initial configuration, while n_0 and T_0 denote the initial density and temperature. The dotted curve at short times has slope 1, while those at later times correspond to the predictions of equation (15): slope $\xi_0 \simeq 0.87$ (upper curve) and slope $2\gamma_0 \simeq 0.26$ (lower curve).

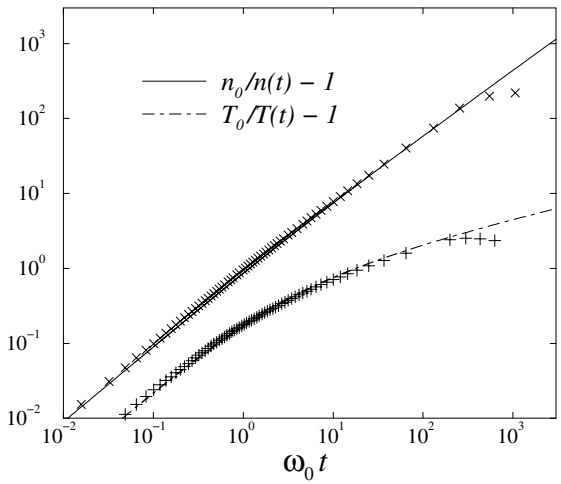

Figure 2. As figure 1, except that the symbols correspond to molecular dynamics simulations ($\times$ for the density and + for the temperature). As in figure 1, the curves show the DSMC results.

The results of two-dimensional DSMC simulations are shown in figure 1. After an initial transient where the density and temperature evolve linearly in time (this feature follows directly from equations (2) and (3)), a well defined scaling regime is entered with characteristic exponents in quantitative agreement with equation (15), which predicts $\xi_0 \simeq 0.87$ and $\gamma_0 \simeq 0.13$ for $d = 2$. A very similar behaviour is observed with molecular dynamics simulations (see figure 2), with the restriction that the time evolution cannot be followed over the same range as in DSMC. Finite-size effects are visible in figure 2 where the MD results saturate for $\omega_0 t$ of the order of 5×10^2, a time for which the mean free path becomes of the order of the system size. In order to avoid spurious but necessarily transient excluded-

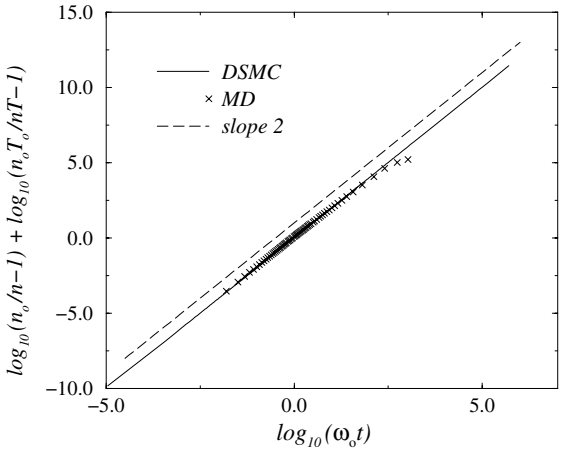

Figure 3. Validity of the scaling relation $\xi + \gamma = 1$ in Monte Carlo and molecular dynamics, for a two-dimensional system.

volume effects, the initial packing fraction needs to be low in MD simulation, whereas the DSMC method simulates the limit of point particles. This constraint also limits the time regime accessible in MD simulation. In figure 2 the DSMC results have been averaged over 10^4 samples with different initial conditions for a system of $N = 5 \times 10^6$ particles, whereas MD simulation has been performed for a single realization of a system with $N = 2 \times 10^5$ (the CPU times needed are comparable in the two cases). Simulations in three dimensions confirm the above picture, with a good agreement between DSMC results and the prediction $\xi_0 \simeq 0.911$ of equation (15). The exponents obtained in 2D both analytically and numerically are close to those reported in the literature ($\xi \simeq 0.8(9)$ in [7] and $\xi \simeq 0.87(5)$ in [15], using a multi-particle lattice gas method).

The validity of the scaling relation $\xi + \gamma = 1$ can be investigated from the time dependence of $n\sqrt{T}$, expected to scale like $1/t$. However, a plot like $\log_{10}(n/n_0) + \log_{10}(T^{1/2}/T_0^{1/2})$ versus $\log_{10}(\omega_0 t)$ would not display any scaling regime at early times. It is possible to extend the validity of the scaling relation by considering $\log_{10}(n_0/n-1) + \log_{10}[n_0T_0/(nT)-1]$, expected to behave like $2\log_{10}(\omega_0 t)$ at late times (from $\xi + \gamma = 1$), but also at short times (where $\omega \simeq \omega_0$), from equations (2) and (3). The results are shown in figure 3, where the asymptotic regime corresponds to the last five decades, and the initial transient to the first five.

The accuracy of the simple Gaussian approximation leading to (15) can be understood by comparing the velocity distribution to the Maxwell–Boltzmann distribution (see figure 4). Although associated with a kinetic process extremely far from equilibrium, $\varphi(\boldsymbol{c})$ is close to the Maxwellian. It can be observed that $\varphi(c_i)$ is overpopulated with respect to the Maxwellian for small velocities, but also for large ones (see figure 5, left graph). The large-c behaviour displayed in figure 5 is in agreement with the analytic prediction $\varphi(\boldsymbol{c}) \propto c^{-1-d+1/\gamma} \exp(-Ac)$ (for $d = 2$, the quantity $-1 - d + 1/\gamma$ is close to 4.7 and, as expected, $c_i^{-4.7}\varphi(c_i)$ shows an exponential tail (figure 5, right graph)). The normalization constraint then implies that $\varphi(c_i)$ is underpopulated compared to the Gaussian for intermediate velocities, which can be observed in figure 4.

4. Conclusions

Within Boltzmann kinetic theory, we have derived a set of exact relations between moments of the velocity distribution and the decay exponents characterizing the asymptotic regime of

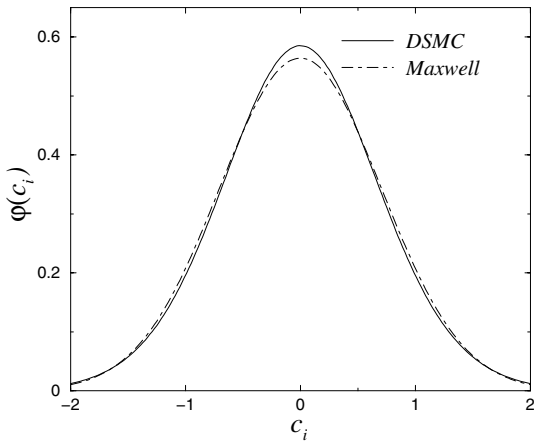

Figure 4. The probability distribution function $\varphi(c_i)$ where c_i is a Cartesian coordinate of the rescaled velocity $\boldsymbol{c}$ and $d = 2$.

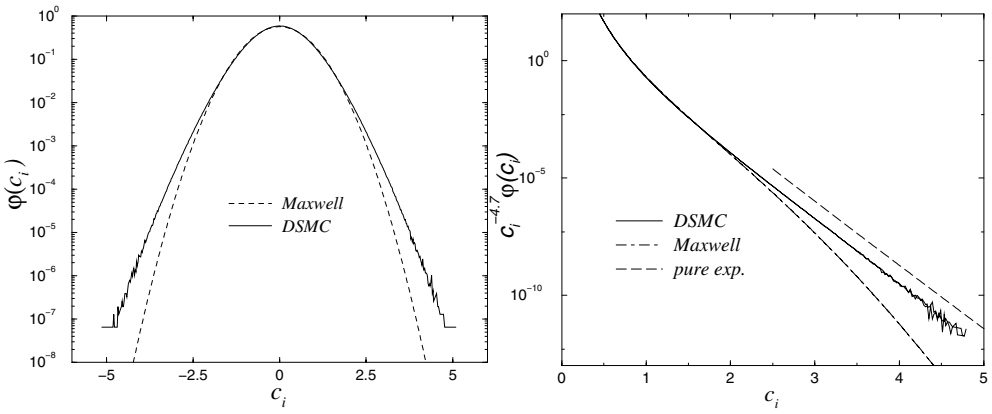

Figure 5. As figure 4, but using a linear–log scale to probe the large velocity tail of the velocity distribution.

the ballistic annihilation process, which turns out to be a good starting point for deriving analytically approximate predictions. In this work, for initial velocity distributions populated and regular near the origin (case $\mu = 0$), we restricted consideration to the Gaussian approximation, which turns out to be accurate compared to the numerical simulations (both molecular dynamics and Monte Carlo), provided that the order of the moments used to compute the energy dissipation exponent α is chosen as low as possible. The numerical velocity statistic φ noticeably differs from the Maxwell–Boltzmann distribution for large velocities associated with low probability densities, which only significantly affects moments of high order of φ. Non-Gaussian corrections can be systematically included in the above analysis, and are expected to improve the quality of the analytical predictions. Work along these lines is in progress [12].

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