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Linear and nonlinear diffusion and reaction–diffusion equations from discrete-velocity kinetic models

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Abstract. Two-velocity kinetic models are used to derive, in the appropriate limit, the equations which govern the macroscopic density of fluid systems. Such equations are obtained from an asymptotic expansion in powers of a small parameter related to the microscopic mean free path. It is shown that the density of a fluid interacting with a non-equilibrium background satisfies a linear diffusion equation, and that the hierarchy of equations arising from the asymptotic expansion can be completely solved by a recursive scheme. For a system of interacting particles, a nonlinear diffusion equation is obtained and some of its solutions are analysed. Finally, the density of a system of particles undergoing chemical reactions is shown to satisfy a nonlinear equation which formally coincides with the reaction–diffusion equation proposed *ad hoc* at the macroscopic level.

1. Introduction

It is well known [1] that the linear diffusion equation (DE)

$$\partial_t n - D \nabla_x^2 n = 0 \quad (1.1)$$

which governs, for example, the evolution of the macroscopic density $n(\mathbf{x}, t)$ of an infinite set of Brownian particles diffusing in a background, can be derived in a proper limit from a more fundamental description level. This is usually performed from the Fokker–Planck kinetic equation

$$(\partial_t + \mathbf{v} \cdot \nabla_x) f(\mathbf{x}, \mathbf{v}, t) = \nu \nabla_v \cdot \left(\mathbf{v} + \frac{k_B T}{m} \nabla_v \right) f(\mathbf{x}, \mathbf{v}, t) \quad (1.2)$$

which determines the evolution of the distribution function $f(\mathbf{x}, \mathbf{v}, t)$ for a system of particles with mass m at temperature T , interacting with the background with a collision frequency ν . By scaling time and space according to $t \rightarrow t/\varepsilon^2$ and $\mathbf{x} \rightarrow \mathbf{x}/\varepsilon$, the DE, equation (1.1), is found to govern the evolution of $n = \int f d\mathbf{v}$ in the limit $\varepsilon \rightarrow 0$, with a diffusion coefficient $D = k_B T / \nu m$ [2, 3].

However, the Fokker–Planck equation is not the only kinetic model able to produce a DE at the macroscopic level. For instance, proper transition frequencies in the Boltzmann equation also describe a macroscopic diffusive behaviour [4]. In general, DEs are expected to arise from scaled kinetic equations of the type

$$(\varepsilon^2 \partial_t + \varepsilon \mathbf{v} \cdot \nabla_x) f(\mathbf{x}, \mathbf{v}, t) = (\partial_t f)_{\text{coll}} \quad (1.3)$$

where the explicit form of the collision operator $(\partial_t f)_{\text{coll}}$ is determined by the underlying kinetics. The small parameter ε defines interrelated *observation scales* on the spatial and temporal coordinates. In fact, ε is eliminated from (1.3) by defining the scaled variables $t' = t/\varepsilon^2$ and $x' = x/\varepsilon$. The limit $\varepsilon \rightarrow 0$ corresponds to interrelated *macroscopic* observation scales for space and time. In this limit, the density associated with the solution $f(x, v, t)$ to (1.3) should satisfy a DE.

The aim of this paper is to derive the DE and related macroscopic equations from some very simple kinetic models, namely, discrete-velocity models (DVMs). In fact, in the frame of DVMs, such derivations can be rigorously performed in a variety of situations of physical interest. In particular, it is possible to study some problems of nonlinear diffusion and to incorporate the effects of reaction processes (like chemical or nuclear reactions) which create or destroy particles.

In view of the high mathematical complexity which characterizes kinetic problems, DVMs [5] have been introduced as a reasonable simplification, preserving the main ingredients of realistic models, such as nonlinearity. Generally, they have been found to give an acceptable qualitative description of real systems. They were used to describe combustion phenomena [6], dynamics of shock waves [7, 8] and chemical reactions in diluted systems [9]. Furthermore, they have inspired the introduction of lattice gases [10], which play a fundamental role in the computational study of fluid dynamics.

In DVMs, it is considered that the velocity of each particle in the gas under study can adopt a value among a discrete set of previously fixed vectors $\{v_i\}_{i=1, \dots, N}$. The distribution function $f(x, v, t)$ reduces to a set of N *partial densities* $f_i(x, t)$, $i = 1, \dots, N$, so that the quantity $f_i(x, t) dx$ represents the number of particles with velocity v_i in the elementary volume dx around x , at time t . The evolution of each distribution function f_i is given by an equation of the type [11]

$$(\partial_t + v_i \cdot \nabla_x) f_i(x, t) = \sum_{j, m, n} [W(n, m \rightarrow i, j) f_n(x, t) f_m(x, t) - W(i, j \rightarrow n, m) f_i(x, t) f_j(x, t)] \quad (1.4)$$

where the summation indices run from 1 to N . The transition frequency $W(i, j \rightarrow n, m)$ indicates the probability per unit time for occurrence of the binary collision with incoming velocities v_i and v_j and outgoing velocities v_n and v_m . These probabilities are required to satisfy the *detailed balance* property, namely

$$W(i, j \rightarrow n, m) = W(n, m \rightarrow i, j) \quad (1.5a)$$

which stands for microscopic time-reversibility. If the interacting particles are of the same species, the transition frequencies also verify the symmetries

$$W(i, j \rightarrow n, m) = W(j, i \rightarrow n, m) = W(j, i \rightarrow m, n). \quad (1.5b)$$

A particular choice of the transition frequencies, satisfying (1.5a) and, eventually, (1.5b), specifies an *interaction model* and defines the explicit form of equations (1.4), to be solved with appropriate initial and boundary data.

In the simplest one-dimensional DVM, $N = 2$, and, without loss of generality, the velocities are taken to be $v_1 = -v$ and $v_2 = v$ [6, 7, 9]. The corresponding distribution functions are denoted by $f_-(x, t)$ and $f_+(x, t)$, respectively. In the case of binary interaction between identical particles, the general form of the kinetic equations (1.4) for two-velocity models is [12]

$$(\partial_t \pm v \partial_x) f_{\pm} = \pm [a_- f_-^2 + (a_+ - a_-) f_- f_+ - a_+ f_+^2] \quad (1.6)$$

where the positive constants a_{\pm} are directly related with the transition frequencies. Here, the analysis will be restricted to the Carleman interaction model [13], which takes $a_- = a_+$. This is the only two-velocity model satisfying the symmetry of *spatial inversion*. Observe that, independently of the values of a_{\pm} a particular stationary solution to equations (1.6) is given by $f_- = f_+ = n/2$, where n is the spatially homogeneous density associated with such an equilibrium state.

The general solution to equations (1.6) is not known, even though some exact similarity solutions have been found [14], and the boundary-free, spatially homogeneous problem can be solved generally [15]. Then, because of both the intrinsic mathematical interest and the potential applications of DVMs, it is relevant to develop methods for the analysis of the solutions to the related kinetic equations. In the following, it is shown that, in an appropriate limit, the particle density in a two-velocity model satisfies a diffusion-like (macroscopic) equation. According to the particular situation under study, different macroscopic equations are obtained and, eventually, solved. These equations suggest the type of evolution laws to be satisfied by the density field in more realistic models.

2. The diffusion equation

Diffusive behaviour is known to be exhibited by a dilute (guest) fluid immersed in a (host) background, when the interaction between guest particles and the effect of the guest species on the background dynamics are neglected. The evolution of the guest species is then driven by the interaction with the background, which is supposed to be in thermal equilibrium.

In order to introduce guest-background interaction in the frame of two-velocity kinetic models, equations (1.6) must be modified. Let the background be considered as a two-velocity species with velocities $\pm V$. The corresponding distribution functions, $F_{\pm}(x, t)$, satisfy a set of equations of the type (1.6). If the host medium is in its equilibrium state, $F_- = F_+ = N/2$, where N is the equilibrium background density.

Neglecting the guest-guest interaction, the *scaled* kinetic equations for the guest distribution functions, $f_{\pm}(x, t)$, are

$$(\varepsilon^2 \partial_t \pm \varepsilon v \partial_x) f_{\pm} = \pm [f_-(w_{-+} F_+ + w_{--} F_-) - f_+(w_{++} F_+ + w_{+-} F_-)] \tag{2.1}$$

where w_{ij} is the transition probability for the collision between a guest particle with velocity iv and a host particle with velocity jV , producing an outgoing guest particle with velocity $-iv$. The invariance under spatial inversion requires that $w_{++} = w_{--}$ and $w_{-+} = w_{+-}$. Since $F_- = F_+ = N/2$, equations (2.1) reduce to

$$(\varepsilon^2 \partial_t \pm \varepsilon v \partial_x) f_{\pm} = \pm \frac{wN}{2} (f_- - f_+) \tag{2.2}$$

with $w = w_{--} + w_{-+}$. At this point, it is convenient to introduce the ‘macroscopic’ density $n(x, t) = f_+(x, t) + f_-(x, t)$ and current $j(x, t) = v[f_+(x, t) - f_-(x, t)]$. For two-velocity models, the macroscopic description in terms of n and j is equivalent to the kinetic description in terms of the distribution functions. The evolution equations for the density and the current are

$$\varepsilon^2 \partial_t n + \varepsilon \partial_x j = 0 \tag{2.3a}$$

$$\varepsilon^2 \partial_t j + \varepsilon v^2 \partial_x n = -wNj. \tag{2.3b}$$

In (2.3a), one recognizes the (scaled) continuity equation.

The solutions to equations (2.3) in the limit $\varepsilon \rightarrow 0$ can be analysed by expanding n and j in powers of ε , namely

$$n(\mathbf{x}, t) = \sum_{i=0}^{\infty} \varepsilon^i n_i(\mathbf{x}, t) \quad (2.4)$$

$$j(\mathbf{x}, t) = \sum_{i=0}^{\infty} \varepsilon^i j_i(\mathbf{x}, t).$$

Entering these expansions in (2.3), one obtains

$$\sum_{i=2}^{\infty} \varepsilon^i \partial_t n_{i-2} + \sum_{i=1}^{\infty} \varepsilon^i \partial_x j_{i-1} = 0 \quad (2.5a)$$

$$\sum_{i=2}^{\infty} \varepsilon^i \partial_x j_{i-2} + \sum_{i=1}^{\infty} \varepsilon^i v^2 \partial_x n_{i-1} = -wN \sum_{i=0}^{\infty} \varepsilon^i j_i. \quad (2.5b)$$

For $i=0$ and $i=1$, these equations imply

$$j_0 = 0 \quad (2.6a)$$

and

$$\begin{aligned} \partial_x j_0 &= 0 \\ v^2 \partial_x n_0 &= -wN j_1 \end{aligned} \quad (2.6b)$$

respectively. For $i \geq 2$, instead, one has the hierarchy

$$\begin{aligned} \partial_t n_{i-2} + \partial_x j_{i-1} &= 0 \\ \partial_x j_{i-2} + v^2 \partial_x n_{i-1} &= -wN j_i. \end{aligned} \quad (2.6c)$$

Equation (2.6a) indicates that the macroscopic current j_0 (i.e. the value of j in the limit $\varepsilon \rightarrow 0$) vanishes, as expected for an isotropic diffusing system. Meanwhile, the spatial derivative of the second of equations (2.6b) can be combined with the first of equations (2.6c) for $i=2$, which provides the value of $\partial_x j_1$. This manipulation yields

$$\partial_t n_0 - \frac{v^2}{wN} \partial_x^2 n_0 = 0 \quad (2.7)$$

i.e. a *diffusion equation* to be satisfied by the macroscopic density n_0 . The diffusion coefficient $D = v^2/wN$, is proportional to the square modulus of the guest particle velocity v , which measures the kinetic energy—and, in some sense, the temperature—of the guest fluid. On the other hand, it is inversely proportional to the interaction rate w and the background density N . Indeed, an increase in its density or in the intensity of the interaction with the guest fluid would impede the transport of this latter species.

Higher order densities satisfy, in general, *inhomogeneous* DEs. In fact, combining the second of equations (2.6c) for the i th order with the first equation for the next order, one obtains

$$\partial_t n_i - D \partial_x^2 n_i = \partial_t \partial_x j_{i-1} \quad (2.8)$$

for $i \geq 1$. In particular, since $j_0 = 0$, the first-order density n_1 is also governed by (2.7).

The solutions for j_0 , n_0 and j_1 , as given by equations (2.6a), (2.6b) and (2.7), provide the initial step for calculating a given current order j_i from j_{i-2} and n_{i-1} through the second of equations (2.6c). The corresponding density order n_i is given by (2.8),

in terms of the previous current order j_{i-1} . This recursion scheme can then be used to formally obtain the *general* solution to the diffusion two-velocity problem, up to an arbitrary order in the expansion in powers of ϵ . Successive orders in that hierarchy determine corrections to the macroscopic behaviour governed by the DE, equation (2.7).

3. A nonlinear diffusion equation

The procedure introduced in section 2 can be applied to a more interesting situation, namely, the evolution of a self-interacting gas. In fact, the Carleman model, as stated by equations (1.6) with $a_- = a_+$, stands for the kinetics of a system of identical interacting particles. At the macroscopic level, this interaction should imply *nonlinear* features in the evolution of the system, which, in particular, should not be described by a linear DE like (2.7). Such a nonlinear macroscopic behaviour, defined in the sense of the scalings studied in section 2, will be hereafter referred to as *nonlinear diffusion*.

Taking $a_- = a_+ \equiv \omega/2$, equations (1.6) reduce to the Carleman kinetic equations, namely

$$(\partial_t \pm v \partial_x) f_{\pm} = \pm \frac{\omega}{2} (f_{-}^2 - f_{+}^2). \tag{3.1}$$

In terms of the density n and the current j , and with proper scalings in space and time, these equations become

$$\epsilon^2 \partial_t n + \epsilon \partial_x j = 0 \tag{3.2a}$$

$$\epsilon^2 \partial_t j + \epsilon v^2 \partial_x n = -\omega n j \tag{3.2b}$$

i.e. a continuity equation for n and a nonlinear evolution equation for j . Expanding the density and the current as in (2.4), the first two orders imply

$$j_0 = 0 \tag{3.3a}$$

$$v^2 \partial_x n_0 = -\omega n_0 j_1 \tag{3.3b}$$

so that, as in the linear diffusion case, the macroscopic state carries no current. For $i \geq 2$, one gets

$$\partial_t n_{i-2} + \partial_x j_{i-1} = 0 \tag{3.3c}$$

$$\partial_t j_{i-2} + v^2 \partial_x n_{i-1} = -\omega \sum_{k=0}^i n_k j_{i-k}.$$

The combination of (3.3b) and the first of equations (3.3c) with $i=2$, yields the following partial differential equation for the macroscopic density $n_0(x, t)$:

$$\partial_t n_0 - \frac{v^2}{\omega} \partial_x (n_0^{-1} \partial_x n_0) = 0 \tag{3.4}$$

i.e. a nonlinear diffusion equation. It corresponds to a DE with a density-dependent diffusion coefficient. $D(n_0) = v^2/\omega n_0$. As was found in the linear case, this diffusion coefficient is proportional to the square of particle velocity and inversely proportional to the collision frequency. The proportionality with the inverse of density can also be interpreted as in the linear case: high particle densities difficult diffusion.

The hierarchy of equations for densities and currents, equations (3.3), can be solved recursively by a straightforward extension of the scheme described at the end of section 2. The density orders are then governed by inhomogeneous diffusion-type equations, involving lower density and current orders. For example, the first order density $n_1(x, t)$ satisfies

$$\partial_t n_1 - \frac{v^2}{\omega} \partial_x (n_0^{-1} \partial_x n_1) + \frac{v^2}{\omega} \partial_x (n_0^{-2} n_1 \partial_x n_0) = 0. \quad (3.5)$$

Once n_0 is known, (3.5) is a *linear* DE for n_1 , with a drift term. The diffusion coefficient coincides with that encountered for the nonlinear DE (3.4). The drift term involves a 'velocity field' given by

$$u(x, t) \equiv \frac{v^2}{\omega} n_0^{-2} \partial_x n_0. \quad (3.6)$$

Since (3.4) is a non-standard DE, it is now worthwhile discussing its solutions [16]. Because of their physical interest, two similarity solutions are considered here. The first one, with a similarity variable of the type x/t , is

$$n_0(x, t) = (t - t_0)^{-1} \left[\eta_0^{-1} + \frac{\omega}{2v^2} \left(\frac{x - x_0}{t - t_0} \right)^2 \right]^{-1} \quad (3.7)$$

where x_0 , t_0 and $\eta_0 > 0$ are arbitrary constants. In particular, η_0 can be seen as the density for $x = x_0$ at time $t = t_0 + 1$. The right-hand side of (3.7) is positive and well defined for all $t > t_0$. For such values of t , $n_0(x, t)$ is a symmetric bell-shaped distribution, centred at $x = x_0$. Because of the prefactor $(t - t_0)^{-1}$, the total area under the curve is preserved for all times, as required by the conservation of the particle number. This area is $N = \pi(2v^2\eta_0/\omega)^{1/2}$, which provides a new interpretation for the constant η_0 in terms of the total number of particles present in the system.

It must be remarked that the width of $n_0(x, t)$ as a function of space grows *linearly* with t , namely, $\sigma \approx vt$. This result has to be confronted with the typical $(Dt)^{1/2}$ -behaviour of linear diffusion. In this sense, the solution to the nonlinear DE (3.4) cannot be considered to exhibit diffusive evolution. It exhibits, instead, *ballistic* behaviour. This difference between the evolution in linear and nonlinear diffusion could be interpreted as the macroscopic reflex of the different single-particle dynamics involved in each system at the very microscopic level.

The second solution to (3.4) to be considered here is a travelling wavefront, for which $n_0(x, t)$ depends on space and time through the combination $\xi = x - ct$. In terms of the new variable, (3.4) reads

$$cn_0' + \frac{v^2}{\omega} (n_0^{-1} n_0')' = 0 \quad (3.8)$$

where the primes indicate differentiation with respect to ξ . The general solution to (3.8) reads

$$n_0(\xi) = \frac{k}{c} (1 + K e^{-k\omega\xi/v^2})^{-1} \quad (3.9)$$

where k and K are two arbitrary integration constants. Physically meaningful solutions are obtained with $k/c > 0$ and $K > 0$. Equation (3.9) represents a step-shaped function which, for positive (negative) values of c , grows (decreases) from zero to k/c as ξ

varies from $-\infty$ to $+\infty$. In the original x, t coordinates, this wavefront moves in such a way that, for a fixed point x , the density decreases from k/c to zero.

The existence of a wavefront solution for the nonlinear DE (3.4) has to be seen as a new peculiarity with respect to the linear DE, entirely due to the nonlinear ingredient. Indeed, linear diffusion does not support (bounded) shape-preserving, travelling solutions.

In order to describe systems of interacting particles in the presence of a background medium, linear and nonlinear diffusion can be combined into a single equation. The collision term in the kinetic equations for such a situation is simply given by the sum of the collision terms describing each interaction process. In this case, from equations (2.2) and (3.1), one gets

$$(\partial_t \pm v\partial_x)f_{\pm} = \pm \frac{\omega}{2}(f_{-}^2 - f_{+}^2) \pm \frac{wN}{2}(f_{-} - f_{+}). \tag{3.15}$$

The macroscopic density $n_0(x, t)$ is found to satisfy the following nonlinear DE:

$$\partial_t n_0 - \frac{v^2}{\omega} \partial_x [(wN + \omega n_0)^{-1} \partial_x n_0] = 0 \tag{3.16}$$

with a diffusion coefficient $D(n_0) = v^2(wN + \omega n_0)^{-1}$. This equation reduces to the previously studied cases either for $wN \rightarrow 0$ or for $\omega \rightarrow 0$.

In order to seek for solutions to (3.16), one can first observe that a redefinition of the unknown as $\omega \hat{n}_0 = wN + \omega n_0$ reduces the equation to (3.4) for \hat{n}_0 and, therefore, provides a solution of the type (3.7). In the second place, (3.16) admits also a set of travelling wavefront solutions. However, all these solutions prove to be negative on some intervals of x and t , and, in consequence, they are not physically meaningful. To the author's knowledge, the problem of finding a non-negative solution to (3.16), which would clarify the interplay between linear and nonlinear diffusion, remains open.

It is interesting to note that nonlinear diffusion equations of the type (3.4), which are used to describe transport processes in population dynamics [17], have been proven to exhibit solutions with non-diffusive behaviour, as in (3.7). In particular, it is shown in [17] that for a density-dependent diffusion coefficient $D(n) \propto n^k$ (with $k > 0$), there exist a similarity solution whose width grows as $t^{1/(2+k)}$. According to the results obtained here, (3.7), this scaling holds also for $k = -1$. Such nonlinear diffusion equations are also known to have wavefront similarity solutions.

As in the case of gas kinetics, the nonlinear character of the equations, which gives place to pathological solutions of the types studied here, is due to the interaction of the system components. Furthermore, in population dynamics, processes in which these components are created or destroyed play a fundamental role. Such processes are also found in gas kinetics, when chemical or other reaction events are present. An extension of the formalism studied so far to the case where reaction processes occur, is presented in the next section.

4. The reaction-diffusion equation

Because of its intrinsic mathematical interest and its relevance in some applications, much attention has been paid in recent years to the interaction between transport and reaction processes [18]. At the macroscopic level, this interaction has been usually

modelled by means of the so called reaction-diffusion equations (RDEs), which govern the macroscopic density $n(\mathbf{x}, t)$ of a system of particles undergoing Brownian motion and subject to events where particles are created or destroyed. These models have provided insight on the complex dynamics of pattern formation, oscillations and self-organization in chemical kinetics.

For a single-species system, the RDE is typically written as

$$\partial_t n - D \partial_x^2 n = F(n) \quad (4.1)$$

where the function $F(n)$ stands for the contribution of reaction processes to the evolution of the density. For chemical reactions, the form of $F(n)$ is given by the mass-action law of chemical kinetics: $F(n)$ is a polynomial in the density, whose coefficients depend on the reaction rates and on the densities of other mediating species (whose evolution is not taken into account).

Modelling reaction processes at the microscopic level provides a derivation of RDEs from a more fundamental stage. In fact, it is known that if appropriate reaction terms are added to the kinetic equations with a scaling of order ε^2 [19], the asymptotic expansion in powers of ε provides for the zeroth-order density a RDE coinciding with that proposed *ad hoc* at the macroscopic level [20].

Consider then a guest species X diffusing in an equilibrium background, whose particles undergo a chemical reaction of the type



where the mediating species A and B represent, in general, a set of chemical species whose evolution is given from outside of the system. Equations (2.2) are generalized to

$$(\varepsilon^2 \partial_t \pm \varepsilon v \partial_x) f_{\pm} = \pm \frac{wN}{2} (f_- - f_+) + \varepsilon^2 R_{\pm}^{(r)}(f_-, f_+) \quad (4.3)$$

including the effects of reaction (4.2) through the operators $R_{\pm}^{(r)}$. The superindex r stands for the number of incoming particles involved in the reaction. If the system undergoes a set of reactions of type (4.2), the corresponding reaction operators are simply added to the RHS of the kinetic equations. Therefore, it is sufficient to consider a single reaction, as in (4.3).

The most general form for the operators $R_{\pm}^{(r)}$ must take into account all the velocity combinations of r interacting guest particles, and can be written as

$$R_{\pm}^{(r)}(f_-, f_+) = \sum_{k=0}^r \alpha_{\pm}^{(r,k)} f_{\pm}^k f_{\mp}^{r-k} \quad (4.4)$$

where the coefficients $\alpha_{\pm}^{(r,k)}$ measure the contribution of each velocity combination to the reaction. In general, the sign of $\alpha_{\pm}^{(r,k)}$ indicates whether particles are created or destroyed by the chemical process. In order to preserve the symmetry under spatial inversion, these coefficients must satisfy the relation

$$\alpha_{-}^{(r,k)} = \alpha_{+}^{(r,r-k)}. \quad (4.5)$$

The continuity and the current equations read now

$$\varepsilon^2 \partial_t n + \varepsilon \partial_x j = \varepsilon^2 [R_{+}^{(r)} + R_{-}^{(r)}] \quad (4.6a)$$

$$\varepsilon^2 \partial_x j + \varepsilon v^2 \partial_x n = -wNj + \varepsilon^2 v^2 [R_{+}^{(r)} - R_{-}^{(r)}]. \quad (4.6b)$$

In terms of n and j the sum and the difference of the reaction operators, as appearing

in (4.6), result

$$R_+^{(r)} \pm R_-^{(r)} = 2^{-r} \sum_{k=0}^r [\alpha_+^{(r,k)} \pm \alpha_-^{(r,k)}] \sum_{q=0}^k \sum_{s=0}^{r-k} \binom{k}{q} \binom{r-k}{s} n^{q+s} \left(\frac{j}{v}\right)^{r-q-s}. \quad (4.7)$$

The highly nonlinear character of the RHS of (4.6) inhibits the full explicit expansion in powers of ε . However, for the first few orders in the hierarchy, it is possible to find

$$j_0 = 0 \quad (4.8a)$$

$$v^2 \partial_x n_0 = -wNj_1 \quad (4.8b)$$

$$\partial_t n_0 + \partial_x j_1 = 2^{-r} v^2 n_0^r \sum_{k=0}^r [\alpha_+^{(r,k)} + \alpha_-^{(r,k)}]. \quad (4.8c)$$

Again, the macroscopic state is characterized by a vanishing current. This fact implies that, in the expansion of the reaction operators $R_{\pm}^{(r)}$, the terms involving successive powers of j_0 vanish, except for the zeroth power. In the first expansion order, this power multiplies the r th power of n_0 , producing the reaction term displayed in (4.8c). Combining this equation with (4.8b), which provides the value of j_1 , yields the RDE

$$\partial_t n_0 - \frac{v^2}{wN} \partial_x^2 n_0 = 2^{-r} v^2 n_0^r \sum_{k=0}^r [\alpha_+^{(r,k)} + \alpha_-^{(r,k)}] \equiv \alpha^{(r)} n_0^r \quad (4.9)$$

to be satisfied by the macroscopic density $n_0(x, t)$.

For a system undergoing a set of chemical reactions of type (4.2), with various values of r , $n_0(x, t)$ is governed by a RDE in which the reaction term is given by the sum of the contributions due to each reaction, namely

$$\partial_t n_0 - \frac{v^2}{wN} \partial_x^2 n_0 = \sum_r \alpha^{(r)} n_0^r. \quad (4.10)$$

Formally, this equation coincides with the RDE proposed *ad hoc* for describing the evolution of the macroscopic density. A full identification between both RDEs is easily achieved by relating the coefficients $\alpha_{\pm}^{(r,k)}$ with the reaction rates and the densities of mediating species.

It is worthwhile to stress that a RDE for the zeroth-order density n_0 is obtained *only* in the case in which reaction terms are weighted by ε^2 [20]. In fact, if, for instance, one chooses to intensify the effects of chemical reactions by scaling reaction terms with ε , the asymptotic expansion yields, in the limit $\varepsilon \rightarrow 0$, the equation

$$\sum_r \alpha^{(r)} n_0^r = 0. \quad (4.11)$$

This algebraic equation represents, precisely, chemical equilibrium, so that the macroscopic behaviour of the system is dominated by chemical kinetics.

On the other hand, if chemical processes are weakened by a scaling ε^3 or even higher power of ε , the macroscopic density satisfies the linear DE, equation (2.7), and the effects of chemical reaction, in the form of the reaction terms of (4.10), shift to higher-order densities.

5. Conclusion

It has been shown that introducing appropriate scalings for space and time in the simplest discrete-velocity kinetic models, namely, one-dimensional two-velocity models, yields macroscopic diffusion equations for the particle density, whose forms depend on the underlying kinetic processes. An asymptotic expansion in powers of the (small) scaling parameter, provides a set of equations to be satisfied by the successive density and current orders, among which the lowest order represents precisely the density and the current observed at macroscopic level.

The linear diffusion equation has been obtained for the macroscopic density of a fluid system interacting with a background medium. In this situation, the kinetic equations are linear, as well as each order in the hierarchy of equations arising from the asymptotic expansion of density and current. In particular, every density order satisfies an inhomogeneous linear diffusion equation, except for the two first orders, which exhibit purely diffusive behaviour. The linear character of the set of equations makes it possible to solve the whole hierarchy up to an arbitrary order by means of a recursive scheme, once appropriate initial and boundary conditions have been fixed.

Linear diffusion has been used as a test situation for evaluating the possibility of deriving, in the proper limit, diffusive evolution from discrete-velocity kinetic models. In a more interesting situation, namely, a system of binary-interacting particles, it was shown that the macroscopic density satisfies a nonlinear diffusion equation with a density-dependent diffusion coefficient, $D \sim n^{-1}$. It can be conjectured that this nonlinear diffusion equation governs the density of more complex models of binary-interacting particle systems. Even when the general solution to this equation seems to be unknown, two physically relevant solutions have been identified. The first one corresponds to a bell-shaped density distribution, whose width grows linearly with time. This ballistic behaviour has to be compared with the $t^{1/2}$ -dependence of the distribution width obtained for linear diffusion. The second solution studied here corresponds to a class of travelling wavefront density, which has no parallel in the linear diffusion case. In fact, it is the nonlinear character of (3.4) that supports the existence of such a solution.

The combination of linear diffusion in a background and binary interaction yields a generalized nonlinear diffusion equation, for which, unfortunately, no physically acceptable solution has been found. It is worthwhile to stress that having at least one solution to this equation could help to clarify the relevant problem of interplay between linear and nonlinear diffusion.

Finally, reaction-diffusion equations have been obtained for the macroscopic density of a system undergoing reaction processes, in which particles are created or destroyed. For two-velocity models, it was possible to write the reaction terms to be added to the kinetic equations in full generality, i.e. considering all the possible microscopic collisions involving a given number of particles (equation (4.4)). The reaction-diffusion equations obtained from the asymptotic expansion coincide with those proposed *ad hoc* at the macroscopic level to describe the evolution of the density. Such a result agrees with those of [20], where it is shown that macroscopic reaction-diffusion equations arise from some more complex kinetic models for reaction processes. As well as in the case of linear diffusion, this suggest that the macroscopic behaviour exhibited by discrete-velocity models accurately imitates that of more realistic systems. As conjectured before, this conclusion is also expected to apply within more complicated situations as, for instance, nonlinear diffusion.

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