

# KINETIC MODELS FOR DUST COAGULATION IN INTERSTELLAR CLOUDS

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## Abstract

In this paper we propose some kinetic models which take into account different mechanisms of coagulation between two populations of dust particles inside interstellar nebulae. These models are in general nonlinear; however, at the end of the paper we perform an approximate procedure to obtain a linear transport equation even for the model which considers the most general mechanism of coagulation.

## 1. Introduction

Dust coagulation is an important phenomenon in astrophysical research [7] since it plays an essential role in the chemical and dynamical evolution of interstellar nebulae.

Measurements of the *extinction curve* [9] of light through interstellar clouds show that the nature of interstellar dust consists of two distinct populations of solid particles, small and relatively large grains (hereinafter indicated with  $a$  and  $b$ , respectively). The bimodal nature of the grain size distribution has become well established, in the sense that the greatest masses of the small grains are of several order of magnitude less than the masses of large particles [9].

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Dust particles experience a great variety of phenomena which may significantly modify their morphological properties, see, for instance, papers [6, 10, 11, 13, 14]. In particular, within these phenomena, *growth* of large grains, due to *coagulation* when they interact with each of the two populations of dust particles, plays a relevant role [5]. Moreover, studies on the microphysics of the coagulation process has shown that sticking of two colliding particles occurs when the relative collision velocity is less than a critical velocity, depending on mass, elastic properties and surface energy of the dust material. Such a physical process leads to the disappearance of the lighter components, which are removed by the large particles from the grain mass distribution.

More precisely, in [5] it is suggested that the critical velocity  $v_{\text{cr}}$  of coagulation is given by the following law:

$$v_{\text{cr}} = K_b R^{-5/6}, \quad R = \frac{R_a R_b}{R_a + R_b}, \quad K_b = 3.86 \frac{\gamma_b^{5/6}}{E_b^{1/3} \rho_b^{1/2}} \quad (1)$$

where  $E_b$  is the Young's modulus,  $\gamma_b$  the surface energy,  $\rho_b$  the density and  $R_b$  the radius of the large grain  $b$ .  $R_a$ , obviously, is the radius of the small particle  $a$ .

We observe that typical critical velocities range between  $10^2$  to  $5 \cdot 10^4$  m/s, whereas  $R_a$  can vary between 1 nm and 10 nm and  $R_b$  is generally greater than 100 nm.

According to the literature quoted above, it seems of some interest a kinetic approach to sticking phenomena of dust particles, at least in the early coagulation process of interstellar matter. A first attempt to build a kinetic model for dust coagulation was performed in [3]. Very recently, this model has been improved in [2], where well-posedness of the Cauchy problem in unbounded domains and numerical simulations of the coagulation process have been performed. Such a model, hereinafter called the *simplest model*, is basically determined assuming that the large particles are at rest and consequently coagulation occurs only when small particles, with a relative velocity less than a suitable critical velocity, collide with the large ones. Under these assumptions the whole system of large grains is viewed as a background which enlarge its total mass but preserve the number of individual particles. Therefore the evolution of small particles is shown to be governed by a linear integro-differential equation.

In the present paper we remove these constraints, first considering the motion of large particles and then allowing coagulation also between large grains.

The paper is organized as follows: in Section 2 we resume the main features of the *simplest model* proposed in [2]. In Section 3 we extend this model by allowing the motion of large particles, but assuming that collisions between these particles are negligible and that collisions between small and large grains do not alter the velocity of these last ones.

In the last section we assume that also large particles may experience coagulation and scattering, by introducing a critical velocity  $w_{\text{cr}}$ . In this case we obtain a nonlinear Boltzmann-like model. Under some further assumptions, including that scattering between large particles can be neglected, we derive a linear transport model which has the same mathematical structure as the *simplest model*, except for a correction term due to the sticking of large grains.

## 2. The Simplest Model

We resume here the main features of the *simplest model*, considered in [2], for an interstellar dust composed of two different populations.

1. *Small particles (or particles a)*. These are characterized by having a mass  $\mu$ ,  $0 < \mu \leq \mu^o$ , and a number density  $n = n(\mathbf{r}, \mathbf{v}, \mu, t)$ ,  $n(\mathbf{r}, \mathbf{v}, \mu, t) d\mathbf{r} d\mathbf{v} d\mu$  representing the number of particles with masses between  $\mu$  and  $\mu + d\mu$  contained, at time  $t$ , in the volume element  $d\mathbf{r}$  around the location  $\mathbf{r}$  and having velocities in the volume element of the velocity space  $d\mathbf{v}$  around the velocity  $\mathbf{v}$ . Since the cross sections for small particles are very small, the contribution of  $a - a$  collisions may be considered negligible.
2. *Large particles (or particles b)*. The second population is characterized by having a mass  $m$ ,  $m_o \leq m < +\infty$ , and number density  $N = N(\mathbf{r}, m, t)$ , where  $N(\mathbf{r}, m, t) d\mathbf{r} dm$  denotes the number of particles with masses between  $m$  and  $m + dm$  contained, at time  $t$ , in the volume element  $d\mathbf{r}$  around the location  $\mathbf{r}$ . In such a model, the dependence of  $N$  from the velocity variable is disregarded, since large particles are considered at rest with respect to some suitable reference frame. Thus, there are no  $b - b$  collisions. Moreover it is assumed that  $\mu^o \ll m_o$ .

3. *Coagulation collisions.* Assume that a small particle of mass  $\mu$ , with a speed  $v := |\mathbf{v}|$  less than a critical speed  $v_{\text{cr}}$ , collides with a large particle of mass  $m$ . The result consists in the formation of a single large particle of mass  $m + \mu$ . Moreover, considering  $\mu = (4/3)\pi\rho_a R_a^3$  (i.e., sphericity of particles) and under the assumption that  $R_a \ll R_b$ , formula (1) gives

$$v_{\text{cr}} = \beta \mu^{-5/18}, \quad \beta = K_b \left( \frac{4\pi\rho_a}{3} \right)^{5/18}, \quad (2)$$

where  $\rho_a$  is the density of the small particle.

4. *Scattering collisions.* Assume that a small particle of mass  $\mu$ , with a speed  $v$  larger than  $v_{\text{cr}}$ , collides with a large particle. This leads to an inelastic scattering of the small particle.
5. *Free streaming.* During the time interval between two consecutive collisions there are no forces acting on small particles, which move with constant velocity.

From the above assumptions, the following *balance equation* for the density of small particles is obtained

$$\begin{aligned} \frac{\partial}{\partial t} n(\mathbf{r}, \mathbf{v}, \mu, t) &= -\mathbf{v} \cdot \nabla_{\mathbf{r}} n(\mathbf{r}, \mathbf{v}, \mu, t) \\ &\quad -v[\sigma_{\text{cg}}(v, \mu) + \sigma_{\text{sc}}(\mathbf{v}, \mu)]n(\mathbf{r}, \mathbf{v}, \mu, t) \left[ \int_{m_0}^{+\infty} N(\mathbf{r}, m', t) dm' \right] \\ &\quad + \int_{\mathbb{R}^3} d\mathbf{v}' \{v' \sigma_{\text{s}}(\mathbf{v}' \rightarrow \mathbf{v}, \mu) n(\mathbf{r}, \mathbf{v}', \mu, t)\} \left[ \int_{m_0}^{+\infty} N(\mathbf{r}, m', t) dm' \right], \end{aligned} \quad (3a)$$

$\mathbf{r} \in \mathbb{R}^3$ ,  $\mathbf{v} \in \mathbb{R}^3$  and  $t > 0$ . Equation (3a) must be supplemented by the following initial condition

$$n(\mathbf{r}, \mathbf{v}, \mu, 0) = n_0(\mathbf{r}, \mathbf{v}, \mu). \quad (3b)$$

The first term on the right hand side of (3a) takes into account the free streaming of small particles. The second one is a loss term describing the disappearance of small particles from the phase-space point  $(\mathbf{r}, \mathbf{v}, \mu)$  due to coagulation, with isotropic coagulation cross-section  $\sigma_{\text{cg}}(v, \mu) \geq 0$ , and to out-scattering, with total scattering cross-section  $\sigma_{\text{sc}}(\mathbf{v}, \mu) \geq 0$ . The third term is a gain term due to in-scattering, because small particles appear in the phase-space point  $(\mathbf{r}, \mathbf{v}, \mu)$  after a scattering collision with a large particle that changes their velocity from  $\mathbf{v}'$  to  $\mathbf{v}$ . The scattering mechanism is intended to be inelastic, so that  $a$ -particles, which initially have a velocity

greater than  $v_{\text{cr}}$ , may loose their velocity after some collisions and then coagulate when the velocity critical value is reached. Moreover in (3a)

$$\sigma_{\text{sc}}(\mathbf{v}, \mu) = \int_{\mathbb{R}^3} \sigma_{\text{s}}(\mathbf{v} \rightarrow \mathbf{v}', \mu) d\mathbf{v}', \quad (4)$$

where  $\sigma_{\text{s}}$  is the differential scattering cross-section,

$$\sigma_{\text{sc}}(\mathbf{v}, \mu) = 0 \quad \forall |\mathbf{v}| < v_{\text{cr}}(\mu) \quad (5)$$

$$\sigma_{\text{cg}}(v, \mu) = 0 \quad \forall v > v_{\text{cr}}(\mu). \quad (6)$$

We observe that the coagulation process is assumed to be isotropic so that the corresponding cross section depends only on  $v = |\mathbf{v}|$ . In addition, let us remark that the cross-sections depend only on the mass  $\mu$  of small particles. This approximation is coherent with the fact that the main physical parameter in the interaction mechanism is the reduced mass  $\mu m / (\mu + m)$  which, when  $\mu \ll m$ , coincides with  $\mu$ . For the same reason also the critical velocity  $v_{\text{cr}}$  of coagulation depends on  $\mu$  only. This approximation, however, allows to reduce (3a) to a linear form, as we shall see later.

The balance equation for large particles reads

$$\begin{aligned} \frac{\partial}{\partial t} N(\mathbf{r}, m, t) = & -N(\mathbf{r}, m, t) \int_{\mathbb{R}^3} d\mathbf{v}' \int_0^{\mu^{\circ}} d\mu' [v' \sigma_{\text{cg}}(v', \mu') n(\mathbf{r}, \mathbf{v}', \mu', t)] \\ & + \int_{\mathbb{R}^3} d\mathbf{v}' \int_0^{\mu_*} d\mu' [v' \sigma_{\text{cg}}(v', \mu') n(\mathbf{r}, \mathbf{v}', \mu', t) N(\mathbf{r}, m - \mu', t)] \end{aligned} \quad (7a)$$

for  $\mathbf{r} \in \mathbb{R}^3$  and  $t > 0$ . As for equation (3a), an initial condition has to be given for (7a), such as

$$N(\mathbf{r}, m, 0) = N_0(\mathbf{r}, m). \quad (7b)$$

In equation (7a)  $\mu_* := \min\{\mu^{\circ}, m - m_{\circ}\}$  since  $N(\mathbf{r}, m, t)$  is only defined for  $m \geq m_{\circ}$ . The first term on the right hand side of equation (7a) is a loss term describing the disappearance of large particles from the phase-space point  $(\mathbf{r}, m)$ , due to coagulation collisions with small particles of any mass  $\mu'$ , that change the mass from  $m$  to  $m + \mu'$  (*out-growing*). The second term is a gain term describing the appearance, in the phase-space point  $(\mathbf{r}, m)$  after coagulation with small particles of mass  $\mu'$ , of large particles that change the mass from  $m - \mu'$  to  $m$  (*in-growing*).

Equations (3) and (7) give the dynamics of the *simplest model*. Nevertheless, as shown in [2], such equations can be re-written by introducing the integrated density

$$\widehat{N}(\mathbf{r}, t) := \int_{m_0}^{+\infty} N(\mathbf{r}, m, t) dm, \quad (8)$$

which represents the total number density of large particles in  $\mathbf{r}$  at time  $t$ . Moreover it was easy to show that

$$\widehat{N}(\mathbf{r}, t) = \widehat{N}_0(\mathbf{r}) := \int_{m_0}^{+\infty} N_0(\mathbf{r}, m) dm \quad (9)$$

for all  $\mathbf{r} \in \mathbb{R}^3$ . Thus, the total number of large particles is constant for all  $t \geq 0$ , since the coagulation process does not change the total number of these particles, but increases only their total mass.

This result allows to re-write equation (3a) as follows

$$\begin{aligned} \frac{\partial}{\partial t} n(\mathbf{r}, \mathbf{v}, \mu, t) &= -\mathbf{v} \cdot \nabla_{\mathbf{r}} n(\mathbf{r}, \mathbf{v}, \mu, t) \\ &\quad -v \widehat{N}_0(\mathbf{r}) [\sigma_{cg}(v, \mu) + \sigma_{sc}(\mathbf{v}, \mu)] n(\mathbf{r}, \mathbf{v}, \mu, t) \\ &\quad + \widehat{N}_0(\mathbf{r}) \int_{\mathbb{R}^3} d\mathbf{v}' \{v' \sigma_s(\mathbf{v}' \rightarrow \mathbf{v}, \mu) n(\mathbf{r}, \mathbf{v}', \mu, t)\}, \quad (10) \end{aligned}$$

for  $\mathbf{r} \in \mathbb{R}^3$ ,  $\mathbf{v} \in \mathbb{R}^3$  and  $t > 0$ . In paper [2] well-posedness of the Cauchy problems (3) and (7) has been proven under the assumption that the quantities  $v\sigma_{sc}(\mathbf{v}, \mu)$  and  $v\sigma_{cg}(v, \mu)$  are bounded non-negative and measurable functions. Moreover some numerical simulations have also been performed in order to evaluate the rate of decrease versus time of the  $a$ -particle population.

### 3. Coagulation with Motion of Large Particles

In this section, we partially remove one of the assumptions made in the previous section, considering now that large particles can move in the space with velocity  $\mathbf{w}$ . However we continue to assume that  $b-b$  interactions (i.e., interactions between large particles) are negligible. The distribution function of these particles is now defined by  $N = N(\mathbf{r}, \mathbf{w}, m, t)$ . Consequently,

equation (3a) becomes:

$$\begin{aligned} \frac{\partial}{\partial t} n(\mathbf{r}, \mathbf{v}, \mu, t) &= -\mathbf{v} \cdot \nabla_{\mathbf{r}} n(\mathbf{r}, \mathbf{v}, \mu, t) \\ &- n(\mathbf{r}, \mathbf{v}, \mu, t) \int_{|\mathbf{v}-\mathbf{w}'| < v_{\text{cr}}} d\mathbf{w}' |\mathbf{v}-\mathbf{w}'| \sigma_{\text{cg}}(|\mathbf{v}-\mathbf{w}'|, \mu) \widehat{N}(\mathbf{r}, \mathbf{w}', t) \\ &- n(\mathbf{r}, \mathbf{v}, \mu, t) \int_{\mathbb{R}^3} d\mathbf{v}' \int_{|\mathbf{v}-\mathbf{w}'| > v_{\text{cr}}} d\mathbf{w}' |\mathbf{v}-\mathbf{w}'| \sigma_{\text{s}}(\mathbf{v} \rightarrow \mathbf{v}', \mathbf{w}', \mu) \widehat{N}(\mathbf{r}, \mathbf{w}', t) \\ &+ \int_{\mathbb{R}^3} d\mathbf{v}' \int_{|\mathbf{v}'-\mathbf{w}'| > v_{\text{cr}}} d\mathbf{w}' |\mathbf{v}'-\mathbf{w}'| \sigma_{\text{s}}(\mathbf{v}' \rightarrow \mathbf{v}, \mathbf{w}', \mu) \widehat{N}(\mathbf{r}, \mathbf{w}', t) n(\mathbf{r}, \mathbf{v}', \mu, t), \end{aligned} \quad (11)$$

where, similarly to the previous section, we put

$$\widehat{N}(\mathbf{r}, \mathbf{w}, t) := \int_{m_0}^{+\infty} N(\mathbf{r}, \mathbf{w}, m, t) dm. \quad (12)$$

In the above equation, the first two integral terms account for the loss of small particles of velocity  $\mathbf{v}$  due to coagulation and scattering, respectively, whereas the third integral term is a gain term produced by scattering of small particles that after collision assume velocity  $\mathbf{v}$ . Observe that now the critical velocity  $v_{\text{cr}}$ , in the integrals, is obviously compared to the incoming relative speed  $|\mathbf{v}-\mathbf{w}'|$  or  $|\mathbf{v}'-\mathbf{w}'|$  of the colliding dust particles. In (11), the differential scattering cross-section  $\sigma_{\text{s}}$  now depends also on the velocity  $\mathbf{w}'$  of the  $b$ -particles. We observe that, thanks to the different order of magnitude of the masses of the particles  $a$  and  $b$ , interactions between them are assumed not altering the incoming velocity  $\mathbf{w}'$  of grains  $b$ . Note also that the coagulation cross-section  $\sigma_{\text{cg}}$  depends, as usual, on the modulus of the incoming relative velocity.

We can now deduce the evolution equation of large grains which turns out to be only a simple generalization of equation (7a) for moving particles of type  $b$ :

$$\begin{aligned} \frac{\partial}{\partial t} N(\mathbf{r}, \mathbf{w}, m, t) &= -\mathbf{w} \cdot \nabla_{\mathbf{r}} N(\mathbf{r}, \mathbf{w}, m, t) \\ &- N(\mathbf{r}, \mathbf{w}, m, t) \int_0^{\mu_0} d\mu' \int_{|\mathbf{v}'-\mathbf{w}| < v_{\text{cr}}} d\mathbf{v}' |\mathbf{v}'-\mathbf{w}| \sigma_{\text{cg}}(|\mathbf{v}'-\mathbf{w}|, \mu') n(\mathbf{r}, \mathbf{v}', \mu', t) \\ &+ \int_0^{\mu_*} d\mu' \int_{|\mathbf{v}'-\mathbf{w}| < v_{\text{cr}}} d\mathbf{v}' |\mathbf{v}'-\mathbf{w}| \sigma_{\text{cg}}(|\mathbf{v}'-\mathbf{w}|, \mu') n(\mathbf{r}, \mathbf{v}', \mu', t) N(\mathbf{r}, \mathbf{w}, m-\mu', t). \end{aligned} \quad (13)$$

Thus, by following the same line of Lemma 3 of paper [2], it is easy to show

that integration of equation (13) over  $m$  yields

$$\frac{\partial}{\partial t} \widehat{N}(\mathbf{r}, \mathbf{w}, t) = -\mathbf{w} \cdot \nabla_{\mathbf{r}} \widehat{N}(\mathbf{r}, \mathbf{w}, t), \quad (14)$$

so that

$$\widehat{N}(\mathbf{r}, \mathbf{w}, t) = \widehat{N}_0(\mathbf{r} - \mathbf{w}t, \mathbf{w}), \quad (15)$$

where

$$\widehat{N}(\mathbf{r}, \mathbf{w}, 0) = \widehat{N}_0(\mathbf{r}, \mathbf{w}), \quad (16)$$

with  $\widehat{N}_0(\mathbf{r}, \mathbf{w})$  given. Hence,

$$\int_{m_0}^{+\infty} N(\mathbf{r}, \mathbf{w}, m, t) dm = \widehat{N}_0(\mathbf{r} - \mathbf{w}t, \mathbf{w}) = F(\mathbf{r}, \mathbf{w}, t) \quad (17)$$

where  $F$  is a known function.

By using (17), equation (11) can be re-written in the following form

$$\begin{aligned} \frac{\partial}{\partial t} n(\mathbf{r}, \mathbf{v}, \mu, t) &= -\mathbf{v} \cdot \nabla_{\mathbf{r}} n(\mathbf{r}, \mathbf{v}, \mu, t) \\ &- n(\mathbf{r}, \mathbf{v}, \mu, t) \int_{|\mathbf{v}-\mathbf{w}'| < v_{\text{cr}}} d\mathbf{w}' |\mathbf{v} - \mathbf{w}'| \sigma_{\text{cg}}(|\mathbf{v} - \mathbf{w}'|, \mu) F(\mathbf{r}, \mathbf{w}', t) \\ &- n(\mathbf{r}, \mathbf{v}, \mu, t) \int_{\mathbb{R}^3} d\mathbf{v}' \int_{|\mathbf{v}-\mathbf{w}'| > v_{\text{cr}}} d\mathbf{w}' |\mathbf{v} - \mathbf{w}'| \sigma_{\text{s}}(\mathbf{v} \rightarrow \mathbf{v}', \mathbf{w}', \mu) F(\mathbf{r}, \mathbf{w}', t) \\ &+ \int_{\mathbb{R}^3} d\mathbf{v}' \int_{|\mathbf{v}'-\mathbf{w}'| > v_{\text{cr}}} d\mathbf{w}' |\mathbf{v}' - \mathbf{w}'| \sigma_{\text{s}}(\mathbf{v}' \rightarrow \mathbf{v}, \mathbf{w}', \mu) F(\mathbf{r}, \mathbf{w}', t) n(\mathbf{r}, \mathbf{v}', \mu, t). \end{aligned} \quad (18)$$

We observe that the last equation is linear since the function  $F$ , as already said, is known.

**Remark.** If we assume that  $\widehat{N}_0$  is independent from space, i.e.  $\widehat{N}_0 = \widehat{N}_0(\mathbf{w})$ , then we find from (15)

$$\widehat{N}(\mathbf{r}, \mathbf{w}, t) = \widehat{N}_0(\mathbf{w}), \quad (19)$$

namely the total number of large particles, with velocity  $\mathbf{w}$ , is constant for all  $t \geq 0$ .

#### 4. Coagulation between Large Particles

In this section we will assume that large grains  $b$  can move and can also

experience coagulation. At this end we introduce, in the same fashion as for interactions between particles  $a$  and  $b$ , a critical velocity of coagulation  $w_{\text{cr}}$  between  $b$ -particles. Assuming that two spherical  $b$ -particles of masses, say  $m$  and  $m'$ , have the same density  $\rho_b$ , then the reduced radius  $R$  turns out to be

$$R = \left[ \frac{3mm'}{4\pi\rho_b(m+m')} \right]^{1/3},$$

and formula (2) this time becomes

$$w_{\text{cr}} = \beta \left( \frac{mm'}{m+m'} \right)^{-5/18}, \quad \beta = K_b \left( \frac{4\pi\rho_b}{3} \right)^{5/18}. \quad (20)$$

Moreover, considering two  $b$ -particles of masses  $m, m'$ , moving with velocities  $\mathbf{w}, \mathbf{w}'$ , we define a suitable coagulation cross-section  $\Sigma_{\text{cg}} = \Sigma_{\text{cg}}(|\mathbf{w}' - \mathbf{w}|, m, m')$  such that

$$\Sigma_{\text{cg}}(|\mathbf{w}' - \mathbf{w}|, m, m') = 0 \quad \forall |\mathbf{w}' - \mathbf{w}| > w_{\text{cr}}(m, m'). \quad (21)$$

Note that  $\Sigma_{\text{cg}}$  is related to the probability that two particles with velocities  $\mathbf{w}, \mathbf{w}'$  and masses  $m, m'$  undergo a coagulation event that produces a single particle of mass  $m + m'$ .

After these definitions, we are able to re-write equation (13) adding to this equation new gain and loss terms. In particular we have to consider

- *a loss term* (in the balance equations of grains of mass  $m$ ) due to coagulation between two grains  $b$  that, before collision, have masses  $m, m'$  and velocities  $\mathbf{w}, \mathbf{w}'$ , respectively, i.e.

$$- N(\mathbf{r}, \mathbf{w}, m, t) \int_{m_0}^{+\infty} dm' \int_{|\mathbf{w}' - \mathbf{w}| < w_{\text{cr}}} d\mathbf{w}' |\mathbf{w}' - \mathbf{w}| \Sigma_{\text{cg}}(|\mathbf{w}' - \mathbf{w}|, m, m') \times N(\mathbf{r}, \mathbf{w}', m', t); \quad (22)$$

- *a gain term* due to coagulation between two particles  $b$  which, before collision, have masses  $m', m''$  and velocities  $\mathbf{w}', \mathbf{w}''$ , and which coagulate in a single grain of mass  $m = m' + m'' > 2m_0$  and velocity  $\mathbf{w}$ , i.e.

$$+ H(m - 2m_0) \int_{m_0}^{m - m_0} dm' \int_{|\mathbf{w}' - \mathbf{w}''| < w_{\text{cr}}} d\mathbf{w}' |\mathbf{w}' - \mathbf{w}''| \Sigma_{\text{cg}}(|\mathbf{w}' - \mathbf{w}''|, m - m', m') \times N(\mathbf{r}, \mathbf{w}', m', t) N(\mathbf{r}, \mathbf{w}'', m - m', t), \quad (23)$$

where  $H$  is the Heaviside function (coagulation between  $b$ -particles cannot lead to particles with mass smaller than  $2m_o$ ); in (23) momentum conservation implies that

$$\mathbf{w}'' = \frac{m\mathbf{w} - m'\mathbf{w}'}{m - m'}; \quad (24)$$

- *a loss term* due to inelastic scattering between two large grains of masses  $m, m'$  that, before collision, have velocities  $\mathbf{w}, \mathbf{w}'$ , and after collision have velocities  $\mathbf{w}_*, \mathbf{w}'_*$ , i.e.

$$\begin{aligned} & - N(\mathbf{r}, \mathbf{w}, m, t) \int_{\mathbb{R}^3 \times \mathbb{R}^3} d\mathbf{w}_* d\mathbf{w}'_* \int_{m_o}^{+\infty} dm' |\mathbf{w}' - \mathbf{w}| \\ & \quad \times \Sigma_s((\mathbf{w}, \mathbf{w}') \rightarrow (\mathbf{w}_*, \mathbf{w}'_*), m, m') N(\mathbf{r}, \mathbf{w}', m', t), \quad (25) \end{aligned}$$

where  $\Sigma_s$  is the scattering differential cross-section (which vanishes if  $|\mathbf{w}' - \mathbf{w}| < w_{\text{cr}}(m, m')$ ) and  $\mathbf{w}' = \mathbf{w}'(\mathbf{w}, \mathbf{w}_*, \mathbf{w}'_*, m, m')$ , through momentum conservation;

- *a gain term* due to inelastic scattering between two particles  $b$  of masses  $m, m'$  that, before collision, have velocities  $\mathbf{w}_*, \mathbf{w}'_*$  such that  $|\mathbf{w}_* - \mathbf{w}'_*| > w_{\text{cr}}$ , and after collision have velocities  $\mathbf{w}, \mathbf{w}'$ , i.e.,

$$\begin{aligned} & + \int_{\mathbb{R}^3 \times \mathbb{R}^3} d\mathbf{w}_* d\mathbf{w}'_* \int_{m_o}^{+\infty} dm' |\mathbf{w}_* - \mathbf{w}'_*| \\ & \quad \times \Sigma_s((\mathbf{w}_*, \mathbf{w}'_*) \rightarrow (\mathbf{w}, \mathbf{w}'), m, m') N(\mathbf{r}, \mathbf{w}_*, m, t) N(\mathbf{r}, \mathbf{w}'_*, m', t), \quad (26) \end{aligned}$$

where we recall that  $\mathbf{w}' = \mathbf{w}'(\mathbf{w}, \mathbf{w}_*, \mathbf{w}'_*, m, m')$ .

Equation (13) with these new terms assumes a nonlinear form, so that it can be considered a true Boltzmann-like equation [4], to be coupled with equation (11) for  $a$ -particles. Such an equation is very similar to that studied in [8] and analogous to kinetic equations appearing in papers [1, 12], concerning coalescence of droplets in sprays, where also breakup is considered.

In order to obtain an evolution equation which includes coagulation for large grains and, at the same time, can be reduced to a linear transport equation, one has to neglect scattering between particles  $b$ . Such a requirement can be justified by the following conjecture. Temperature inside an interstellar cloud results to be of only some Kelvin degree [5]. Therefore, the characteristic velocity of large grains, as for instance the thermal velocity [4], can be very small if compared to the coagulation critical velocity  $w_{\text{cr}}$ .

Consequently, one can argue that the number of  $b - b$  collisions with scattering is of some order of magnitude less than that producing coagulation. If this hypothesis is assumed, then the evolution equation for grains  $b$  can be written disregarding the terms (25) and (26). Thus, we obtain

$$\begin{aligned}
\frac{\partial}{\partial t} N(\mathbf{r}, \mathbf{w}, m, t) &= -\mathbf{w} \cdot \nabla_{\mathbf{r}} N(\mathbf{r}, \mathbf{w}, m, t) \\
&- N(\mathbf{r}, \mathbf{w}, m, t) \int_0^{\mu^o} d\mu' \int_{|\mathbf{v}' - \mathbf{w}| < v_{\text{cr}}} d\mathbf{v}' |\mathbf{v}' - \mathbf{w}| \sigma_{\text{cg}}(|\mathbf{v}' - \mathbf{w}|, \mu') n(\mathbf{r}, \mathbf{v}', \mu', t) \\
&+ \int_0^{\mu^*} d\mu' \int_{|\mathbf{v}' - \mathbf{w}| < v_{\text{cr}}} d\mathbf{v}' |\mathbf{v}' - \mathbf{w}| \sigma_{\text{cg}}(|\mathbf{v}' - \mathbf{w}|, \mu') n(\mathbf{r}, \mathbf{v}', \mu', t) N(\mathbf{r}, \mathbf{w}, m - \mu', t) \\
&- N(\mathbf{r}, \mathbf{w}, m, t) \int_{m_o}^{+\infty} dm' \int_{|\mathbf{w}' - \mathbf{w}| < w_{\text{cr}}} d\mathbf{w}' |\mathbf{w}' - \mathbf{w}| \Sigma_{\text{cg}}(|\mathbf{w}' - \mathbf{w}|, m, m') N(\mathbf{r}, \mathbf{w}', m', t) \\
&+ H(m - 2m_o) \int_{m_o}^{m - m_o} dm' \int_{|\mathbf{w}' - \mathbf{w}''| < w_{\text{cr}}} d\mathbf{w}' |\mathbf{w}' - \mathbf{w}''| \Sigma_{\text{cg}}(|\mathbf{w}' - \mathbf{w}''|, m - m', m') \\
&\times N(\mathbf{r}, \mathbf{w}', m', t) N(\mathbf{r}, \mathbf{w}'', m - m', t). \tag{27}
\end{aligned}$$

This equation, together with (11) for small grains, constitutes the objective of this section. Nevertheless (27) is still a nonlinear equation; however, in (11), the quantity  $\widehat{N}(\mathbf{r}, \mathbf{w}, t)$ , defined by (12), is what is needed. We then integrate both sides of (27) with respect to  $m$ , obtaining after standard calculations

$$\begin{aligned}
\frac{\partial}{\partial t} \widehat{N}(\mathbf{r}, \mathbf{w}, t) &= -\mathbf{w} \cdot \nabla_{\mathbf{r}} \widehat{N}(\mathbf{r}, \mathbf{w}, t) \\
&- \int_{m_o}^{+\infty} dm \int_{m_o}^{+\infty} dm' \int_{|\mathbf{w}' - \mathbf{w}| < w_{\text{cr}}} d\mathbf{w}' |\mathbf{w}' - \mathbf{w}| \Sigma_{\text{cg}}(|\mathbf{w}' - \mathbf{w}|, m, m') \\
&\times N(\mathbf{r}, \mathbf{w}, m, t) N(\mathbf{r}, \mathbf{w}', m', t) \\
&+ \int_{m_o}^{+\infty} dm' \int_{m_o}^{+\infty} dm'' \int_{|\mathbf{w}' - \mathbf{w}''| < w_{\text{cr}}} d\mathbf{w}' |\mathbf{w}' - \mathbf{w}''| \Sigma_{\text{cg}}(|\mathbf{w}' - \mathbf{w}''|, m'', m') \\
&\times N(\mathbf{r}, \mathbf{w}', m', t) N(\mathbf{r}, \mathbf{w}'', m'', t), \tag{28}
\end{aligned}$$

where now  $\mathbf{w}'' = \mathbf{w} + m'(\mathbf{w} - \mathbf{w}')/m''$ , since we have used the substitution  $m'' = m - m'$ .

Note that the second and third term on the r.h.s. of (27) cancel each other, after integration with respect to  $m$ , because coagulation between small and large particles does not change  $\widehat{N}$ . We also remark that (28) is not an equation for the “unknown”  $\widehat{N}(\mathbf{r}, \mathbf{w}, t)$  because it involves also  $N(\mathbf{r}, \mathbf{w}, m, t)$ .

In the following section, we shall derive an approximate version of (28) involving only  $\widehat{N}$ .

### 5. An Approximate Procedure

If we assume, for simplicity, that  $w_{cr}$  does not depend on  $m$  and  $m'$  (which is coherent with the assumption that all  $b$ -particles coagulate when they interact) and that

$$\Sigma_{cg}(|\mathbf{w}' - \mathbf{w}|, m, m') \simeq \Sigma_{cg,o}/|\mathbf{w}' - \mathbf{w}|, \quad \Sigma_{cg,o} = const. ,$$

which corresponds to the so-called Maxwellian molecules for the classical Boltzmann equation [4]. With this assumption, (28) becomes

$$\begin{aligned} \frac{\partial}{\partial t} \widehat{N}(\mathbf{r}, \mathbf{w}, t) &= -\mathbf{w} \cdot \nabla_{\mathbf{r}} \widehat{N}(\mathbf{r}, \mathbf{w}, t) - \Sigma_{cg,o} \widehat{N}(\mathbf{r}, \mathbf{w}, t) \int_{|\mathbf{w}' - \mathbf{w}| < w_{cr}} d\mathbf{w}' \widehat{N}(\mathbf{r}, \mathbf{w}', t) \\ &+ \Sigma_{cg,o} \int_{m_o}^{+\infty} dm' \int_{m_o}^{+\infty} dm'' \int_{|\mathbf{w}' - \mathbf{w}''| < w_{cr}} d\mathbf{w}' N(\mathbf{r}, \mathbf{w}', m', t) N(\mathbf{r}, \mathbf{w}'', m'', t), \end{aligned} \quad (29)$$

recalling that  $\mathbf{w}'' = \mathbf{w} + m'(\mathbf{w} - \mathbf{w}')/m''$ .

Assume also that the collision mechanism of two  $b$ -particles is dominated by collisions between particles having almost the same mass, i.e.  $m' \simeq m'' \simeq m/2$ . Correspondingly, the momentum balance becomes:  $\mathbf{w}''/2 + \mathbf{w}'/2 = \mathbf{w}$ , and so  $\mathbf{w}'' - \mathbf{w}' = 2(\mathbf{w} - \mathbf{w}')$ . We then obtain from eq.(29)

$$\begin{aligned} \frac{\partial}{\partial t} \widehat{N}(\mathbf{r}, \mathbf{w}, t) &= -\mathbf{w} \cdot \nabla_{\mathbf{r}} \widehat{N}(\mathbf{r}, \mathbf{w}, t) - \Sigma_{cg,o} \widehat{N}(\mathbf{r}, \mathbf{w}, t) \int_{|\mathbf{w}' - \mathbf{w}| < w_{cr}} d\mathbf{w}' \widehat{N}(\mathbf{r}, \mathbf{w}', t) \\ &+ \Sigma_{cg,o} \int_{|\mathbf{w} - \mathbf{w}'| < w_{cr}/2} d\mathbf{w}' \widehat{N}(\mathbf{r}, \mathbf{w}', t) \widehat{N}(\mathbf{r}, 2\mathbf{w} - \mathbf{w}', t). \end{aligned} \quad (30)$$

The (rather rough) derivation of (30) is not important in itself. What is interesting is that (30) suggests the following approximate form of eq.(28)

$$\frac{\partial}{\partial t} \widehat{N}(\mathbf{r}, \mathbf{w}, t) = -\mathbf{w} \cdot \nabla_{\mathbf{r}} \widehat{N}(\mathbf{r}, \mathbf{w}, t) - \lambda [\widehat{N}(\mathbf{r}, \mathbf{w}, t)]^2, \quad (31)$$

where  $\lambda$  is a suitable non-negative constant. As shown in what follows, the solution of (31) gives some clue about the behavior of the density  $\widehat{N}$ . As far as  $\lambda$  is concerned, it should be chosen so that

$$\lambda \simeq -\left\{ -\Sigma_{\text{cg,o}} \widehat{N}(\mathbf{r}, \mathbf{w}, t) \int_{|\mathbf{w}'-\mathbf{w}|<w_{\text{cr}}} d\mathbf{w}' \widehat{N}(\mathbf{r}, \mathbf{w}', t) + \Sigma_{\text{cg,o}} \int_{|\mathbf{w}-\mathbf{w}'|<w_{\text{cr}}/2} d\mathbf{w}' \widehat{N}(\mathbf{r}, \mathbf{w}', t) \widehat{N}(\mathbf{r}, 2\mathbf{w} - \mathbf{w}', t) \right\} / [\widehat{N}(\mathbf{r}, \mathbf{w}, t)]^2. \quad (32)$$

Hence, if we assume that  $\widehat{N}$  is “almost independent” on  $\mathbf{w}$  (see Section 2) we have

$$\begin{aligned} \lambda &\simeq \Sigma_{\text{cg,o}} \int_{|\mathbf{w}'-\mathbf{w}|<w_{\text{cr}}} d\mathbf{w}' - \Sigma_{\text{cg,o}} \int_{|\mathbf{w}-\mathbf{w}'|<w_{\text{cr}}/2} d\mathbf{w}' \\ &= \Sigma_{\text{cg,o}} \left( \frac{4\pi}{3} w_{\text{cr}}^3 - \frac{4\pi}{3} \frac{w_{\text{cr}}^3}{8} \right) = \frac{7\pi}{6} \Sigma_{\text{cg,o}} w_{\text{cr}}^3. \end{aligned}$$

Since (31) (with  $\mathbf{r}$  substituted by  $\mathbf{r} + \mathbf{w}t$ ) becomes

$$\frac{d}{dt} \widehat{N}(\mathbf{r} + \mathbf{w}t, \mathbf{w}, t) = -\lambda [\widehat{N}(\mathbf{r} + \mathbf{w}t, \mathbf{w}, t)]^2, \quad (33)$$

integration, with the initial condition

$$\widehat{N}(\mathbf{r}, \mathbf{w}, 0) = \widehat{N}_0(\mathbf{r}, \mathbf{w}) = \int_{m_o}^{+\infty} N(\mathbf{r}, \mathbf{w}, m, 0) dm,$$

gives

$$\widehat{N}(\mathbf{r} + \mathbf{w}t, \mathbf{w}, t) = \frac{\widehat{N}_0(\mathbf{r}, \mathbf{w})}{1 + \lambda \widehat{N}_0(\mathbf{r}, \mathbf{w}) t}$$

and thus

$$\widehat{N}(\mathbf{r}, \mathbf{w}, t) = \frac{\widehat{N}_0(\mathbf{r} - \mathbf{w}t, \mathbf{w})}{1 + \lambda \widehat{N}_0(\mathbf{r} - \mathbf{w}t, \mathbf{w}) t} = \Phi(\mathbf{r}, \mathbf{w}, t). \quad (34)$$

Substitution of the integrals over  $m'$  of eq.(11) with  $\widehat{N}$ , given by (34), leads to a “reasonable” *linear* approximate equation for the density  $n(\mathbf{r}, \mathbf{v}, \mu, t)$  into eq.(11) itself, that is

$$\begin{aligned} \frac{\partial}{\partial t} n(\mathbf{r}, \mathbf{v}, \mu, t) &= -\mathbf{v} \cdot \nabla_{\mathbf{r}} n(\mathbf{r}, \mathbf{v}, \mu, t) \\ &- n(\mathbf{r}, \mathbf{v}, \mu, t) \int_{|\mathbf{v}-\mathbf{w}'|<v_{\text{cr}}} d\mathbf{w}' |\mathbf{v} - \mathbf{w}'| \sigma_{\text{cg}}(|\mathbf{v} - \mathbf{w}'|, \mu) \Phi(\mathbf{r}, \mathbf{w}', t) \\ &- n(\mathbf{r}, \mathbf{v}, \mu, t) \int_{\mathbb{R}^3} d\mathbf{v}' \int_{|\mathbf{v}-\mathbf{w}'|>v_{\text{cr}}} d\mathbf{w}' |\mathbf{v} - \mathbf{w}'| \sigma_{\text{s}}(\mathbf{v} \rightarrow \mathbf{v}', \mathbf{w}', \mu) \Phi(\mathbf{r}, \mathbf{w}', t) \end{aligned}$$

$$+ \int_{\mathbb{R}^3} d\mathbf{v}' \int_{|\mathbf{v}' - \mathbf{w}'| > v_{cr}} d\mathbf{w}' |\mathbf{v}' - \mathbf{w}'| \sigma_s(\mathbf{v}' \rightarrow \mathbf{v}, \mathbf{w}', \mu) \Phi(\mathbf{r}, \mathbf{w}', t) n(\mathbf{r}, \mathbf{v}', \mu, t). \quad (35)$$

We remark that (35) is linear as (18) and has the same mathematical structure. The only difference consists in the presence of the unknown function  $\Phi$  (instead of  $F$ ) which takes into account the dominant mechanism of coagulation between  $b$ -particles through the parameter  $\lambda$ .

We finally observe that a further approximate procedure on (35), similar to that leading to (31), might be used to derive a simpler equation for  $\hat{n}(\mathbf{r}, \mathbf{v}, t) = \int_0^{\mu^0} n(\mathbf{r}, \mathbf{v}, \mu, t) d\mu$ .

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