Nontrivial Polydispersity Exponents in Aggregation Models

Stéphane Cueille and Clément Sire
Laboratoire de Physique Quantique (UMR C5626 du CNRS), Université Paul Sabatier
31062 Toulouse Cedex, France.
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We consider the scaling solutions of Smoluchowski’s equation of irreversible aggregation, for a non-gelling collision kernel. The scaling mass distribution \( f(s) \) diverges as \( s^{-\tau} \) when \( s \to 0 \). \( \tau \) is non trivial and could, until now, only be computed by numerical simulations. We develop here new general methods to obtain exact bounds and good approximations of \( \tau \). For the specific kernel \( K^D(x, y) = (x^{1/D} + y^{1/D})^d \), describing a mean-field model of particles moving in \( d \) dimensions and aggregating with conservation of “mass” \( s = R^D \) (\( R \) is the particle radius), perturbative and nonperturbative expansions are derived. For a general kernel, we find exact inequalities for \( \tau \) and develop a variational approximation which is used to carry out the first systematic study of \( \tau(d, D) \) for \( K^D \). The agreement is excellent both with the expansions we derived and with existing numerical values. Finally, we discuss a possible application to 2\( d \) decaying turbulence.

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INTRODUCTION

Aggregation phenomena are widespread in Nature. They have such an impact on material sciences, chemistry, astrophysics, that a large amount of literature has been devoted to them [1–4]. In such dynamical processes, particles or objects as different in geometry and size as crystals, colloidal particles, galaxies, small molecules, vortices in fluids, droplets, polymers, can merge to form a new entity when they come into close contact or interpenetrate, through diffusion (Brownian coagulation [5,6]), ballistic motion (ballistic agglomeration [7–9]), exogenous growth (droplets growth and coalescence [10]) or droplet deposition [11].

One is usually interested in the evolution of the statistical distribution of the “mass” \( s \), a quantity characteristic of each particle, that is conserved in the coalescence process: it can be either the actual mass, the volume, the area, the electric charge, or any other physical quantity, depending on the underlying physics.

A great progress was achieved when it was proposed [12] and observed both in real experiments and in numerical simulations that the mass distribution \( N(s, t) \) exhibits scale invariance at large time:

\[
N(s, t) \sim S(t)^{-\beta} f \left( \frac{s}{S(t)} \right), \quad S(t) \sim t^z \tag{0.1}
\]

The divergence of the mass scale \( S(t) \) bears on the oblivion of initial conditions and physical cut-off or discreteness, as does the diverging correlation length of critical phenomena: universality arises in dynamics as well, with new universality classes.

The exponents \( z \) and \( \beta \) are easily derived from conservation laws and physical arguments, but in many cases a polydispersity exponent \( \tau \) defined by \( f(x) \sim x^{-\tau} \) when \( x \to 0 \) is observed, whose value is nontrivial though universal. The prediction of \( \tau \) is still a challenge.

Except for a few (usually 1D) exactly solvable model [13,14], analytical results are still lacking. The most popular, and the earliest, approach to these aggregation problems is Smoluchowski’s equation [5], a master equation [15] for the one-body distribution \( N(s, t) \):

\[
\frac{\partial N(s, t)}{\partial t} = \frac{1}{2} \int_0^s N(s_1, t)N(s-s_1, t)K(s_1, s-s_1) \, ds_1
- N(s, t) \int_{s}^{+\infty} N(s_1, t)K(s, s_1) \, ds_1 \tag{0.2}
\]

where the aggregation kernel \( K(x, y) \) is symmetric and is characteristic of the physics of the aggregation process on a more or less coarse-grained level. Such kinetic equations are usually derived within a mean-field approximation, where density fluctuations are ignored. Mean-field approximation is expected to be valid above an upper critical spatial dimension. This dimension is usually 2 for reaction-diffusion models, but van Dongen showed that it can depend on the kernel [16]. Including some proper approximation of the density-density correlations in the kernel may improve Smoluchowski’s approach [17].

Mean-field as it may be, Smoluchowski’s equation is still highly nontrivial. No exact solution is available, except in a very few specific cases (see below), and extracting the nontrivial exponent \( \tau \) for a specific system from the proper kinetic equation is not an easy task. The problem was clarified by van Dongen and Ernst [18] who classified the kernels according to their homogeneity and asymptotic behavior:

\[
K(bx, by) = b^{\lambda} K(x, y) \tag{0.3}
\]

\[
K(x, y) \sim x^{\mu} y^{\nu} \quad (y \gg x) \tag{0.4}
\]

For a given physical system, the homogeneity \( \lambda \) is easily determined using scaling arguments. We consider only nongelling systems with \( \lambda \leq 1 \) [18]. For \( \mu > 0 \), the exponent \( \tau \) is trivial and found to be \( \tau = 1 + \lambda \), whereas for
\( \mu = 0, \tau \) depends on the whole solution \( f \) of the scaling equation derived from Eq. (1.2) (see Eq. (1.5) below). \( \mu < 0 \) does not lead to any power law behavior but rather to a bell-shaped scaling function \( f \). In the following, we shall focus on the \( \mu = 0 \) case for which the exponent \( \tau \) has so far only been determined numerically by direct simulation of Smoluchowski’s equation \[20,21\], not an easy task \[2,20\], by time series \[22\], and of course by direct simulation of the physical system supposed to be described by the considered Smoluchowski’s equation \[21\]. In the latter case, direct comparison with mean-field results is in principle rather delicate. These methods are quite heavy, which makes it possible to carry out extensive studies, making it possible to carry out extensive studies, are certainly needed to use Smoluchowski’s approach in a predictive way. The purpose of this article is to provide both and use them to perform the first complete study of \( \tau(d,D) \) for the kernel \( K_D^p = (x^{1/D} + y^{1/D})^d \). These analytical methods consist of exact bounds, perturbative and nonperturbative expansions around exactly solvable limits, while we introduce a variational scheme, leading to excellent approximations of \( \tau \) at extremely low computational cost, without directly solving Smoluchowski’s equation. We end the paper with a practical application of our results in the field of two-dimensional turbulence.

In section II, we present a variational approximation based on integral equations for the moments of \( f \), and valid for any homogeneous kernel. This method reproduces some known exact results, and is used to compute \( \tau \) for a wide range of \( d \) and \( D \), the results being summarized on Fig. 3. The approximation is compared to the few existing numerical results \[21,22\] as well as with analytical expansions derived in section III, with excellent agreement and very low computational cost.

Section IV presents a possible application in the field of two-dimensional turbulence. We consider a model of diffusing and merging coherent vortices, and Smoluchowski’s equation leads to non Batchelor energy spectra with exponents in qualitative agreement with direct simulations found in the literature \[30,31\].

I. MODEL AND SCALING

Consider hyperspherical particles in a \( d \)-dimensional box, of polydisperse radii \( R \) with distribution \( F(R,t) \), evolving the following way: at time \( t \) we choose the positions of their centers with uniform probability in \( d \)-space. Then each pair of overlapping spheres of radii \( R_1 \) and \( R_2 \) merges to form a new sphere of radius,

\[
R = (R_1^D + R_2^D)^{1/D} \tag{1.1}
\]

where \( D \) is a parameter with \( D \geq d \). \( D \) can be the actual dimension of the spheres, as for instance in the case of \( D = 3 \) spheres deposited on a \( d = 2 \) plane \[13\]. Once each coalescence has been resolved, we have reached time \( t + \delta t \).

A. Derivation of Smoluchowski’s equation

The conserved variable is \( s = R^D \), and is continuous. We shall call \( s_0 \) the physical lower cut-off, that is the charge of the smallest sphere in the initial condition. Since the radius of a surviving sphere can only increase through coalescence, \( N(s,t) = 0 \) for \( s < s_0 \) and for any time \( t > 0 \). Smoluchowski’s equation consists just in a balance of collisions. The number of collisions between two spheres of radius \( s_1^{1/D} \) and \( s_2^{1/D} \) randomly and independently deposited in the \( d \) dimensional medium being \( N(s_1,t)N(s_2,t)\Omega_d(s_1^{1/D} + s_2^{1/D})^d \) where \( \Omega_d \) is the \( d \)-dimensional total solid angle. We obtain the equation,

\[
N(s, t + \delta t) - N(s, t) = \Omega_d \left\{ \frac{1}{2} \int_0^t N(s_1, t)N(s - s_1, t)K_D^p(s_1, s - s_1) \, ds_1 \right\}
\]
with \( K^d_D(x, y) = (x^{1/D} + y^{1/D})^d \). We can get rid of the multiplicative constant, by properly choosing the time unit \( \delta t \) and by replacing the finite difference in time by a partial derivative to exactly obtain Eq. (1.2). We notice that the only approximation used to derive the equation is to neglect multiple collisions, for the system is intrinsically mean-field.

The kernel \( K^d_D(x, y) = (x^{1/D} + y^{1/D})^d \) has been introduced in many contexts from molecular coagulation \([17]\) to cosmology \([21, 23]\) for specific values of \( d \) and \( D \), and is one of the most studied in the literature \([17, 18, 21, 23, 26–28]\) although very few analytical results are known. This kernel has \( \lambda = \frac{1}{D} \) and \( \mu = 0 \). Exact solutions are available in the case \( d = 0 \) or \( D = \infty \) (constant kernel) \([3]\), and \( d = D = 1 \) \([20]\).

**B. Scaling**

Now, we introduce the scaling form of \( N(s, t) \). We first write the conservation law. The total mass in the system is \( \int_0^{\infty} N(s, t) ds \sim S(t)^{2-\beta} \int_0^{\infty} f(x) dx \) and is conserved which implies \( \beta = 2 \), implicitly assuming that the integral of \( x f(x) \) converges, i.e., in terms of the small \( x \) divergence of \( f \), that \( \tau < 2 \), which will be shown below. We consider the total number of particles in the system \( n(t) = \int_0^{\infty} N(s, t) ds \). It behaves at large time like \( S(t)^{1-\beta} \int_0^{\infty} f(x) dx \). If \( \tau < 1 \), \( n(t) \sim S(t)^{1-\beta} \int_0^{\infty} f(x) dx \) whereas if \( \tau > 1 \), \( n(t) \sim S(t)^{\frac{1}{\tau}} \int_0^{\infty} f(x) dx \).

Another way of taking care of these divergences is to be found in \([18, 19]\).

As we are only interested in the exponent affecting the small \( s \) behavior of \( f \), we shall set \( w \) to unity by changing \( f \) to \( w f \). If \( f(s) \) is a solution of Eq. (1.3), then \( b^{1+\lambda} f(b s) \) is also a solution. The value of \( b \) is often fixed by imposing \( \int f(x) dx = 1 \), but we will make a different choice for reasons that will become clear later.

A careful study of the large \( s \) behavior of \( f \) shows that if \( \lambda < 1 \) \((d < D)\), \( f(s) \propto c_\infty \delta s^{-\lambda} e^{-\delta s} \), with \( c_\infty = \int_0^{1/2} K^d_D(x, 1 - x)x^{-\lambda}(1 - x)^{-\lambda} dx \) \([14]\). We choose the solution corresponding to \( \delta = 1 \), which fixes \( b \), and leads to a nontrivial value for \( \int f(x) dx \). This asymptotic behavior is not valid for \( \lambda = 1 \) \((d = D)\).

For \( d = 0 \) or \( D = \infty \), Eq. (1.3) reduces to the constant kernel equation with exact solution \( f_0(x) = 2e^{-s} \) and \( f_\infty(s) = 2^{1-d} e^{-s} \) (note that the large \( s \) asymptotics become the exact solution for all \( s \) in these cases). For \( d = 1 \) and \( D = 1 \), an exact analytic solution is also known for the time dependent equation; the scaling function being \( f(s) \propto s^{-3/2} e^{-s} \) \([24]\), with \( z = \infty \) and \( S(t) \propto e^t \).

Now, for given \( d \) and \( D \), and plugging the expected small \( s \) behavior \( f(s) \sim s^{-\tau} \) into Eq. (1.3), one first gets that \( \tau < 1 + \lambda = 1 + d/D \). Then, matching the behavior of both sides of Eq. (1.3) \([13, 18, 19]\), one finds,

\[
\tau = 2 - \int_0^{\infty} f(x) x^\lambda dx. \tag{1.7}
\]

If \( \alpha > \tau - 1 \) we obtain by multiplying Eq. (1.3) by \( x^\alpha \) and integrating \([18, 27]\),

\[
-N(s, t) \int_0^{+\infty} N(s_1, t) K^d_D(s, s_1) ds_1 \tag{1.2}
\]
Most existing analytical results for $\mu = 0$ kernels are to be found in the beautiful series of papers by van Dongen and Ernst. Apart from results mentioned earlier, they determined the small $x$ subleading behavior of the scaling function, and they found some inequalities for $\tau$ in the cases $d = 1$, and $D = 1$. In 1984, Leyvraz proposed the analytical result $\tau = 1 + 1/2D$ for the kernel $K^d_D$ with $d = 1$, but in 1985, using exact inequalities, van Dongen and Ernst showed that this result was erroneous and explained why it was so. The argument of Leyvraz leading to this result is perfectly valid for class I kernels with $\mu > 0$ for which it predicts the correct exponent, but it breaks down for $\mu = 0$ kernels. We mention this fact for some references to the wrong result $\tau = 1 + 1/2D$ can still be found in some recent articles.

We now review various kinds of numerical studies concerning the polydispersity exponent $\tau$. These studies deal with the kernel $K^d_D$. Kang et al. simulated a model of particle diffusion and coalescence (PCM) that can be shown to be exactly equivalent to Smoluchowski’s equation. They also numerically directly computed the solution of the equation itself. Their results concern the $d = 1$ case. They surprisingly found values of $\tau$ in contradiction with the exact bound $\tau \geq 1$ (see section II) (for $D = 4$, they found $\tau = 0.63$). By comparison between their two methods of computation, they concluded that in both cases they observed a pseudo-asymptotic state, with wrong exponents but apparent scaling, and that the actual asymptotic scaling regime appeared at times too large to be seen by their simulations. This illustrates the drawback of considering the direct time evolution of the system: the actual asymptotic regime may not be reached within the accessible numerical simulation time scale.

Krivitsky numerically solved Smoluchowski’s equation for the time dependent distribution for the kernel $K^d_D$, for $D = 1, d \leq 1$, for which he determined 10 values for $\tau$ (see Fig. 1). Comparison with analytical results obtained by analysis of the scaling equation (infinite time limit) in the present article will assess the fact that in this case the asymptotic regime was actually reached by Krivitsky’s solution. These numerical results will be found to be in excellent agreement with our variational method of section II and consider Eq. (1.8) with $\alpha = 0$,

$$2(1 - \alpha) \int_0^\infty x^\alpha f(x) \, dx = \int_0^\infty \int_0^\infty f(x)f(y)K^d_D(x, y) [x^\alpha + y^\alpha - (x + y)^\alpha] \, dx \, dy. \quad (1.8)$$

as a power series in time $t$, and to extract the exponent $\ell'$ by manipulations of this series. They treated only the cases $d = 1, D = 2$ and $d = 2, D = 3$. In the case $d = 1, D = 2$, they present two different results in the text (?). They first consider $K^d_2$ and find $1/\ell' = 0.57 \pm 0.01$, then they extend their method two $K^d_2$ and in the case $d = 2$, which is exactly the same as previously, they find $1/\ell' = 0.588$ (they do not give any error estimate in this case). In the following, we shall see that we believe the first result to be closer to the exact one. In the next section, we shall see that their result in $d = 2, D = 3$ strongly violates exact inequalities, and thus is wrong.

The conclusion of this section, is that no complete study of the value of $\tau$ had been performed until now because of a lack of appropriate numerical tools. More precise analytical results would also certainly be welcome to guide numerical works. We see that simulating or solving for the time evolution of the distribution function may not enable to reach the asymptotic scaling regime, and a guideline of the present work will be to directly rely on the scaling equation corresponding to the infinite time asymptotic state itself.

II. EXACT BOUNDS

In the next three sections, our workhorses will be both Eq. (1.7) and (1.8).

We first show that $\tau \geq 1$, for $d \geq 1$. Suppose $\tau < 1$ and consider Eq. (1.8) with $\alpha = 0$,

$$2 \int_0^\infty f(x) \, dx = \int_0^\infty \int_0^\infty f(x)f(y)K^d_D(x, y) \, dx \, dy. \quad (2.1)$$

For $d \geq 1$, we have $(x^\tau + y^\tau)^d \geq x^d + y^d$, which leads to $\int f(x) \, dx \geq \int f(x) \, dx \int f(x) x^\tau \, dx$ (in the bulk of the text, all integrals should be understood from 0 to $\infty$). Comparing with Eq. (1.7), this leads to $1 \geq 2 - \tau$ or $\tau \geq 1$, which is contradictory. Notice that Eq. (1.8) with $\alpha = 2$ for $d = 1$ and $D = 1$ leads to $\int f(x) \, dx = 2\int x^2 f(x) \, dx \int f(x) x^\tau \, dx$, and we recover the exact result $\tau = 2 - \int f(x) \, dx = 3/2$ in a very simple way. These results were already obtained by van Dongen and Ernst, who were able to find in the case $D = 1$ the exact inequality, $2d < \tau < 2 - 2^{1-d}(1-d)/(2-d)^d$, which shows that $\tau = 2d + O(d^2)$ when $d \rightarrow 0$. This interesting result will be generalized to any $D$ in next section and the $O(d^2)$ term will be computed in $D = 1$. They also found weaker inequalities in $d = 1$, but no result was obtained for general $d$ and $D$. 

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In order to deal with a general $\mu = 0$ kernel $K$, we introduce an extremely simple method to get lower and upper bounds for $\tau$. We rely on Eq. (1.8) valid for $\alpha > \tau - 1$. Combining Eq. (1.7) and (1.8), we get:

$$
\tau = 2 - (1 - \alpha) \frac{\int_0^\infty g(x,y) \, dx \, dy}{\int_0^\infty g(x,y) A(x/y) \, dx \, dy} \quad (2.2)
$$

where $A(u) = (1 + u^\alpha - (1 + u)^\alpha)K(x,y)/(u^\alpha + u^\alpha)$ satisfies $A(u) = A(1/u)$ and $g(x,y) = (x^\alpha y^\alpha + x^\alpha y^\alpha)f(x)f(y)$. The ratio in Eq. (2.2) can then be interpreted as the inverse of a kind of average of $A(x/y)$ with the weight $g(x,y)$. For a given $\alpha < \lambda$, we numerically determine the maximum $M_\alpha$ and minimum $m_\alpha$ of the function $A(u)$. Using Eq. (2.2), this gives

$$
2 - (1 - \alpha)/m_\alpha \leq \tau \leq 2 - (1 - \alpha)/M_\alpha \quad (2.3)
$$

We then choose the best values of $\alpha \leq \lambda$ compatible with $\alpha > \tau - 1$ leading to the tightest bounds. More precisely, we proceed the following way: we start with $\alpha = \lambda$ (as $\tau < 1 + \lambda$), from which we obtain some upper and lower bound $\tau_m$ and $\tau_M$. If $\tau_M < 1 + \lambda$, Eq. (2.3) holds for $\tau_M - 1 < \alpha \leq \lambda$, and we can compute new bounds for each $\alpha$ in this interval, and find the tightest bounds. The upper bound obtained for $\alpha = \lambda$ cannot be improved since $A(0) = 1$ for $\alpha < \lambda$, hence $2 - (1 - \alpha)/M_\alpha \geq 1 + \alpha$, but in many cases we can find a better lower bound.

For $R^2_{d/\alpha}$, a superficial plot of the function $A(u)$ may lead to the incorrect conclusion that its minimum is always obtained at $u = 0$ with $A(0) = 1$. In fact a more careful study of $A$ shows that for certain values of $\alpha$, the actual minimum is at $u > 0$ but very close to 0. For $u \to 0$, $A(u) \sim 1 + d\mu^1/D - u^d/D - \alpha$, and we see that if $\alpha > (d - 1)/D$, there is a local minimum for $u_m > 0$ with $A(u_m) < 1$. For $d > 1$, and $\alpha = (d - 1)/D + \varepsilon$, we get $u_m \sim \exp(-\ln(d)/\varepsilon)$, which vanishes exponentially when $\varepsilon \to 0$ ($d > 1$). Indeed, even when $\alpha$ is not so close to $(d - 1)/D$, $u_m$ may be very small. For instance, for $d = 2$, $D = 3$, and $\alpha = 0.58598 > (d - 1)/D = 0.333...$, we find that $u_m = 1.365 \times 10^{-4}$, and $A(u_m) = 0.7322$, which leads to a nontrivial lower bound of 1.4349 for $\tau$.

Actually, it is easily seen that the inequalities obtained by van Dongen and Ernst (in the case $d = 1$ or $D = 1$) correspond to $\alpha = d/D$. In fact even in this case, $M_\alpha$ and $m_\alpha$ are nontrivial, and they used some explicit bounds of $M_\alpha$ and $m_\alpha$, which do not lead to the tightest bounds for $\tau$.

Thus, our method consists in computing the actual value of $m_\alpha$ and $M_\alpha$, and varying $\alpha$ to optimize these bounds, which allows us to greatly improve van Dongen and Ernst’s explicit inequalities for $D = 1$ or $d = 1$, and to obtain new exact bounds for $d > 1$. For instance, for the physically interesting cases (see below) ($d = 1$, $D = 2$), ($d = 1$, $D = 4$) and ($d = 2$, $D = 4$) we respectively found $1.084 \leq \tau \leq 1.147$, $1 \leq \tau \leq 1.075$ (compared to $1 \leq \tau \leq 1.28$ and $1 \leq \tau \leq 1.109$ in [27]) and $1.25 \leq \tau \leq 1.5$.

For $d = 2$, $D = 3$, we find $1.4349 \leq \tau \leq 1.585$, which just discards the value $\tau = 1.244$ found by Song and Poland [22], and strongly questions the validity of their approach. The exact bounds we obtained in $d = 1$, $D = 2$ are violated by their alternative value 1.150 for $\tau$ but not by their first result 1.123 (see subsection 1C).

It is useful to note that for any $D$, with $\alpha = d/D$, $A(u) \to 1/2$ when $d \to 0$, which entails that $\tau \to 0$ (from Eq. (2.3)) in this limit.

To conclude with this topic of inequalities, let us consider Eq. (2.3) with $\alpha = d/D$. In this case, when $D \to \infty$,

$$
A(u) = \frac{1}{2} (1 + u^{-d})^{d} \left[ 1 + u^{-d} - (1 + u^{-d})^{-d} \right] = \begin{cases} 2^{d-1}, & 0 < u \leq 1 \\ u = 0 & \end{cases} \quad (2.4)
$$

hence $m_\alpha \to 1/2$ and $M_\alpha \to 2^{d-1}$. Therefore, the upper bound for $\tau$ in Eq. (2.3) tends to $2 - 2^{1-d}$. This is strictly less than 1 for $d < 1$, which means that for any $d < 1$, there exists a finite critical $D_c(d)$, such that $\tau < 1$ for any $D > D_c$. This result will be used in section 11.

### III. PERTURBATIVE AND NONPERTURBATIVE EXPANSIONS

In this section we use the exactly solvable limits $d = 0$ and $D = \infty$ as a basis for a perturbative expansion. We also consider the case $d \to \infty$, keeping $d/D = \lambda$ constant, for which we find a nonperturbative expansion.

We saw that $\lim_{d \to 0} \tau = 0$. What about the $D \to \infty$ limit of $\tau$? In fact, although strictly at $D = \infty$, $\tau$ is equal to 0, as $f(x) = 2^{1-d}e^{-x}$, we will see that $\tau_\infty = \lim_{D \to \infty} \tau > 0$. This result was already noticed by van Dongen and Ernst in $d = 1$ [27]. Since $\tau < 1 + d/D$ we get that,

$$
\tau_\infty \leq 1 \quad (3.1)
$$

What can we learn from equation (1.7) in the large $D$ limit? We see that the limit for $\tau$ is

$$
\tau_\infty = 2 - \int_0^\infty f_\infty(x) \, dx = 2 - 2^{1-d} \quad (3.2)
$$

provided that:

$$
\lim_{D \to \infty} \int_0^\infty (f_D(x) - f_\infty(x)) x^d \, dx = 0 \quad (3.3)
$$

For $d < 1$, this result is consistent, since, from the last remark of section 1, we get $\tau_\infty \leq 2 - 2^{1-d} < 1$.

However, for $d \geq 1$ we know that $\tau \geq 1$, hence $\tau_\infty = 1$, which means that for $d > 1$,

$$
\lim_{D \to \infty} \int_0^\infty (f_D(x) - f_\infty(x)) x^d \, dx = 1 - 2^{1-d} > 0 \quad (3.4)
$$
while in \(d = 1\), (3.3) is true.

Now that we know the large \(D\) limit of \(\tau\) \(\tau_{\infty} = 1\) for \(d > 1\) and \(\tau_{\infty} = 2 - 2^{1-d}\) for \(d \leq 1\), as well as its small \(d\) limit \((\tau \to 0)\), let us compute the corresponding asymptotic corrections.

A. Small \(d\) Expansion

First, consider the limit \(d \to 0\). We expand \(f\) in series in \(d\): \(f(x) = f_0(x) + df_1(x) + O(d^2)\), \(f_0(x) = e^{-x}\). A systematic way of expanding \(\tau\) would be to write down a linear (self-consistent) differential equation for \(f_1\) to solve it and plug the result into (1.7).

However, as far as the first order is concerned we can get it without solving for \(f_1\). By developing the integral expression of \(\tau\), Eq. (1.7), we get,\(\tau = 2 - \int_0^{+\infty} f(x) x \frac{\text{d}f}{\text{d}x} dx\)

\[= -d \int_0^{+\infty} f_0(x) \ln x \, dx - d \int_0^{+\infty} f_1(x) dx + O(d^2).\] (3.5)

Then we expand both sides of Eq. (2.1) to get an equation for \(\int f_1(x) dx\),

\[\int_0^{+\infty} f_1(x) dx = \frac{1}{2} \int_0^{+\infty} f_0(x) f_0(y) \ln(x^{1/2} + y^{1/2}) dx dy - \int_0^{+\infty} f_0(x) dx \int_0^{+\infty} f_1(x) dx\] (3.6)

hence \(\int f_1(x) dx = - \int e^{-x-y} \ln(x^{1/2} + y^{1/2}) dx dy\). After eliminating \(\int f_1(x) dx\), we get:

\[\tau = 2dJ_D + O(d^2)\]

\[J_D = \int_0^1 \ln \left(1 + \left(\frac{1 - u}{u}\right)^{1/2}\right) du\] (3.7)

Let us mention that this result can be systematically generalized to the case of any homogeneous kernel of the form: \((g(x,y))d\), leading to, \(\tau = 2d \int_0^1 \ln g(1, \frac{1-u}{u}) du + O(d^2)\).

Although it may seem a bit tedious, it is interesting to recover this result in another way, as it shows that the small \(x\) behavior of \(f_1\) is consistent with the \(d \to 0\) expansion of the power law \(x^{-\tau} = 1 - 2dJ_D \ln x + O(d^2)\). Let us write down the linear equation for \(f_1\),

\[xf_1(x) + 2e^{-x} \int_0^x f_1(y) e^y dy = 2e^{-x} \int_0^{+\infty} f_1(y) dy + 4e^{-x} \int_0^{+\infty} e^{-y} \ln(y^{1/D} + x^{1/D}) dy\]

\[= 2e^{-x} \int_0^{+\infty} \ln(y^{1/D} + (x - y)^{1/D}) dy\] (3.8)

With \(u = e^x f_1\) we get the following equation:

\[x(u' - u) + 2 \int_0^x u(y) dy = 2 \int_0^{+\infty} u(y) e^{-y} dy + 4 \int_0^{+\infty} e^{-y} \ln(y^{1/D} + x^{1/D}) dy\]

\[= 2 \int_0^{+\infty} \ln(y^{1/D} + (x - y)^{1/D}) dy - 2xJ_D - \frac{2}{D} (x \ln x - x)\] (3.9)

which implies, after taking the derivative of Eq. (3.9),

\[xu'' + (1 - x)u' + u = \frac{4}{D} \int_0^{+\infty} e^{-y} \frac{x^{1/D-1}}{y^{1/D} + x^{1/D}} dy\]

\[-\frac{2}{D} \ln x - 2J_D\] (3.10)

the solution of (3.10) involves two integration constants, one being fixed by the fact that \(f_1\) should go to zero at large \(x\), the other, \(c_0\), by writing the compatibility with Eq. (3.9), which can be done by taking the \(x \to 0\) limit the latter equation. From the expression of the solution (appendix I), or directly from Eq. (3.10), it is easily seen that \(u\) has the asymptotic expansion for \(x \to 0\):

\[u(x) = b_0 \ln x + O(1)\] (3.11)

with \(b_0 = c_0 - 2/D\).

We know that \(f(x) \sim cx^{-\tau}\) when \(x \to 0\). When \(d \to 0\), \(c \to 2\) and \(\tau = d\tau_1 + O(d^2)\), hence up to order \(d\) we expect,

\[f(x) \sim 2\tau_1 \ln x\] (3.12)

so that we interpret \(b_0\) as \(-2\tau_1\),

\[\tau = -d\frac{b_0}{2} + O(d^2)\] (3.13)

The \(x \to 0\) limit of (3.9) is:

\[b_0 = 2 \int_0^{+\infty} f_1(x) dx - \frac{4}{D} \int_0^{+\infty} e^{-x} \ln x dx\] (3.14)

The integration of Eq. (3.10) between 0 and \(+\infty\) yields,
\[ b_0 + \int_0^{+\infty} f_1(x) dx = 2J_D - \frac{2}{D} \int_0^{+\infty} e^{-x} \ln x \, dx \]

(3.15)

The combination of Eqs. (3.14) and (3.15) yields \( b_0 \), which, substituted into Eq. (3.13), eventually leads to the same result for \( \tau \) as previously obtained through the expansion of Eq. (2.4) and Eq. (1.7).

For \( D = 1 \), we get \( \tau = 2d + O(d^2) \), in good agreement with direct numerical integration of Smoluchowski’s equation performed by Krivitsky [21] and shown on Fig. I (see below). This result for \( O(d) \) is Euler’s constant, while from Eq. (1.7), \( \tau = 2 \), expanding \( f(x) = f_\infty(x) + \frac{1}{2\pi} f_1(x) + \frac{1}{12} f_2(x) + O(1/D^3) \).

The order \( O(d^2) \) requires the computation of \( f_1 \). However, in the special case \( D = 1 \) it is possible to obtain explicitly the \( O(d^2) \) term by expanding Eq. (1.8) for \( \alpha = d/D \) (see appendix I). We obtain,

\[
\int_0^{+\infty} f_1(x) dx = d \int_0^{+\infty} f_\infty(x) f_\infty(y) (\ln x + \ln y) \, dx \, dy + 2d \int_0^{+\infty} f_\infty(x) dx \int_0^{+\infty} f_1(x) dx,
\]

(3.17)

hence :

\[
\int_0^{+\infty} f_1(x) dx = -d \int_0^{+\infty} f_\infty(x) \ln(x) \, dx = 2^{1-d} d \gamma,
\]

(3.18)

where \( \gamma \) is Euler’s constant, while from Eq. (1.7),

\[
\tau = \tau_\infty - \frac{d}{D} \int_0^{+\infty} f_\infty(x) \ln(x) \, dx - \frac{1}{D} \int_0^{+\infty} f_1(x) dx + O\left(\frac{1}{D^2}\right).
\]

(3.19)

\[
\int_0^{+\infty} f_2(x) dx = \frac{1}{2} \int_0^{+\infty} f_\infty(x) f_\infty(y) \frac{2d}{8} [(d + 1)(\ln x)^2 + (\ln y)^2 + 2(d - 1) \ln(x) \ln(y)] \, dx \, dy + 2^{1-d} d \int_0^{+\infty} f_1(x) f_1(y) (\ln x + \ln y) \, dx \, dy + 2^{1-d} \left( \int_0^{+\infty} f_1(x) dx \right)^2 + 2 \int_0^{+\infty} f_2(x) dx
\]

(3.21)

Using the known value of \( \int f_1 \) and our favourite integral table, we get:

\[
- \int_0^{+\infty} f_2(x) dx = \frac{d^2}{4} \int_0^{+\infty} f_\infty(x) (\ln x)^2 \, dx + d \int_0^{+\infty} f_1(x) \ln(x) \, dx + \frac{2^{1-d} d}{12} \left( \frac{\pi^2}{6} + d \gamma^2 \right)
\]

(3.22)

(\( \gamma \) being Euler’s constant), which leads to:

\[
\tau = 2 - 2^{1-d} + \frac{\pi^2 2^{-d} d(1 - d)}{12D^2} + O\left(\frac{1}{D^3}\right)
\]

(3.23)

Once again we were able to obtain a highly nontrivial expansion for \( \tau \) without solving for \( f_1 \) and \( f_2 \) themselves, although this can also be achieved this way. Note that in the limit of large \( D \) and small \( d \), Eq. (3.7) and (3.23) coincide up to order \( O(d/D^2) \).

**B. Large D expansion**

Now, we perform an expansion in powers of \( 1/D \) for \( d \leq 1 \), expanding \( f(x) = f_\infty(x) + \frac{1}{2\pi} f_1(x) + \frac{1}{12} f_2(x) + O(1/D^3) \).

**Perturbative expansion in \( d < 1 \) - In \( d < 1 \), as mentioned in section II, \( \tau < 1 \) for any \( D \) above a finite critical \( D_c(d) \). As a consequence, Eq. (1.8) can be written for any \( D > D_c(d) \). Therefore, we can develop this equation for large \( D \) in powers of \( 1/D \), and we find at first order,
have shown that \( \tau \geq 1 \) and since \( \tau < 1 + d/D \), we see that \( \tau \to 1 \) for \( D \to \infty \) and finite \( d \geq 1 \). As \( f_1 \) is non integrable, Eq. (3.8) cannot be used with \( \alpha = 0 \), and the previous perturbation breaks down.

Nevertheless we can try to obtain an estimate of \( \tau \) in the following way: we make the ansatz \( f \sim f_\infty + c/s^{1+\varepsilon}e^{-s} \). We plug it into Eq. (3.7) and Eq. (3.8) for \( \alpha = d/D \), and after some algebra (see appendix [1]) we see that for consistency \( \varepsilon \) must be of order \( 1/D \) and that \( c = (1 - 2^{-1/d})(d/D - \varepsilon) \), and eventually that \( \varepsilon = \kappa/D + O(1/D^2) \) where \( \kappa \) is the solution of the nonlinear equation:

\[
\frac{2}{1 + 2^{1-d}} = \int_0^1 (1 + v^{1-\lambda})^d dv \tag{3.24}
\]

This equation always has a solution consistent with the exact bound \( 1 < \tau < 1 + d/D \). For instance in the case \( d = 2, D = 4 \) we obtain \( \tau \approx 1.462 \). Though it is still of order \( 1/D \), the obtained perturbative estimate depends on the choice of \( \alpha \). \( \alpha = d/D \) seems however to be the most natural choice.

In \( d = 1, c \) vanishes and we do not learn much. All terms of the \( d < 1 \) series for \( \tau \) in powers of \( 1/D \) vanish for \( d \to 1 \), as can be seen in Eq. (3.13) for the two leading ones. The reason is the following: the perturbation is derived from Eq. (2.1) under the assumption that \( \tau < 1 \). In \( d = 1 \), such an assumption yields \( 2 \int f(x)dx = 2(\int x^{1/D}f(x)dx)/(\int f(x)dx) \) hence \( \tau = 1 \). Consequently the perturbative value of \( \tau \) tends to 1 when \( d \to 1^- \). As will be illustrated below by numerical results, for a given \( d > 1 \) there is a critical \( D = D_c(d) \) above which \( \tau < 1 \), and \( D_c(d) \) tends to infinity when \( d \to 1^- \), entailing the vanishing of the perturbation validity domain in \( D \). Thus, the correction to \( \tau = 1 \) for large \( D \) may be nonperturbative in \( d = 1 \).

If we now take the \( d \to \infty \) limit in Eq. (3.24), we obtain, \( \tau \approx 1 + \lambda - 2^{-d}\lambda (\lambda = d/D) \), a nonperturbative behavior in \( d \) which is to be related to the results below, obtained for \( d \to \infty \), \( D \to \infty \), keeping \( \lambda \) constant.

C. Large \( d \) and \( D \)

We now present a nonperturbative calculation in the limit of large \( d \) and \( D \), keeping the ratio \( \lambda = d/D \) fixed. In this limit, the kernel can be written,

\[
(x^{1/d} + y^{1/d})^d = 2^d(xy)^{1/d} (1 + O(d/D^2)) \tag{3.25}
\]

and surprisingly transforms into the well-studied “product” kernel [18, 22, 28]. Assuming scaling (a still controversial subject [21]), one can easily show that \( \tau = 1 + \lambda = 1 + d/D \) [18] (see also Eq. (1.3) and (1.4) and the discussion below them, as it corresponds to \( \mu = \lambda/2 \geq 0 \)).

We can show that including higher order corrections in power of \( 1/D \) does not change the value of \( \tau \) such that the correction to \( \tau = 1 + \lambda \) is certainly nonperturbative. Consider the expansion of the kernel:

\[
K(x, y) = 2^d(xy)^{1/d} [1 + 2^{-d}O(1/d^2)] \tag{3.26}
\]

The rescaled function \( \tilde{f} = 2^d f \) is the solution of the scaling form of Smoluchowski’s equation with the kernel \( \tilde{K} = 2^{-d} K(x, y) \), which is equal to \( (xy)^{1/d} \) at every order in \( 1/d = 1/(AD) \). In fact, we can estimate this correction by assuming that for finite \( d \) and \( D \),

\[
\tilde{f}(s) \sim c_\lambda s^{1+\lambda - \varepsilon_d} \tag{3.27}
\]

for \( s \to 0 \). Plugging this estimate into Eq. (1.7) with the limit kernel of Eq. (3.25), we first get

\[
\varepsilon_d \approx 2^{-d} \frac{c_\lambda}{(1 - \lambda)} \tag{3.28}
\]

\( c_\lambda \) can be determined by matching the coefficients of the leading terms in Eq. (1.3) using the kernel of Eq. (3.25). After a straightforward calculation, one gets in the \( d \to \infty \) limit,

\[
c_\lambda = 2(1 - \lambda)I_\lambda^{-1} \tag{3.29}
\]

\[
I_\lambda = \int_0^1 [u(1-u)]^{-1-\lambda/2} [u^\lambda + (1-u)^\lambda - 1] du \tag{3.30}
\]

which leads to

\[
\tau = 1 + \lambda - 2^{1-d}I_\lambda^{-1} \tag{3.31}
\]

We thus find a nonperturbative (exponentially small) correction to \( \tau \) in the large \( d \) and large \( D \) limit, consistent with the result obtained above for \( d > 1 \) and large \( D \). Note that Eq. (3.23) is also consistent with the exact result that \( \tau \to 1 \) as \( D \to \infty \) for finite \( d > 1 \), a result that we obtain by setting \( \lambda = 0 \) (as \( I_\lambda \) diverges).

D. Summary of the results

We have shown that when \( D \to \infty \), \( \tau \to 1 \) for \( d \geq 1 \), whereas \( \tau \to 2 - 2^{1-d} < 1 \) for \( d < 1 \). We were able to derive an \( O(1/D^2) \) perturbative expansion in \( d < 1 \), and we convinced ourselves that the leading corrective term in \( d > 1 \) was of order \( 1/D \), by giving an estimate of this correction. In \( d = 1 \) both approaches break down and the large \( D \) corrections to \( \tau_\infty = 1 \) are probably nonperturbative.

When \( d \to 0 \), \( \tau \) goes to zero, and we gave a first order perturbative expression in \( d \), for any \( D \). For \( D = 1 \), we also found the explicit coefficient in \( d^2 \).

Eventually, we showed that for a fixed homogeneity \( \lambda = d/D \), \( \tau \) tends exponentially to \( 1 + \lambda \) at large \( d \). In the following section we present a new general numerical method to compute \( \tau \) and we confirm our analytical result by performing the first extensive study of the function \( \tau(d, D) \).
IV. VARIATIONAL APPROACH

In this section, we present a practical way of obtaining good approximate values for $\tau$, without explicitly solving Smoluchowski’s equation. Once again, we rely on Eq. (2.2), which holds for the exact scaling function (solution of Eq. (1.3)), for any $\alpha > \tau - 1$. This equation is general, and does not depend on the specific kernel we study in this article. As a consequence, the methods we develop are general and do apply to any homogeneous kernel. We emphasize the fact that this method does not intend to approach the whole scaling function, but sets the focus on the computation of $\tau$ (in fact, numerically solving the scaling equation Eq. (1.3) for the scaling function seems to be at least as difficult as directly solving the time-dependent equation [29]).

A. Principles of the method

The simplest way of approximating $\tau$ is to evaluate the “average” in Eq. (2.2) using a reasonable trial weight function $g(x, y)$ instead of the unknown exact one. As a simple start, we will expose a crude, but straightforward algorithm, that illustrates the basic idea. Then we will develop the variational method itself, which is not much more intricate, but much more effective.

A one parameter choice for a trial weight function is obtained by replacing in the above expression of $g(x, y)$ the exact $f(x)$ by $f_{\tau}(x) = x^{-\tau} \exp(-x)$ which has the correct leading asymptotics for small $x$ (by definition of $\tau$) and decays exponentially at large $x$, although not with the exact asymptotics $x^{-\lambda}e^{-x}$ ($\lambda < 1$) [4]. Still, this functional form is known to be a good approximation of the actual $f(x)$ obtained in simulations [21], and is even the exact solution, but for a multiplicative constant, for the constant kernel ($\tau = 0$) and in the $d = D = 1$ case, which belongs to the special class $\lambda = 1$ [21]. The first idea that comes to mind is just to determine $\tau$ self-consistently such that Eq. (2.2) holds for $f_{\tau}$, with a specific choice of $\alpha$, for instance $\alpha = \lambda$. This is readily done, by an iterative method: starting from an initial $\tau_0$, verifying previously obtained exact bounds, we construct the sequence.

$$\tau_{n+1} = (1 - \varepsilon) + \varepsilon(2 - (1 - \alpha)R_\alpha(f_{\tau_n}))$$

(4.1)

with

$$R_\alpha(\phi) = 2\frac{\int_0^{\infty} x^\alpha \phi(x) y^\lambda \phi(y) dy dx}{\int_0^{\infty} \phi(x) \phi(y) K(x, y) [(x + y)\alpha - x\alpha - y\alpha]}$$

(4.2)

which converges, with a proper choice of $1 > \varepsilon > 0$, to a fixed point corresponding to an $f_{\tau}$ verifying Eq. (2.2). The numerical evaluation of $R(\tau)$ can be achieved with utter celerity and arbitrary precision, since it reduces to the calculation of one-dimensional integrals, and of a few values of the gamma function, thanks to a very convenient transformation (see appendix [3]). We notice that it is unnecessary to include any multiplicative constant into $f_{\tau}$, since it would just cancel out in Eq. (2.2).

Of course, this algorithm should yield different values of $\tau$ for different choices of $\alpha$, except in the special case when the exact solution is of the form $f_{\tau}$. This corresponds to $d = 0, D = \infty$ and $d = 1, D = 1$, and this method converges by construction, to the exact value of $\tau$, but for the round-off errors. In the generic case, the variation can be non negligible (in $d = 2, D = 4$, $\tau \approx 1.371$ for $\alpha = d/D$, while $\tau \approx 1.398$ for $\alpha = 0.403$) and the fixed point $\tau$ may even violate exact bounds. For instance, in the case $d = 1, D = 3$ with $\alpha = d/D$ we get $\tau = 0.9894$ whereas we know that $\tau > 1$. The variation with $\alpha$ makes the method unreliable. In $d = 2, D = 4$, it gives $\tau \approx 1.385 \pm 0.015$, compared to $\tau \approx 1.434 \pm 0.004$ with the variational approximation, that we now introduce, which, starting from the same basic idea, proves to be much more effective.

Variational approximation - A much better and hardly more intricate method is to choose a reasonable sample of values of $\alpha$, and minimize an error function measuring the violation of the corresponding Eq. (2.2). This method can be systematically improved by allowing for $n$ free ‘fitting’ parameters (including $\tau$ itself) in the trial weight $g(x, y)$. In the following we will proceed by replacing the exact $f$ by a variational function of the form,

$$f_\nu(x, \tau_0, \tau_1, \ldots, \tau_n, c_1, c_2) = x^{-\tau_0}e^{-x} + \sum_{j=1}^{n} c_j x^{-\tau_j} e^{-x}$$

(4.3)

and we will minimize the error function,

$$\chi^2(f_\nu) = \sum_i (\tau_0 - 2 + (1 - \alpha_i)R_{\alpha_i}(f_\nu))^2$$

(4.4)

to get a variational approximation $\tau_0 = \tau_0$ of $\tau$. Brute force should not be used in the evaluation of $\chi^2$: once again, Eq. (1.1) makes it possible to drastically reduce the computation time, and to perform the evaluation of $\chi^2$ with an excellent precision.

Of course, the values of the exponents in $f_\nu$ should not be blindly chosen. van Dongen and Ernst [19] showed that the subleading term in the small $x$ asymptotic expansion of $f$ is

$$\propto \begin{cases} x^{1+\lambda-2\tau}, & \text{if } \tau > 1 + \lambda - \mu_1, \\
\quad x^\mu_1 - \tau, & \text{if } \tau < 1 + \lambda - \mu_1 \\
\quad x^{-\tau} \ln x, & \text{if } \tau = 1 + \lambda - \mu_1 
\end{cases}$$

(4.5)

with $K(x, y) = x^{\lambda} \propto y^{\mu_1} x^{\lambda-\mu_1}$ when $x \to \infty$, whereas the exact asymptotic at large $x$ is $\propto x^{\lambda} e^{-x}$. Therefore, a good three-parameters class of trial functions should be:

$$f_\nu(x, \tau_0, c_1, c_2) = \left( \frac{1}{x^{\tau_0}} + \frac{c_1}{x^{\tau_1(\tau_0)}} + \frac{c_2}{x^{\lambda}} \right) e^{-x}$$

(4.6)
\(\tau_1\) being either \(2\tau_0 - 1 - \lambda\) (if \(\tau_0 > 1 + \lambda - \mu_1\)), or \(\tau_0 - \mu_1\) (if \(\tau_0 < 1 + \lambda - \mu_1\)). The small \(x\) leading term in \(f_\tau\) is \(\tau_0\) provided that \(\tau_0 > \lambda\). The approximate value \(\tau_v\) is the value of \(\tau_0\) at the minimum.

By construction, this method reproduces the exact results for the constant kernel and \(d = 1, D = 1\), since the exact scaling function is contained in those cases in the class of variational function we chose. In general, this method is inadequate to approach \(f\) itself, and is just designed to compute \(\tau\), in the same way as the variational approach in quantum mechanics is designed to obtain eigenvalues but, in principle, not eigenfunctions.

**B. Implementation**

With a small number \(n\) of variational parameters, we choose to perform the minimization with the downhill simplex method described in \([32]\) (steepest descent, conjugate gradient or other methods could also be used, with the drawback that these methods require extra evaluations of \(\chi^2\) to compute its gradient). This method starts from a \(n\)-dimensional simplex, i.e. \(n + 1\) points in the \(n\)-dimensional parameter space, and performs a sequence of geometric deformations until it contracts to a local minimum of the function. It is not the fastest algorithm, but it easily converges, and in our case where the computational burden is low we do not need more sophisticated devices.

As in any optimization problem, the initial condition is a crucial parameter, but here there is the additional complication that the smallest moment \(\alpha_{\text{min}}\) used in the computation of \(\chi^2\), should be bigger than \(\tau - 1\), and bigger than \(\tau_0 - 1\) at any step of the algorithm. What information on the value of \(\tau\) we may a priori gather (exact bounds, perturbation expansion), should guide our choice. Anyway, we do know that \(\tau < 1 + \lambda\): starting with an initial \(\tau_0\) smaller than \(1 + \lambda\) and \(\alpha_{\text{min}} > \lambda\) should avoid any trouble. As we get a first approximation of \(\tau\) we will be able to decrease the value of \(\alpha_{\text{min}}\) and make it closer to \(\tau_v - 1\), while refining the initial conditions. A few Monte-Carlo minimization steps can also be used to find a proper initial condition (but we scarcely needed this functionality in this work).

Why should we choose as small an \(\alpha_{\text{min}}\) as possible? The answer is that small moments probe the small \(x\) divergence of \(f(x)\), which is precisely what we are interested in. However, we also need some intermediate and higher moments to probe the intermediate \(x\) and the large \(x\) decay to stabilize consistent values of \(c_1\) and \(c_2\). There should be at least as many moments as variational parameter, otherwise there would be an infinite number of minima. Too many moments would cause excessive numerical round-off errors in the computation of \(\chi^2\).

We tested round-off errors by computing \(\tau_v\) for the exactly solvable model \(K^1\) for which \(f(x) \propto x^{-3/2}e^{-x}\), since, were we endowed with infinite numerical precision, our algorithm would yield the exact result in this case, as said before, whatever the \(\alpha\) may be, provided that they all are bigger than \(1/2 = \tau - 1\).

With the three parameter function introduced above, and moments 0.55, 0.667, 0.783, 0.9 and 2, we find \(\tau = 1.49997 \pm 4 \times 10^{-6}\) (\(\chi^2 = 1.94 \times 10^{-8}\)), the uncertainty being due to variations with different choices for the initial values of the parameters and the tolerance on the size of the simplex (the minimization algorithm stop criterion). The round-off errors increase with the number of moments and the number of variational parameters. The error is much bigger on \(c_1\) and \(c_2\), we find \(c_1 = 0.11 \pm 0.1\) and \(c_2 = -0.12 \pm 0.1\), instead of strictly 0. This means that the sensitivity on \(c_1\) and \(c_2\) is small in the vicinity of the minimum, and this method is not the right one to determine the scaling function (a negative \(c_2\) is unphysical here), but it just was not devised for this purpose: we just meant to compute \(\tau\), and for this quantity the accuracy is excellent.

**C. Numerical results**

We used this method to determine approximations of \(\tau\) for the kernel \((x^{1/D} + y^{1/D})^d\). We compared our results to numerical values obtained for \(d \leq 1, D = 1\) by Krivitsky \([21]\), and to our perturbative and nonperturbative expansions.

All values were obtained from the three-parameter variational functions introduced earlier in this text. We used 8 moments, 6 in the interval \([\alpha_{\text{min}} = 0.9]\), plus \(\alpha = 2\) and \(\alpha = 3\). \(\alpha_{\text{min}}\) was adjusted to be as close to \(\tau_v - 1\) as possible. The computation time was from 1 to 10 seconds per run on a HP workstation. 2 to 5 runs per points were necessary to adjust the parameters.

We also computed a few points with a different reparametrization of moments: 5 in the range \([\tau - 1, d/D]\), \(\alpha = 0.9, 2, 3\), as well as with only 2 variational parameters \((c_1 = 0)\), and with 4 variational parameters (the additional exponent being \(\mu_1 - \tau\) in the case when \(\tau > 1 + (d - 1)/D\)). The observed relative variations of \(\tau_v\) were at most of a few \(10^{-3}\). In all cases, \(\tau\) was found to be consistent with exact bounds.

First, we consider the case \(D = 1\). Fig. \([1]\) shows the comparison between variational approximations of \(\tau\) obtained with the modus operandi we just exposed, values extracted by Krivitsky \([21]\) from a numerical solution of Smoluchowski’s equation, and the \(O(d^2)\) perturbative expansion. The agreement between the variational approximation and Krivitsky’s results is excellent, which confirms the effectiveness and efficiency of the method: the ratio computation time (a few seconds)/accuracy is impressive. Actually, the variational approximation looks smoother than Krivitsky’s curve, which has two visible accidents (small cusps) near \(d = 1\) and \(d = 0.4\), and the variational approximation is fully consistent with the exact \(O(d^2)\) expansion at small \(d\) to
which it clearly tends asymptotically, whereas Krivitsky’s result tends to remain parallel to the perturbative curve, though close to it. Its good agreement with our infinite time results assesses the fact that Krivitsky’s solution actually reached the scaling regime, which, as said in section I, was not obvious a priori. We conclude that in this regime, the variational approximation recovers and confirms the results obtained by numerical integration of Smoluchowski’s equation.

FIG. 1. In $d = 1$, the comparison between the results obtained in [21] by Krivitsky, the variational approximation with 3 parameters and 8 moments, and the $O(d^2)$ perturbative expansion of $\tau$, illustrates the efficiency of the variational approximation. Indeed, the agreement between the numerical solution of Smoluchowski’s equation [21] and the variational approximation is excellent. The variational approximation is even in closer agreement with the small $d$ perturbative expansion than Krivitsky’s result, and although both methods recover the exact result $\tau = 3/2$ for $D = 1$, Krivitsky’s curve seems to have an accident in the vicinity of $D = 1$, whereas the variational result is smooth.

Once the effectiveness of the method was established, we were able to carry out the first systematic study of $\tau(d, D)$, and to control its validity thanks to the analytical results obtained in sections I and II.

We show on Fig. 2 the function $\tau(d, D)$ ($0.25 \leq d \leq 3$, $d \leq D < 8$) plotted in a $(\tau, D)$ diagram. Two kinds of curves are shown. Solid lines represent some iso-$d$ lines, i.e. the function $\tau(D)$ for a fixed value of $d$, whereas dashed lines are iso-$\lambda$ ($\lambda = d/D$) lines. The reliability of the approximation is assessed by the comparison with analytical results. As established in section I, iso-$d$ lines tend to $\tau = 2 - 2^{1-d}$ (stars on the right axis of Fig. 2) if $d < 1$, and to 1 if $d \geq 1$. As expected, the critical $D$ above which $\tau$ becomes smaller than 1 tends to infinity when $d \to 1^-$, entailing the breakdown of the large $D$ perturbative expansion in $D \geq 1$. The $d = 1$ iso-$d$ line seems to tend exponentially to 1, which is consistent with a nonperturbative decay in $1/D$ (see below). For $d > 1$ the large $D$ decay is slower as analytically predicted (we found a $1/D$ perturbative correction, see below). For $d \geq 2$ the curves shape qualitatively changes and an inflexion point appears.

Iso-$\lambda$ lines exponentially saturate to $1 + \lambda$ at large $D$, as analytically established before. Fig. 3 shows the comparison between the variational approximation and the nonperturbative large $d$ expansion of Eq. (3.31) in two cases, $\lambda = 1/2$ and $\lambda = 2/3$. The agreement is once again excellent at large $d$.

In $d = 1$, $D = 2$, Song and Poland [22] found $\tau = 1.123 \pm 0.016$ (using their first result), which compares well with our $\tau = 1.109$. In $d = 2$, $D = 3$, we find $\tau = 1.528$ which, unlike their result (1.243), is perfectly consistent with the exact bounds $1.4349 < \tau < 1.585$. In $d = 2$, $D = 4$, we find $\tau = 1.434$, which is in fair agreement with the perturbative large $D$ estimate $\tau = 1.462$ of section II. In fact, as shown on Fig. 3, the perturbative estimate is indeed a good approximation of $\tau$ in $d = 2$ for $D \leq 6$, and the $1/D$ decay is confirmed by the variational results. The cusp on the variational curve is confirmed by the existence of an inflexion point on $d > 2$ curves, as mentioned above. In $d = 1$, a nonperturbative exponential large $D$ decay to $\tau_{\infty} = 1$, is confirmed by Fig. 4. We roughly find $\tau - 1 \propto e^{-1.15D}$.

FIG. 2. The exponent $\tau$ was computed by the variational method for various values of $d$ and $D$. We show here some iso-$d$(solid lines) and iso-$\lambda$ (dashed) ($\lambda = d/D$) lines. The iso-$d$ lines tend to $\tau = 2 - 2^{1-d}$ (stars on the right axis) if $d < 1$, and to 1 if $d \geq 1$. The critical $D$ above which $\tau$ becomes smaller than 1 tends to infinity when $d \to 1^-$, entailing the breakdown of the large $D$ perturbative expansion in $D \geq 1$. The $d = 1$ iso-$d$ line seems to tend exponentially to 1, while for $d > 1$ the relaxation to 1 is slower. An inflexion point appears above $d \approx 2$. The iso-$\lambda$ lines exponentially saturate to $1 + \lambda$ at large $D$. 

FIG. 3. The comparison between the variational approximation and the nonperturbative large $D$ expansion of Eq. (3.31) in two cases, $\lambda = 1/2$ and $\lambda = 2/3$. The agreement is once again excellent at large $d$. 

FIG. 4. We roughly find $\tau - 1 \propto e^{-1.15D}$.
FIG. 3. Iso-$\lambda$ curves computed by the variational method (solid lines), as a function of $d$, for $\lambda = 1/2$ and $\lambda = 2/3$. As analytically established, $\tau$ tends to $1 + \lambda$ at large $D$. The agreement is good at large $d$ with the nonperturbative expansion (dashed lines).

Eventually, we show on Fig. 6 (for $d = 0.25$), that the variational result is also in good agreement with the large $D$ second order perturbative expansion in $d < 1$ ($\propto 1/D^2$).

As this section draws to a close, we shall say that this variational method, although very simple, seems to be very well adapted to the determination of the exponent $\tau$, as it is fast and, at least in the case we studied in this article, very accurate. It made it possible to acquire for the first time quantitative knowledge of $\tau$ in the whole parameter space of the $K_D^d$ kernel, the most studied and the prototype of the notorious class II kernels. The method is general and could help shedding some light on the whole class of kernels, thus increasing the practical use of Smoluchowski’s approach to understand aggregation phenomena. This point is worth an example. This is precisely what is dealt with in section V.

FIG. 4. In $d = 2$, the exponents computed by the variational approximation are in good agreement with the perturbative large $D$ estimate $\tau = 1 + 1.849/D$. From data, the actual asymptotic correction seems to be closer to $1.82/D$. The cusp on the variational curve corresponds to the change of behavior with the occurrence of an inflexion point for above $d = 2$.

FIG. 5. For $d = 1$, the exponents computed by the variational approximation displays a much faster decay to their $D = \infty$ limit ($\tau_\infty = 1$), than for $d > 1$. Indeed, as shown on this figure, the decay seems to be exponential in $D$, with roughly $\tau - 1 \propto e^{-1.15D}$, a nonperturbative behavior to be related to the break-down of the large $D$ perturbative approaches for $d = 1$. 
reduce the fact that starting from a Batchelor spectrum \[31\], the simulation of this model was able to reproduce a steeper spectrum range \(\gamma\) which describes the dynamics and the merger of vortices due to mergers by means of Eq. (1.5) with \(1 + d\) and \(D\) as the radius of the \(i\)-th vortex) through-out the merging processes. This model reproduces the main features observed in direct numerical simulations (see \[31\] for details). For instance, after noting that a distribution of vortex radii satisfying \(P(R) \sim R^{-\beta}\) is equivalent to a Gaussian energy spectrum \(E(k) \sim k^{\beta - 6}\) \[31\], the simulation of this model was able to reproduce the fact that starting from a Batchelor spectrum \(E(k) \sim k^{-3}\) (\(\beta = 3\)), the system evolves systematically to a steeper spectrum \(E(k) \sim k^{-\gamma}\) with \(\gamma = 6 - \beta\) in the range \(3 \sim 5\) \[31\].

Now, one expects that the collision kernel between two vortices is somewhat intermediate between the ballistic hard-disk form \(\sigma \sim (R_1 + R_2)^2\) \[24\], and the totally un-correlated form \(\sigma \sim (R_1 + R_2)^D\) (where the probability of colliding is proportional to the probability that two randomly placed vortices overlap, see also below Eq. (1.3)). Thus, one can describe approximately the decay of vortices due to mergers by means of Eq. (1.3) with \(1 \leq d \leq 2\) and \(D = 4\), as two colliding vortices merge into a new one with \(R = (R_1^d + R_2^d)^{1/4}\) in order to conserve energy and core vorticity. One thus expects a power law radius distribution \(P(R) \sim R^{-\beta}\), with \(\beta = D(\tau - 1) + 1\) and \(\tau\) given by our model. We find values of \(\gamma\) ranging from \(\gamma \approx 3.26\) for \(d = 2\) (taking \(\tau = 1.434\)) to \(\gamma \approx 4.95\) (taking \(\tau = 1.012\)) for \(d = 4\), in good qualitative agreement with observed exponents. As also found in direct simulations, the actual exponent (and here the value of the effective correct \(d\)) could depend on the actual initial conditions (\(\omega\), area occupied by the vortices \(\sim\) enstrophy). Note that the Batchelor limit case \(\gamma = 3\), is obtained when taking the naive strict upper bound \(\tau = 1 + d/D\) with \(d = 2\) and \(D = 4\).

FIG. 6. In \(d = 0.25\), the exponents computed by the variational approximation are in good agreement with the perturbative large \(D\) estimate \(\tau = 2 - 2^{-d} + (d(1-d))^{d+1}Dd + O(1/D^4)\).

V. APPLICATION IN TWO-DIMENSIONAL DECAYING TURBULENCE

In this section, we would like to illustrate the results obtained in this article by presenting an original application outside the field of massive particle aggregation, namely the dynamics of vortices in two-dimensional decaying turbulence. Recently, a statistical numerical model was introduced \[30,31\] which describes the dynamics and the merger of vortices with the assumption that the typical core vorticity \(\omega\) and the total energy \(E \sim \int v^2 \, d^2x \sim \sum_i \omega^2 R_i^2\) are conserved \((R_i)\) the radius of the \(i\)-th vortex) through-out the merging processes. This model reproduces the main features observed in direct numerical simulations (see \[30,31\] for details). For instance, after noting that a distribution of vortex radii satisfying \(P(R) \sim R^{-\beta}\) is equivalent to a Gaussian energy spectrum \(E(k) \sim k^{\beta - 6}\) \[31\], the simulation of this model was able to reproduce the fact that starting from a Batchelor spectrum \(E(k) \sim k^{-3}\) (\(\beta = 3\)), the system evolves systematically to a steeper spectrum \(E(k) \sim k^{-\gamma}\) with \(\gamma = 6 - \beta\) in the range \(3 \sim 5\) \[31\].

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CONCLUSION

In this article, we tackled the notoriously difficult problem of nontrivial polydispersity exponents in Smoluchowski’s approach to aggregation from an original angle. We chose to directly start from the scaling (infinite time limit) equation, and we did not focus on the determination of the whole scaling function, which is the object of solving Smoluchowski’s equation, to concentrate on \(\tau\) itself, which actually mainly depends on global (integral) equations. We think, and illustrated this point on the example of a simplified model of two-dimensional turbulence, that in some cases, the only knowledge of \(\tau\) would still be a good step towards the understanding of the phenomenon. The choices we made were fruitful and gave birth to new analytical and numerical results.

From an analytical viewpoint, we were able to use integral equations to find some exact bounds for \(\tau\), and, in the specific case of \(K_D = (x^{1/D} + y^{1/D})^d\), we obtained some perturbative and nonperturbative expansions of \(\tau\), without explicitly computing the corresponding expansions for the whole scaling function.

From a numerical viewpoint, we devised a variational approximation scheme, that recovers by construction known exact results, and can be used as a tool for extensive determination of \(\tau\), since it is both very economical and accurate. In addition, it is likely that the scaling function obtained in the variational approach is in many cases qualitatively, if not quantitatively, right. To illustrate its effectiveness, we performed a comprehensive study of \(\tau\) for a wide range of the parameters \((d, D)\) of the kernel \(K_D\). This is a noticeable advance, since very little quantitative knowledge was available for this kernel, although it was the prototype kernels with a non-trivial \(\tau\), and the object of much attention in the past \[17,18,20–28\].

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APPENDIX A: A USEFUL FORMULA

\[ \int \int_0^{+\infty} x^{-\tau_1} y^{-\tau_2} e^{-x-y} K(x,y) [(x+y)^\alpha - x^\alpha - y^\alpha] \, dx \, dy = \Gamma(2 + \lambda + \alpha - \tau_1 - \tau_2) \left[ \lambda(\tau_1, \alpha, \tau_1 + \tau_2) + \lambda(\tau_2, \alpha, \tau_1 + \tau_2) \right], \]  

(1.1)

where \( \Gamma \) is the gamma function, and,

\[ \lambda(t, \alpha, q) = \int_0^1 K(1, u) \frac{[(1 + u)^\alpha - 1 - u^\alpha]}{u^t(1 + u)^{2 + \lambda + \alpha - q}} \, du \]  

(1.2)

To demonstrate this formula is straightforward: just make the change of variable \( x = uv, y = v \), and use the definition of the \( \Gamma \) function:

\[ \Gamma(x) = \int_0^{+\infty} t^{x-1} e^{-t} \, dt \]  

(1.3)

From a numerical viewpoint this formula makes it possible to implement very rapid and accurate code for the variational approximations we developed before.

\[ 4 - 2a_2 = c + 4 \int_0^{+\infty} f_1(x) \ln x \, dx + 4 \int_0^{+\infty} f_2(x) \, dx \]  

(2.1)

\[ -a_2 = \frac{1}{2} \int_0^{+\infty} e^{-x} (\ln x)^2 \, dx + \int_0^{+\infty} f_1(x) \ln x \, dx + \int_0^{+\infty} f_2(x) \, dx, \]  

(2.2)

where \( \tau = 2d + a_2 d^2 + O(d^3) \), and,

\[ c = 4 \int_0^{+\infty} e^{-x} (\ln x)^2 \, dx + 4 \int_0^{+\infty} e^{-x-y} \ln (x+y) \, dx \, dy + 4 \left( \int_0^{+\infty} f_1(x) \, dx \right) \left( \int_0^{+\infty} e^{-y} \ln y \, dy \right) + \left( \int_0^{+\infty} f_1(x) \, dx \right)^2. \]  

(2.3)

\( c \) can be computed since \( \int f_1 \) is known from the first order calculation. After some elementary transformations, we find that \( c - 4 \int e^{-x} (\ln x)^2 \, dx = \frac{2\pi^2}{3} - 4 \). Combining Eq. (2.1) and (2.2), we find \( 4 + 2a_2 = c - 4 \int e^{-x} (\ln x)^2 \, dx \), hence eventually

\[ a_2 = \frac{\pi^2}{3} - 4. \]  

(2.4)

APPENDIX II: THE \( O(D^2) \) TERM IN \( D=1 \)

We derive the \( O(D^2) \) correction to \( \tau = 2d \) for \( D = 1 \), by computing the \( D^2 \) order of respectively Eqs. (1.4) and (2.8) with \( \alpha = d \), to get,

\[ x u'' + (1-x) u' + u = \frac{4}{D} \int_0^{+\infty} e^{-y} \frac{x^{1/D - 1}}{y^{1/D} + x^{1/D}} \, dy - \frac{2}{D} \ln x - 2 J_D. \]  

(3.1)

With \( v(x) = u(x)/(x-1) \), this equation reduces to a first order differential equation for \( v' \), and we find,

\[ \int \int_0^{+\infty} x^{-\tau_1} y^{-\tau_2} e^{-x-y} K(x,y) [(x+y)^\alpha - x^\alpha - y^\alpha] \, dx \, dy = \]  

\[ \Gamma(2 + \lambda + \alpha - \tau_1 - \tau_2) \left[ \lambda(\tau_1, \alpha, \tau_1 + \tau_2) + \lambda(\tau_2, \alpha, \tau_1 + \tau_2) \right], \]  

(1.1)

It would be very awkward and inefficient to use 2-dimensional numerical integration (especially here, as the integrand is singular at the origin). A startlingly economical way of computing the gamma function is due to Lanczos and is described in [32] (it is not much slower than the built-in exponential function...).

APPENDIX III: THE LINEARIZED SCALING FUNCTION

We find the solution of the second order differential equation Eq. (3.10) for the linear coefficient \( f_1(x) \) in

\[ f_1(x) = c_0 u_0(x) e^{-x} + c_1 (x-1) - 2 J_D - \frac{2}{D} (1 + \ln x) \]

\[ + \frac{4}{D} e^{-x} \int_0^x dy_1 \frac{e^{y_1}}{y_1(y_1-1)^2} \int_0^{y_1} dy_2 y_2^{1/D-1} e^{-y_2} (y_2-1) \int_0^{y_2} dy_3 \frac{e^{-y_3}}{y_3^{1/D} + y_2^{1/D}}, \]  

(3.2)
\( u_0(x) = e^x - (x - 1)Vp \left( \int_{-\infty}^{x} \frac{e^y}{y} dy \right) \) (3.3)

(“Vp” means “principal value”).

In fact, the triple integral can be transformed into a simple integral involving special functions. For our purpose, we only need to know that this integral goes to zero when \( x \to 0 \), which is easily seen.

\[
2(1 - \frac{d}{D})(1 - \varepsilon) = 2^{2-2d} \int e^{-x-y}(x^{\frac{\varepsilon}{2}} + y^{\frac{\varepsilon}{2}})d[x^{\frac{\varepsilon}{2}} + y^{\frac{\varepsilon}{2}} - (x+y)^{\frac{\varepsilon}{2}}]dxdyd\varepsilon
\]

\[
\approx \Gamma(1 + 2d/D - \varepsilon) [\mathcal{X}(0, d/D, 1 + \varepsilon) + \mathcal{X}(1 + \varepsilon, d/D, 1 + \varepsilon)]
\]

\[
= 2c^2\Gamma(2d/D - 2\varepsilon)\mathcal{X}(1 + \varepsilon, d/D, 2 + 2\varepsilon)
\]

APPENDIX IV: PERTURBATIVE ESTIMATE

For \( d > 1 \), \( \tau = 1 + \varepsilon(D) \) where \( \varepsilon \to 0 \) when \( D \to \infty \).

We make the ansatz:

\[
f(x) \approx f_\infty(x) + \frac{c}{x^{1+\varepsilon}}e^{-x},
\]

and plug it into Eq. (3.4) to obtain, \( 1 - \varepsilon = 2^{1-d} + c\Gamma(\frac{2}{d} - \varepsilon) \), which means that, when \( D \to \infty \), \( c \approx (1 - 2^{1-d})/(d/D - \varepsilon) \). Then we make use of Eqs. (1.1) and (1.8) to obtain,

\[
\frac{2}{1 + 2^{1-d}} = \int_0^1 (1 + v^{-\frac{\varepsilon}{d}})dv = J(\kappa, d)
\]

\[
\tau = 1 + \frac{\kappa}{D} + O(\frac{1}{D^2})
\]

The equation Eq. (4.3) has a unique solution \( 0 < \kappa < d \) since the integral \( J(\kappa, d) \) is a decreasing function of \( \kappa \), and \( J(0, d) = 2^d > 2/(2^{1-d} + 1) > 1 = J(d, d) \) (for \( d > 1 \)).

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