Singular perturbation techniques in the study of a diatomic gas with reactions of dissociation and recombination

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Abstract

Model equations for the description of chemical reactions of dissociation and recombination through a transition state constitute necessarily singular perturbation problems because of the very short lifetime of the excited molecules, compared to all other characteristic times. Asymptotic solutions are derived and tested versus an accurate numerical solution by resorting to different expansion algorithms, taking initial layer corrections into account. Since the singular problem turns out to be also singularly perturbed, techniques like Hilbert and Chapman–Enskog expansions, typical of the Boltzmann equation for gas kinetic theory, have been considered. The simple stationary state approximation, very popular in chemistry, is shown to provide very good results out of the initial layer if equipped with the proper initial conditions, as obtained from the present analysis.

Key words: Dissociation/recombination reactions, singular perturbation problems, asymptotic expansions, initial layer corrections

1 Introduction

Kinetic theory is being used significantly in last half century in order to understand evolution problems involving chemical reactions. Among the many contributions related to chemically reacting gas flows we may quote a pioneering work like [1] and some recent papers by the authors [2,3] where an extensive bibliography is given. In this respect, recombination/dissociation reactions are very important in the world of applications, but

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quite difficult to deal with from a kinetic point of view, and only few approaches are available in the literature, at least to our knowledge. They are based on either three-body collisions [4], or on a sequence of two-body collisions according to the transition-state theory [5]. It is just along the latter line that a Boltzmann-type model has been proposed in [6] for a mesoscopic description of a diatomic gas, considered as a three species mixture of atoms A (mass $m$), stable molecules $A_2$, and unstable molecules $A_2^*$ (labeled in the sequel by indices 0,1,2, respectively).

A key point of the model is that the third species plays the role of a transition state, created by atom-atom collisions only, and does not survive to any interaction. Since the mean collision times of the unstable molecules are assumed to be much shorter than all other interaction times, the $A_2^* - A_2^*$ encounters may be neglected, and the mathematical problem is affected intrinsically by at least one small parameter, which makes the problem itself of singular perturbation type. It was possible to derive in [6], from the kinetic formulation, both conservation and moment equations at the macroscopic level. The essential step of a closure strategy was also addressed, and indeed self-consistent fluid dynamics equations were obtained either in some simplified physical situations, or in general in the asymptotic limit when the small parameter tends to zero. We shall consider here for simplicity the case of an isothermic reaction in a thermal bath in space homogeneous conditions, when the effective collision frequencies $\nu_{ij}^\alpha$ for an $i - j$ encounter of type $\alpha$ are constant (see [6] for details). In this case the evolution is simply described by a set of three ordinary differential equations for the densities $n_i$. Such a dynamical system retains the essential features of the singular perturbation problem. In particular the problem may be classified as singularly perturbed [7], or as a singular singular perturbation problem [8], since the dominant part of the collision operator has infinite null points, or, in other words, since the reduced problem obtained for vanishing small parameter has an infinity of solutions. This peculiar feature is shared by other important perturbation problems, like derivation of the hydrodynamic limit from the classical Boltzmann equation [9], and in that frame a famous asymptotic expansion, bearing the name of Hilbert, was devised.

In this paper some singular perturbation methods suitable for the presented problem are illustrated, aiming at deriving and comparing approximate analytical solutions. The quite usual assumption of quasi steady-state for the excited species [10], considered already in [6], is taken into account. This is called stationary–state approximation, and represents the simplest approach for applications, but ignores completely the initial layer, and thus needs to be equipped with proper (fictitious) initial conditions in order to provide an accurate description outside the initial layer (the so called bulk region). The singular perturbation analysis presented here has been inspired also by this problem of determining the appropriate initial conditions for such widely used approximation.

The paper is organized as follows. The physical problem and the governing equations to be studied are presented and discussed in Section 2, together with the quasi steady–state approach. The following Section deals with the derivation of an analytical solution, first order approximation with respect to the small parameter, in the spirit of the Hilbert asymptotic expansions. We apply the well know O’Malley-Hoppensteadt procedure [8,11]
in which the solution is sought as a superposition of an outer expansion and an inner expansion, the latter vanishing when time tends to infinity. The inner components involve the stretched time variable and accounts for initial layer corrections. Section 4 is devoted to the reduction of the same set of equations to a regular singular perturbation problem [8], with appearance of slowly varying dependent variables, and to the exploitation of a different asymptotic procedure. More specifically, the kernel of the dominant part of the collision operator allows to introduce suitable projection operators which split the solution as the sum of an hydrodynamic and of a kinetic part [7], with the former showing a slow evolution. The equivalent singular perturbation problem leads of course, by standard asymptotic expansion, to the same approximate solutions as before, but lends itself to a different asymptotic treatment, which shares the same features of the Chapman-Enskog expansion of kinetic theory [9]. It consists in leaving the outer component of the hydrodynamic part of the solution unexpanded with respect to the small parameter, and it leads to a modified (compressed) asymptotic solution, as proposed in [12] and worked out in detail in [7]. Finally numerical comparison of the various approximate solutions is presented in Section 5, in order to emphasize the different trends of the error in the different approaches.

2 The model equations and the stationary-state approximation

According to the adopted physical model, formation of stable molecules $A_2$ from atoms $A$ occurs in two steps according to two irreversible bimolecular chemical reactions. The first is a recombination process $A + A \rightarrow A_2^*$, labelled by superscript $\alpha = r$, while the second is an inelastic scattering ($\alpha = i$) $A_2^* + P \rightarrow A_2 + P$, where $P$ is either $A$ or $A_2$, and where the excitation energy is transformed into extra kinetic energy of the products (exothermic process). The inverse reaction of dissociation occurs in turn via two possible irreversible bimolecular reactions, both with $\alpha = d$, namely $A_2 + P \rightarrow 2A + P$ and $A_2^* + P \rightarrow 2A + P$. Reaction rates for a binary $i - j$ encounter of type $\alpha$ are expressed in terms of microscopic collision frequencies $\nu_{ij}^\alpha$ (relative speeds times cross sections [9]). Elastic scattering between any pair of species is also allowed. Without entering the physical details, for which the interested reader is referred to [6], the simplest possible case for an analytical manipulations is the one described in the Introduction, in which the evolution of the densities $n_i$ is governed by a self-consistent three-dimensional dynamical system, reading as

\[
\begin{align*}
\dot{n}_0 &= -2 \nu_{00}^r n_0^2 + 2 \nu_{01}^d n_0 n_1 + 2 \nu_{11}^d n_1^2 + 2 \nu_{02}^d n_0 n_2 + 2 \nu_{12}^d n_1 n_2 \\
\dot{n}_1 &= -\nu_{01}^d n_0 n_1 - \nu_{11}^d n_1^2 + \nu_{02}^d n_0 n_2 + \nu_{12}^d n_1 n_2 \\
\dot{n}_2 &= - (\nu_{02}^d + \nu_{02}^i) n_0 n_2 - (\nu_{12}^d + \nu_{12}^i) n_1 n_2 + \nu_{00}^r n_0^2.
\end{align*}
\]
Indeed the set (1) is of clear phenomenological interpretation; the vector field on the right hand side represents the collision operator, and the quadratic nonlinearities reflect the fact that all collisions are binary. Initial conditions are taken of the form
\[
  n_0(0) = a \quad n_1(0) = b \quad n_2(0) = c,
\]
and it is easy to see that (1) implies \(\dot{n}_0 + 2\dot{n}_1 + 2\dot{n}_2 = 0\), which quantifies the obvious physical requirement that the total mass is constant, since it is conserved in all underlying reactions. More explicitly
\[
  n_0 + 2n_1 + 2n_2 = a + 2b + 2c = \rho. 
\]

Due to the presence of unstable molecules \(A^*_2\), all collision frequencies \(\nu^{a}_{k2}\), \(k = 0, 1\), in (1) are much larger than any of the \(\nu^{a}_{kl}\), \(k, l = 0, 1\). We may introduce a typical density \(n\), typical slow and fast collision frequencies \(\nu\) and \(\nu^*\), with \(\nu/\nu^* = \epsilon \ll 1\), and then we can measure densities in units of \(n\) \((\bar{n}_i = n_i/n)\), frequencies \(\nu^{a}_{kl}\), \(k, l \neq 2\) in units of \(\nu\) \((\bar{\nu}^{a}_{kl} = \nu^{a}_{kl}/\nu)\), frequencies \(\nu^{a}_{k2}\) in units of \(\nu^*\) \((\bar{\nu}^{a}_{k2} = \nu^{a}_{k2}/\nu^*)\), and time in units of \(n\nu^{-1}\). Such adimensionalization yields a dimensionless dynamical system which differs from (1) only in that the \(\nu^{a}_{k2}\) coefficients are affected by a “large” factor \(1/\epsilon\). We are led thus, as anticipated, to a singular perturbation problem [8,13–15]. With the usual abuse of notation we remove now all tildas. Moreover, we take advantage of (3) in order to reduce the dimensionality of the problem by eliminating \(n_0\). In this way, mass conservation is exactly taken care of “a priori”, before introducing any approximation techniques. There results
\[
  \begin{cases}
    \dot{n}_1 = A_1(n_1, n_2) + \frac{1}{\epsilon} B_1(n_1, n_2) \\
    \dot{n}_2 = A_2(n_1, n_2) + \frac{1}{\epsilon} B_2(n_1, n_2),
  \end{cases}
\]
where the vectors \(\mathbf{A} = (A_1, A_2)\) and \(\mathbf{B} = (B_1, B_2)\) represent respectively the non-dominant and the dominant part of the collision operator. They are given by
\[
  A_1 = (2\nu^{d}_{01} - \nu^{d}_{11})n_1^2 + 2\nu^{d}_{01}n_1n_2 - \rho\nu^{d}_{01}n_1 \\
  A_2 = 4\nu^{r}_{00}n_1^2 + 8\nu^{r}_{00}n_1n_2 + 4\nu^{r}_{00}n_2^2 - 4\rho\nu^{r}_{00}n_1 - 4\rho\nu^{r}_{00}n_2 + \nu^{r}_{00}\rho^2
\]
and
\[
  B_1 = -(2\nu^{i}_{02} - \nu^{i}_{12})n_1n_2 - 2\nu^{i}_{02}n_2^2 + \rho\nu^{i}_{02}n_2 \\
  B_2 = (2\nu^{d}_{02} + 2\nu^{d}_{02} - \nu^{d}_{12} - \nu^{d}_{12})n_1n_2 + 2(\nu^{d}_{02} + \nu^{d}_{02})n_2^2 - \rho(\nu^{d}_{02} + \nu^{d}_{02})n_2.
\]
The phase space for the set (4) of ODE is the triangle of the \((n_1, n_2)\) plane defined by the inequalities \(0 \leq n_1 \leq \rho/2, 0 \leq n_2 \leq \rho/2, n_1 + n_2 \leq \rho/2\). Fixed points for (4) have been determined in [6]. There is indeed a unique equilibrium internal to the phase space, determined by a suitable transcendental equation (representing mass action law for the chemical process). Moreover, another equilibrium exists on the border, given by \(n_1 = 0, n_2 = \rho/2\), but it will be excluded from any further consideration since it corresponds to the completely unphysical situation of absence of any atom and of any stable molecule. Its formal existence in the model is due to the fact that other de-excitation channels have been disregarded. Anyhow, even from a mathematical point of view, it turns out to be unstable [6]. We will assume then from now on that \(n_0 + n_1 > 0\), i.e. \(n_1 + 2n_2 < \rho\). The singular perturbation problem (4) is also singularly perturbed [7]. In fact the limiting equations \(B_1 = 0, B_2 = 0\) admit evidently at least the \(\infty^1\) solutions \(n_2 = 0, n_1\) arbitrary. The kernel of the dominant operator \(B\) is infinite-dimensional, whereas any positive value of \(\epsilon\) implies a single null point for the full operator \(B + \epsilon A\). Asymptotic methods will be applied later for an approximate solution of this singular singular problem. In order to keep all manipulations analytical, all dimensionless collision frequencies will be set in the sequel equal to unity. Then (5) and (6) become

\[
A_1 = n_1^2 + 2n_1 n_2 - \rho n_1
\]

\[
A_2 = 4n_1^2 + 8n_1 n_2 + 4n_2^2 - 4\rho n_1 - 4\rho n_2 + \rho^2
\]

and

\[
B_1 = n_2(\rho - n_1 - 2n_2)
\]

\[
B_2 = -2n_2(\rho - n_1 - 2n_2).
\]

For later use, we report here on the fixed points for this special option. From (1), after excluding the unphysical point \((0, 0, \rho/2)\), we get

\[
n_2 = \frac{n_0^2}{2(n_0 + n_1)\epsilon}
\]

plus the algebraic equation \(n_0^2 - 2n_0 n_1 - 2n_1^2 = 0\), with unique admissible root \(n_0 = n_1(1 + \sqrt{3})\). Upon taking into account the first integral (3), the unique fixed point is then explicitly given by

\[
n_0^* = \frac{1 + \sqrt{3}}{3 + \sqrt{3} + 2\epsilon} \rho \quad n_1^* = \frac{1}{3 + \sqrt{3} + 2\epsilon} \rho \quad n_2^* = \frac{\epsilon}{3 + \sqrt{3} + 2\epsilon} \rho.
\]
In the limiting case $\epsilon = 0$ the point (10) collapses to \( \left( \frac{\rho}{\sqrt{3}}, \frac{\rho}{3 + \sqrt{3}}, 0 \right) \), but fixed points of (1) degenerate, since the only equation \((n_0 + n_1)n_2 = 0\) is left. Having assumed \(n_0 + n_1 > 0\), this is solved actually by (and only by) the $\infty^1$ solutions
\[
n_0 = \rho - 2n_1, \quad n_1 \text{ arbitrary}, \quad n_2 = 0.
\] (11)

The simplest algorithm for a possible approximate analytical solution of problem (1) is provided by the very well known and widely used stationary-state approximation [10], as discussed already in [6]. It amounts to a quasi steady-state assumption on the excited species, which reduces the dimension of the dynamical system by one since the very beginning. It is physically motivated by the fact that, if \(\nu_{k_2}\) collision frequencies are very large, the third species adjusts almost immediately to the collision equilibrium in which the loss rate compensates instantaneously the gain rate due to recombination. From the standpoint of analytical manipulations, if \(\tilde{n}_2 = n_2/\epsilon\) is used instead of \(n_2\) in the dimensionless version of (1), \(\epsilon\) disappears from the first two equations, and is left in the third only as a factor in front of \(\tilde{n}_2\). Therefore, taking the limiting case \(\epsilon = 0\), it reproduces exactly the stationary-state approximation. In any case, this approximation consists quantitatively in setting the third component of the vector field in (1) equal to zero, which yields at once a linear algebraic equation for \(n_2\), solved by (9). This value of \(n_2\) is necessarily $O(\epsilon)$, and is used in the remaining equations. It is clear that this procedure ignores completely the initial layer and can supply only an outer component hopefully fitting the exact solution in the bulk region. In this respect it is remarkable that it prescribes relaxation to the exact equilibrium, since the approximation does not affect the collision terms. However, the stationary-state algorithm is not self-consistent, in the sense that the proper (fictitious) initial conditions to be applied can not be deduced in terms of the actual initial conditions by the algorithm itself.

In order to make this approximation explicit, we start from (4) with \(n_0\) expressed by the first integral (3). We get
\[
n_2 = \frac{(\rho - 2n_1 - 2n_2)^2}{2(\rho - n_1 - 2n_2)} \epsilon,
\] (12)

and the resulting quadratic equation for \(n_2\) has only one admissible solution
\[
n_2 = \frac{\rho - n_1 + 2\epsilon(\rho - 2n_1) - \sqrt{(\rho - n_1)^2 + 4\epsilon n_1(\rho - 2n_1)}}{4(1 + \epsilon)},
\] (13)

to be used in the first of (4). In this way the dynamical system collapses to the single first order autonomous equation for \(n_1\).
\[ \begin{align*}
\dot{n}_1 &= \frac{7 - 6\epsilon - 4\epsilon^2}{4(1 + \epsilon)^2} n_1^2 - \frac{3\rho}{2(1 + \epsilon)^2} n_1 + \frac{\rho - (5 + 2\epsilon)n_1}{4(1 + \epsilon)^2} \sqrt{(\rho - n_1)^2 + 4\epsilon n_1(\rho - 2n_1)} \\
&\quad + \frac{\rho^2}{4(1 + \epsilon)^2},
\end{align*} \] (14)

which is amenable to quadrature, and can be solved numerically without any problem. It is easy to check that the right hand side of (14) vanishes for \( n_1 = n_1^* \) as given by (10). Of course, no information is available on the effective initial conditions for such stationary-state equation, but this will be obtained as a byproduct from the singular perturbation methods proposed in the next Sections, which will provide a detailed and mathematically appropriate analysis of the initial layer.

### 3 Hilbert expansion

The first perturbation method we present is based on the Hilbert expansion. We consider the singular and singularly perturbed problem (4), rewritten as

\[ \begin{align*}
\epsilon \frac{dn_1}{dt} &= f_1(n_1, n_2, \epsilon) = \epsilon (n_1^2 + 2n_1n_2 - \rho n_1) - n_1 n_2 - 2n_2^2 + \rho n_2 \\
\epsilon \frac{dn_2}{dt} &= f_2(n_1, n_2, \epsilon) = \epsilon (4n_1^2 + 8n_1n_2 + 4n_2^2 - 4\rho n_1 - 4\rho n_2 + \rho^2) + \\
&\quad + 2n_1n_2 + 4n_2^2 - 2\rho n_2
\end{align*} \] (15)

with initial conditions

\[ n_1(0) = b, \quad n_2(0) = c, \] (16)

and we determine an asymptotic solution, uniformly valid with respect to time, by following the classical Hilbert expansion method which is often applied in kinetic theory for the asymptotic treatment of the Boltzmann equation [9].

The solution is sought in the composite form

\[ \begin{align*}
n_1(t, \epsilon) &= n_1^o(t, \epsilon) + n_1^i(\tau, \epsilon) \\
n_2(t, \epsilon) &= n_2^o(t, \epsilon) + n_2^i(\tau, \epsilon)
\end{align*} \] (17)

as the sum of an outer (or bulk) solution and of an inner initial layer correction, depending on the stretched time variable \( \tau = t/\epsilon \), which turns out to be the distinguished limit for this problem [15], and vanishing as \( \tau \to +\infty \). This approach is equivalent to resorting to the matching principle [14], which would provide the same results.
It is assumed that $n_{1,2}^0$, $n_{1,2}^i$ and the functions $f_1$, $f_2$ can be expanded in power series of the small parameter $\epsilon$

\begin{align}
n_1^0 &\sim \sum_k \epsilon^k n_{1k}(t), \quad n_1^i \sim \sum_k \epsilon^k N_{1k}(\tau) \\
n_2^0 &\sim \sum_k \epsilon^k n_{2k}(t), \quad n_2^i \sim \sum_k \epsilon^k N_{2k}(\tau) \tag{18}
\end{align}

\begin{align}
f_1(n_1, n_2, \epsilon) &\sim \sum_k \epsilon^k f_{1k}(n_1, n_2), \quad f_{1k} = \frac{1}{k!} \left( \frac{d^k f_1}{d\epsilon^k} \right)_{\epsilon=0} \\
f_2(n_1, n_2, \epsilon) &\sim \sum_k \epsilon^k f_{2k}(n_1, n_2), \quad f_{2k} = \frac{1}{k!} \left( \frac{d^k f_2}{d\epsilon^k} \right)_{\epsilon=0} \tag{19}
\end{align}

such that the terms in series (18) satisfy the initial conditions

\begin{align}
n_{10}(0) + N_{10}(0) &= b \\
n_{20}(0) + N_{20}(0) &= c \tag{20}
\end{align}

\begin{align}
n_{1k}(0) + N_{1k}(0) &= 0 \\
n_{2k}(0) + N_{2k}(0) &= 0, \quad k = 1, 2, \ldots \tag{21}
\end{align}

The outer solution is requested to satisfy (15) for every $t > 0$

\[ \begin{align*}
\epsilon \frac{dn_1^0}{dt} &= f_1(n_1^0, n_2^0, \epsilon) \\
\epsilon \frac{dn_2^0}{dt} &= f_2(n_1^0, n_2^0, \epsilon)
\end{align*} \tag{22} \]

and this implies that the initial layer correction must be the asymptotically vanishing solution of

\[ \begin{align*}
\frac{dn_1^i}{d\tau} &= f_1[n_1^i(\epsilon\tau, \epsilon) + n_1^i(\tau, \epsilon), n_2^i(\epsilon\tau, \epsilon) + n_2^i(\tau, \epsilon), \epsilon] - f_1[n_1^0(\epsilon\tau, \epsilon), n_2^0(\epsilon\tau, \epsilon), \epsilon] \\
\frac{dn_2^i}{d\tau} &= f_2[n_1^i(\epsilon\tau, \epsilon) + n_1^i(\tau, \epsilon), n_2^i(\epsilon\tau, \epsilon) + n_2^i(\tau, \epsilon), \epsilon] - f_2[n_1^0(\epsilon\tau, \epsilon), n_2^0(\epsilon\tau, \epsilon), \epsilon].
\end{align*} \tag{23} \]

By inserting the expansions (18) and (19) into equations (22) and (23) and by equating the terms with the same power in $\epsilon$, we obtain a sequence of equations in the unknown terms of order $k = 0, 1, \ldots$ of the expanded solutions, to be solved with the initial conditions (20) and (21).
Zero order solution

Let us first consider the reduced problem which occurs when we confine ourselves to the simplest possible approximation for representing the solution in powers of \( \epsilon \), namely we truncate the series (18) to the order zero, or, in other words, we consider their limiting values for \( \epsilon = 0 \). This leads to the limiting or zero order solution of problem (15). The terms of order \( k = 0 \) of the outer solution which are deduced from (22) must satisfy the nonlinear algebraic system

\[
0 = f_1(n_{10}, n_{20}, 0) = n_{20}(\rho - n_{10} - 2n_{20}) \tag{24}
\]
\[
0 = f_2(n_{10}, n_{20}, 0) = n_{20}(-2\rho + 2n_{10} + 4n_{20}). \tag{25}
\]

Its solutions are represented by the \( \infty^1 \) family \( (n_{10}, 0) \) with arbitrary \( n_{10} \) and by the unstable point \( (0, \rho/2) \) to be discarded as discussed above.

Owing to the singularity of the kernel of the limiting vector field, this solution, which gives \( n_{20} = 0 \) and leaves \( n_{10} \) undetermined, is then useless. Nevertheless, \( n_{10}(t) \) can be calculated by pushing the expansion one step further, even though the new terms are not needed in the representation of the solution, and by deriving a compatibility condition for the solution of the outer problem of order \( k = 1 \). In fact, by setting \( n_{20} = 0 \), this \( \epsilon \)-order outer problem is defined by the singular system

\[
\frac{dn_{10}}{dt} = f_{11} = (\rho - n_{10})n_{21} - \rho n_{10} + n_{10}^2 \tag{26}
\]
\[
0 = f_{21} = (-2\rho + 2n_{10})n_{21} - 4\rho n_{10} + 4n_{10}^2 + \rho^2. \tag{27}
\]

This linear algebraic set of equations for the unknowns \( n_{11} \) and \( n_{21} \) is singular, like (24) and (25), in the sense that now it leaves \( n_{11} \) undetermined and allows a solution for \( n_{21} \) only if the two inhomogeneous terms are properly related. Specifically, the solution is

\[
n_{21}(t) = \frac{[2n_{10}(t) - \rho]^2}{2[\rho - n_{10}(t)]}, \tag{28}
\]

under the condition that \( n_{10} \) satisfies the following nonlinear differential equation

\[
\frac{dn_{10}}{dt} = 3n_{10}^2 - 3\rho n_{10} + \frac{\rho}{2}, \tag{29}
\]

determining the unknown \( n_{10} \) which was left unspecified at the previous step. It is of Bernoulli type, and has the solution

\[
n_{10}(t) = \frac{\rho[6n_{10}(0) - (3 - \sqrt{3})\rho]}{6\sqrt{3}n_{10}(0)\left(1 - e^{\sqrt{3}\rho t}\right) + 3\rho\left[1 - \sqrt{3} + (1 + \sqrt{3})e^{\sqrt{3}\rho t}\right]} + \frac{3 - \sqrt{3}}{6}\rho \tag{30}
\]
where \( n_{10}(0) = b - N_{10}(0) \) is the initial condition that is still unknown and must be determined by matching this outer solution with the limiting inner one.

Therefore, let us now consider the limiting inner system, which is related to the terms of order zero in (23). It is

\[
\begin{align*}
\frac{dN_{10}}{d\tau} &= f_1(n_{10}(0) + N_{10}(\tau), n_{20}(0) + N_{20}(\tau), 0) - f_1(n_{10}(0), n_{20}(0), 0) \\
&= [\rho - n_{10}(0)]N_{20} - 2N_{20}^2 - N_{10}N_{20} \\
\frac{dN_{20}}{d\tau} &= f_2(n_{10}(0) + N_{10}(\tau), n_{20}(0) + N_{20}(\tau), 0) - f_2(n_{10}(0), n_{20}(0), 0) \\
&= -2[\rho - n_{10}(0)]N_{20} + 4N_{20}^2 + 2N_{10}N_{20} \tag{31}
\end{align*}
\]

and, owing again to its singularity, equation (31) can be replaced by

\[
\frac{dN_{10}}{d\tau} = -\frac{1}{2} \frac{dN_{20}}{d\tau}. \tag{33}
\]

By using the initial conditions \( N_{10}(0) = b - n_{10}(0) \), \( N_{20}(0) = c \) and requiring that

\[
\lim_{\tau \to \infty} N_{10}(\tau) = \lim_{\tau \to \infty} N_{20}(\tau) = 0,
\]

one obtains from (33)

\[
\begin{align*}
n_{10}(0) &= b + \frac{c}{2} = \rho - \frac{k_1}{2}, \quad \text{with} \quad k_1 = 2\rho - 2b - c > 0 \tag{34} \\
N_{10}(\tau) &= -\frac{1}{2} N_{20}(\tau). \tag{35}
\end{align*}
\]

Thus, by inserting this last result into (32) and by integrating, the limiting inner solution is determined as follows

\[
\begin{align*}
N_{10}(\tau) &= -\frac{k_1}{2 \left( \frac{k_1}{c} - 3 \right) e^{k_1 \tau} + 6} \tag{36} \\
N_{20}(\tau) &= \frac{k_1}{\left( \frac{k_1}{c} - 3 \right) e^{k_1 \tau} + 3} \tag{37}
\end{align*}
\]

for \( c > 0 \), and \( N_{10}(\tau) = N_{20}(\tau) = 0 \) in the special case \( c = 0 \).
Moreover, by inserting into (30) the initial condition determined in (34), one also obtains the final result for $n_{10}(t)$

$$n_{10}(t) = \frac{\rho}{e^{\sqrt{3}\rho t} \left[ \frac{6\rho}{(3 + \sqrt{3})\rho - 3k_1} - \sqrt{3} \right] + \sqrt{3}} + \frac{3 - \sqrt{3}}{6} \rho,$$  \hspace{1cm} (38)

and the following composite zero-order approximation to the solution of problem (15)

$$n_1^{(0)}(t, \epsilon) = n_{10}(t) + N_{10}(t/\epsilon)$$
$$n_2^{(0)}(t, \epsilon) = N_{20}(t/\epsilon).$$  \hspace{1cm} (39)

**Solution of order $\epsilon$.**

The $\epsilon$-order outer term $n_{21}(t)$ is given by (28), while $n_{11}(t)$ will be determined, as in the case of the zero-order solution, through a compatibility condition for the outer system of order 2, and by the matching procedure with the correspondent inner solution $N_{11}(\tau)$.

The inner terms $N_{11}, N_{21}$ must satisfy the following singular, linear system obtained by equating the terms of order $k = 1$ in (23)

$$\frac{dN_{11}}{d\tau} = a_1(\tau) N_{11} + a_2(\tau) N_{21} + A_0(\tau)$$  \hspace{1cm} (40)
$$\frac{dN_{21}}{d\tau} = -2a_1(\tau) N_{11} - 2a_2(\tau) N_{21} + B_0(\tau)$$  \hspace{1cm} (41)

with

$$a_1(\tau) = -N_{20}(\tau), \quad a_2(\tau) = k_1/2 - 4N_{20}(\tau) - N_{10}(\tau)$$

and where $A_0(\tau), B_0(\tau)$ are known functions of the zero-order solution, also containing the initial data of the $\epsilon$-order outer terms

$$A_0(\tau) = -\left[ \tau \dot{n}_{10}(0) + n_{11}(0) \right] N_{20} - n_{21}(0)(N_{10} + 4N_{20}) + N_{10}^2 + (\rho - k_1) N_{10} + 2(\rho - k_1/2) N_{20} + 2N_{10} N_{20}$$
$$B_0(\tau) = 2\left[ \tau \dot{n}_{10}(0) + n_{11}(0) \right] N_{20} + 2n_{21}(0)(N_{10} + 4N_{20}) + 4N_{10}^2$$
$$+ 4(\rho - k_1) N_{20} + 4N_{20}^2 + 4(\rho - k_1) N_{10} + 8N_{10} N_{20}.$$  \hspace{1cm} (42)

Equations (40) and (41) are related by

$$\frac{dN_{11}}{d\tau} + \frac{1}{2} \frac{dN_{21}}{d\tau} = A_0(\tau) + \frac{B_0(\tau)}{2} =$$
$$= 3\rho N_{10} + 4\rho N_{20} - 3k_1(N_{10} + N_{20}) + 6N_{10} N_{20} + 3N_{10}^2 + 2N_{20}^2$$
$$= (a - 4b - c) N_{10} - N_{10}^2,$$  \hspace{1cm} (44)
and a formal integration of this equation, with initial conditions satisfying (21) for \( k = 1 \), yields

\[
N_{11}(\tau) + n_{11}(0) + \frac{1}{2} [N_{21}(\tau) + n_{21}(0)] = I(\tau) = (a - 4b - c) \int_0^\tau N_{20}(\tau')d\tau' - \int_0^\tau N_{20}^2(\tau')d\tau'.
\] (45)

Since the initial layer correction terms must vanish as \( \tau \to \infty \), we have

\[
n_{11}(0) = I(+\infty) - \frac{n_{21}(0)}{2} = I(+\infty) + b + \frac{c}{2} - \frac{\rho^2}{2k_1},
\] (46)

and by using the solution (36) of \( N_{10}(\tau) \) it is obtained

\[
I(\tau) = -\frac{k_1}{12[(k_1/c - 3)e^{k_1\tau} + 3]} - k_2 \left[ k_1\tau - \log |(k_1/c - 3)e^{k_1\tau} + 3| \right] - k_2 \log |k_1/c| + \frac{c}{12}
\] (47)

with

\[
k_2 = \frac{1}{6} \left( \frac{4}{3} a - \frac{11}{3} b - \frac{1}{2} c \right).
\]

It has the limit

\[
\lim_{\tau \to +\infty} I(\tau) = I(\infty) = k_2 \log \left( \frac{2a + 2b}{k_1} \right) + \frac{c}{12}
\] (48)

and therefore the initial value of \( n_{11} \) is given by

\[
n_{11}(0) = k_2 \log \left( \frac{2a + 2b}{k_1} \right) + b + \frac{7}{12} c - \frac{\rho^2}{2k_1}.
\] (49)

We can now derive explicitly the solution of the inner system. From (45) we have

\[
N_{21}(\tau) = 2[I(\tau) - I(\infty) - N_{11}(\tau)]
\] (50)

and substitution into (40) provides a differential equation for \( N_{11} \) with the solution

\[
N_{11}(\tau) = -n_{11}(0)e^{\int_0^\tau (a_1 - 2a_2)d\tau'} + \int_0^\tau \{2a_2[I(\tau') - I(\infty)] + A_0(\tau') \} e^{\int_\tau^\tau a_1 - 2a_2 d\tau''} d\tau'.
\] (51)
Finally, let us determine the term \( n_{11}(t) \) by using the singular, nonlinear system of order \( \epsilon^2 \) which results by equating the terms with \( k = 2 \) in (22). It is given by

\[
\frac{dn_{11}}{dt} = f_{12} = (\rho - n_{10})n_{22} + (2n_{10} - \rho)n_{11} + 2n_{10}n_{21} - n_{11}n_{21} - 2n_{21}^2 \tag{52}
\]

\[
\frac{dn_{21}}{dt} = f_{22} = 2(n_{10} - \rho)n_{22} + (8n_{10} - 4\rho)n_{11} + (8n_{10} - 4\rho)n_{21} + 2n_{11}n_{21} + 4n_{21}^2 \tag{53}
\]

and has a unique solution for \( n_{22}(t) \) under the condition that \( n_{11} \) satisfies

\[
\frac{dn_{11}}{dt} = 3[2n_{10}(t) - \rho]n_{11} + 2[3n_{10}(t) - \rho]n_{21}(t) - \frac{1}{2} \frac{dn_{21}}{dt}. \tag{54}
\]

By taking into account that \( n_{10}(t), n_{21}(t) \) and its derivative are known, equation (54) may be rewritten as

\[
\frac{dn_{11}}{dt} = \alpha(t)n_{11} + \beta(t)
\]

with

\[
\alpha(t) = 3(2n_{10} - \rho)
\]

\[
\beta(t) = \frac{2n_{10} - \rho}{n_{10} - \rho} \left[ -(3n_{10} - \rho)(2n_{10} - \rho) + \frac{2n_{10} - 3\rho}{4(n_{10} - \rho)} \cdot \frac{dn_{10}}{dt} \right]
\]

and solved with the initial condition (49), with the result

\[
n_{11}(t) = \left[ k_2 \log \left( \frac{2a + 2b}{k_1} \right) + b + \frac{7}{12}c - \frac{\rho^2}{2k_1} \right] e^{\int_0^t \alpha(t')dt'} + \int_0^t \beta(t')e^{\int_0^t \alpha(\xi)d\xi} dt'. \tag{55}
\]

The \( \epsilon \)-order approximate solution of problem (15) is thus determined as

\[
n_{1}(t, \epsilon) = n_{10}(t) + N_{10}(t/\epsilon) + \epsilon[n_{11}(t) + N_{11}(t/\epsilon)]
\]

\[
n_{2}(t, \epsilon) = N_{20}(t/\epsilon) + \epsilon[n_{21}(t) + N_{21}(t/\epsilon)]. \tag{56}
\]

When \( t \to \infty \) the zero-order solution converges to the point \((n_{1}^{(0)}*, n_{2}^{(0)}*) = \left( \frac{3 - \sqrt{3}}{6}, \rho, 0 \right)\)

and analogously the first order solution converges to a point showing \( O(\epsilon) \) corrections with respect to this. In fact the final equilibria reached by the previous expansions are necessarily asymptotic representations of the exact one, given by (10).

The extension of this solution to higher-order approximations is now a matter of straightforward, though cumbersome, calculations. In fact, the expansions of \( f_1, f_2 \) in power series of \( \epsilon \) lead to linear equations for the unknown terms of order \( k = 2, 3, \ldots \) having the same
coefficient matrix, i.e. the singular Jacobian matrix of the vector field, calculated at $\epsilon = 0$

$$D_f(n_{10}, n_{20}, 0) = \begin{pmatrix} -n_{20} & \rho - n_{10} - 4n_{20} \\ 2n_{20} & -2(\rho - n_{10} - 4n_{20}) \end{pmatrix}.$$  

Consequently, the same procedure used for the $\epsilon$-order approximation can be applied to determine the outer and inner terms of order $k \geq 2$.

4 Fast and slow variables, compressed solution

As seen in the previous Section, the source of singularity, which forces consideration of the step $n + 1$ and a relevant compatibility condition in order to determine the $n$-th order solution, is the operator $\mathcal{B}$, as given by (8). Following the detailed procedure devised in [7], we can easily realize that the null space of $\mathcal{B}$, $N(\mathcal{B})$, is made up by pairs $\mathbf{n} = (n_1, n_2)$ in the phase space such that $n_2 = 0$. Analogously, the range of $\mathcal{B}$, $R(\mathcal{B})$, is constituted by the pairs $\mathbf{n} = (n_1, n_2)$ with $n_2 = -2n_1$. In order to single out the hydrodynamic variable and to proceed to the compressed (Chapman-Enskog) asymptotic expansion, it is crucial the determination of the projection operator $P$ such that $P(\mathcal{B}(\mathbf{n})) = 0$ for any $\mathbf{n}$ in the phase space, and $P(\mathbf{n}) = 0 \forall \mathbf{n} \in R(\mathcal{B})$. In the present case, it is easily seen by inspection that $P$ is determined as

$$P_1(n_1, n_2) = n_1 + \frac{1}{2}n_2$$

$$P_2(n_1, n_2) = 0.$$  \hspace{1cm} (57)

The main feature of the operator $P$ is that its application to equation (4) eliminates the dominant part of the collision operator, by virtue of the identity

$$P(\mathcal{B}(\mathbf{n})) = 0$$  \hspace{1cm} (58)

for any $\mathbf{n}$ in the phase space. Since $P$ and time derivative obviously commute, this leaves an equation with slow evolution for the quantity $P(\mathbf{n})$, the hydrodynamic variable of [7]. The complementary projection operator $Q$ is then

$$Q_1(n_1, n_2) = -\frac{1}{2}n_2$$

$$Q_2(n_1, n_2) = n_2$$  \hspace{1cm} (59)

with $\mathbf{n} = P(\mathbf{n}) + Q(\mathbf{n})$, $P(\mathbf{n}) \in N(\mathcal{B})$ and $Q(\mathbf{n}) \in R(\mathcal{B})$. 

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Such decomposition introduces spontaneously new dependent variables

\[
x_1 = n_1 + \frac{1}{2} n_2
\]
\[
x_2 = n_2
\]

which are respectively the slow and the fast variable in the jargon of singular perturbation theory [8].

The set (15), recast in terms of the variables (60), reads as

\[
\begin{aligned}
\dot{x}_1 &= g_1(x_1, x_2) = 3x_1^2 + 3x_1 x_2 - \frac{1}{4} x_2^2 - 3 \rho x_1 - \frac{1}{2} \rho x_2 + \frac{1}{2} \rho^2 \\
\epsilon \dot{x}_2 &= g_2(x_1, x_2, \epsilon) = 4 \epsilon x_1^2 + 2(1 + 2 \epsilon) x_1 x_2 + (3 + \epsilon) x_2^2 - 4 \epsilon \rho x_1 - 2(1 + \epsilon) \rho x_2 + \epsilon \rho^2,
\end{aligned}
\]

with phase space given by the triangle defined by \(x_2 \geq 0, x_1 \geq \frac{1}{2} x_2, 2x_1 + x_2 \leq \rho\) (the unphysical equilibrium corresponds to the vertex \((\rho/4, \rho/2)\)). It is only matter of some algebra to show that the unique fixed point in the admissible phase space corresponds to the point (10), and that the problem is now regular-singular, since the limiting equations for \(\epsilon = 0\) has the unique fixed point of physical meaning \(x_1 = \frac{3 - \sqrt{3}}{6} \rho\), \(x_2 = 0\), which corresponds to the limiting value of (10) when \(\epsilon \to 0\). We can apply then the standard composite asymptotic expansion

\[
\begin{aligned}
x_1(t, \epsilon) &= x_1^o(t, \epsilon) + x_1^i(\tau, \epsilon) \\
x_2(t, \epsilon) &= x_2^o(t, \epsilon) + x_2^i(\tau, \epsilon)
\end{aligned}
\]

and the initial conditions \(x_1(0) = b + \frac{c}{2}, x_2(0) = c\). Outer and inner components are expanded in power series of \(\epsilon\)

\[
\begin{aligned}
x_j^o &= \sum_k \epsilon^k x_{jk}(t), & \quad x_j^i &= \sum_k \epsilon^k X_{jk}(\tau) & j &= 1, 2
\end{aligned}
\]

with initial values

\[
\begin{aligned}
x_{10}(0) + X_{10}(0) &= b + \frac{c}{2} & x_{20}(0) + X_{20}(0) &= c \\
x_{1k}(0) + X_{1k}(0) &= 0 & x_{2k}(0) + X_{2k}(0) &= 0 & k &= 1, 2, ...
\end{aligned}
\]

and with initial layer corrections \(X_{ij}(\tau)\) bound to vanish when \(\tau \to \infty\).
We will not give all detailed manipulations. The main variation with respect to the previous Section is that now each step determines the unknowns relevant to that step, reducing the amount of standard but lengthy algebra. Another advantage is that for the present approach several results about asymptoticity of the series and error estimates are well established in [8,11], providing an adequate mathematical setting to the present formal developments. Of course, after truncation either to the zero order or to the first order, upon going back to the density variables $n_1$ and $n_2$, the two analytical approximate solutions coincide.

It suffices to mention here that in the solution of the set (61) the zero order outer and inner components have to satisfy respectively

\[
\frac{dx_{10}}{dt} = 3x_{10}^2 + 3x_{10}x_{20} - \frac{1}{4}x_{20}^2 - 3\rho x_{20} - \frac{1}{2}\rho x_{20} + \frac{\rho^2}{2} \tag{65}
\]
\[
0 = 2x_{10}x_{20} + 3x_{20}^2 - 2\rho x_{20} \tag{66}
\]

\[
\frac{dX_{10}}{d\tau} = 0 \tag{67}
\]
\[
\frac{dX_{20}}{d\tau} = 2x_{10}(0)X_{20} + 2X_{10}X_{20} + 3X_{20}^2 - 2\rho X_{20} \tag{68}
\]

From (66) one has $x_{20}(t) = 0$ and therefore also $n_{20}(t) = 0$; $n_{10} = x_{10}$. Since $X_{10}$ must vanish asymptotically, from (67) it is obtained $X_{10}(\tau) = 0$. Thus we have $N_{10} = -N_{20}/2$, already obtained in (35), and moreover the initial condition

\[
x_{10}(0) = X_{10}(0) + b + \frac{c}{2} = b + \frac{c}{2} \tag{69}
\]

for Eq. (65), that after suppression of $x_{20}$ reads as

\[
\frac{dx_{10}}{dt} = 3x_{10}^2 - 3\rho x_{10} + \frac{\rho^2}{2}, \tag{70}
\]

and is coincident with (29) since $x_{10} = n_{10}$. Finally, by replacing $x_{10}(0)$ and suppressing $X_{10}$ in (68) one obtains

\[
\frac{dX_{20}}{d\tau} = -k_1X_{20} + 3X_{20}^2, \tag{71}
\]

whose solution satisfying the initial condition $X_{20}(0) = c$ is the same as $N_{20}(\tau)$ given by (37).

In analogous fashion, the $\epsilon$-order terms in the expansions (63) can be determined by solving the following sets of equations, that result by equating in system (61) the terms of the same order $\epsilon$
\[
\frac{dx_{11}}{dt} = 3(2x_{10} - \rho)x_{11} + \left(3x_{10} - \rho \right) x_{21} + 4x_{10}^2 - 4\rho x_{10} + \rho^2
\] (72)

\[
0 = 2(x_{10} - \rho)x_{21} + 4x_{10}^2 - 4\rho x_{10} + \rho^2
\] (73)

\[
\frac{dX_{11}}{d\tau} = -\left(\frac{a}{2} - 2b - \frac{c}{2}\right) X_{20} - \frac{1}{4} X_{20}^2
\] (74)

\[
\frac{dX_{21}}{d\tau} = 2X_{20}X_{11} + (6X_{20} - k)X_{21} + \tilde{B}_0(\tau)
\] (75)

with

\[
\tilde{B}_0(\tau) = [2\dot{x}_{10}(0)\tau + 2x_{11}(0) + 6x_{21}(0) - 2(a + c)]X_{20} + X_{20}^2.
\]

Equation (73) gives \(x_{21}(t) = n_{21}(t)\) already obtained in (28), and the solution of (74) satisfying the asymptoticity condition requested to the initial layer corrections is \(X_{11}(\tau) = I(\tau) - I(\infty)\), where \(I(\cdot)\) are the same integrals shown in (47) and (48). Substitution of these results into (72) and (75) and calculation of the respective initial conditions, yield the following two linear first order ordinary differential equations

\[
\frac{dx_{11}}{dt} = 3(2x_{10} - \rho)x_{11} + \frac{(6x_{10} - \rho)(2x_{10} - \rho)^2}{4(\rho - x_{10})},
\] (76)

\[
x_{11}(0) = -X_{11}(0) = I(\infty)
\]

\[
\frac{dX_{21}}{d\tau} = (X_{20} - k)X_{21} + 2X_{20}[I(\tau) - I(\infty)] + \tilde{B}_0(\tau),
\] (77)

\[
X_{21}(0) = -x_{21}(0) = -\frac{(\rho - k)^2}{k}.
\]

whose solution yields the remaining unknown terms at the \(\epsilon\) stage. Thus, by restoring the original density variables, the first order approximate solution of (15) is determined as

\[
n^{(1)}_1(t, \epsilon) \simeq x_{10}(t) - \frac{1}{2} X_{20} \left(\frac{t}{\epsilon}\right) + \epsilon \left[ x_{11}(t) - \frac{1}{2} x_{21}(t) + X_{11} \left(\frac{t}{\epsilon}\right) - \frac{1}{2} X_{21} \left(\frac{t}{\epsilon}\right) \right]
\] (78)

\[
n^{(1)}_2(t, \epsilon) \simeq X_{20} \left(\frac{t}{\epsilon}\right) + \epsilon \left[ x_{21}(t) + X_{21} \left(\frac{t}{\epsilon}\right) \right].
\] (79)

A rather tedious algebra allows to verify that it is indeed equivalent to the Hilbert approximation of the same order.

As mentioned in the Introduction, once the problem is reduced to the form (61) and the slow (hydrodynamic) part has been singled out, an alternative algorithm is provided by the compressed asymptotic expansion [7], by leaving the outer component of the slow variable unexpanded. This allows to determine \(x^o_1\) by solving a unique \(\epsilon\)-dependent differential equation, which hopefully retains more information with respect to a truncation after few
powers of $\epsilon$. We shall follow this procedure according to the recipe proposed in [12]. We write

\[ x_1^0(t) = \bar{x}_1(t) \]
\[ x_2^0(t) = \sum_k \epsilon^k \varphi_k(\bar{x}_1) \] (80)

and try to determine the unknown functions $\bar{x}_1$ and $\varphi_k$ by requiring the outer solution to satisfy the set (61). We have

\[ \frac{d\bar{x}_1}{dt} = g_1(\bar{x}_1, \sum_k \epsilon^k \varphi_k(\bar{x}_1)) = \sum_k \epsilon^k g_{1,k} \] (81)
\[ \epsilon \frac{dx_2^0}{dt} = \epsilon \sum_k \epsilon^k \frac{d\varphi_k}{dx_1} \frac{d\bar{x}_1}{dt} = \epsilon \sum_k \epsilon^k \frac{d\varphi_k}{dx_1} \sum_j \epsilon^j g_{1,j} = \sum_k \epsilon^k g_{2,k} \] (82)

with

\[ g_{1,0} = g_1(\bar{x}_1, \varphi_0(\bar{x}_1)) = 3\bar{x}_1^2 + 3\bar{x}_1 \varphi_0 - \frac{1}{4} \varphi_0^2 - 3\rho \bar{x}_1 - \frac{1}{2} \rho \varphi_0 + \frac{1}{2} \rho^2 \]
\[ g_{2,0} = g_2(\bar{x}_1 \varphi_0(\bar{x}_1), 0) = 2\bar{x}_1 \varphi_0 + 3\varphi_0^2 - 2\rho \varphi_0 \]
\[ g_{1,1} = \left( \frac{dg_1}{d\epsilon} \right)_{\epsilon=0} = \varphi_1(\bar{x}_1) \left( 3\bar{x}_1 - \frac{\varphi_0}{2} - \frac{\rho}{2} \right) \]
\[ g_{2,1} = \left( \frac{dg_2}{d\epsilon} \right)_{\epsilon=0} = \varphi_1(\bar{x}_1) (2\bar{x}_1 + 6\varphi_0 - 2\rho) + 4\bar{x}_1^2 + 4\bar{x}_1 \varphi_0 + \varphi_0^2 - 2\rho \varphi_0 - 4\rho \bar{x}_1 + \rho^2. \]

By equating in (82) the coefficients of $\epsilon^0$ and $\epsilon$ it is obtained the system

\[ \begin{cases} g_{2,0} = [2\bar{x}_1 + 3\varphi_0 - 2\rho] \varphi_0 = 0 \\ g_{2,1} = \frac{d\varphi_0}{d\bar{x}_1} g_{1,0} \end{cases} \] (83)

which has the solution

\[ \varphi_0 = 0, \quad \varphi_1(\bar{x}_1) = -\frac{(2\bar{x}_1 - \rho)^2}{2(\bar{x}_1 - \rho)} \] (84)

where $\bar{x}_1$ is determined by solving

\[ \frac{d\bar{x}_1}{dt} = g_1(\bar{x}_1, \epsilon \varphi_1(\bar{x}_1)) = 3\bar{x}_1(\bar{x}_1 - \rho) + \frac{\rho^2}{2} + \epsilon (\rho - 6\bar{x}_1) \left[ \bar{x}_1 + \frac{\rho^2}{4(\bar{x}_1 - \rho)} \right] - \frac{(2\bar{x}_1 - \rho)^4}{16(\rho - \bar{x}_1)^2} \epsilon^2. \] (85)
The initial condition for (85) and the ones of the inner terms \( X_{1k}, X_{2k} \) are now related, up to the \( \epsilon \)-order approximation, as follows

\[
\bar{x}_1(0) + X_{10}(0) + \epsilon X_{11}(0) = b + \frac{c}{2} \tag{86}
\]
\[
\varphi_0[\bar{x}_{1,0}(0)] + X_{20}(0) = c \tag{87}
\]
\[
\varphi_1[\bar{x}_{1,0}(0)] + X_{21}(0) = 0 \tag{88}
\]

where \( \bar{x}_{1,0}(0) = b + c/2 \) is the initial value of \( \bar{x}_1(t) \) in the limit \( \epsilon \to 0 \). They are calculated, as usual, by matching the outer solution with the inner one, which must satisfy the following system

\[
\begin{cases}
\frac{dx_1^i}{d\tau} = \epsilon \left( g_1[\bar{x}_1 + x_1^i, \epsilon \varphi_1(\bar{x}_1) + x_2^i] - g_1[\bar{x}_1, \epsilon \varphi_1(\bar{x}_1)] \right) \\
\frac{dx_2^i}{d\tau} = g_2[\bar{x}_1 + x_1^i, \epsilon \varphi_1(\bar{x}_2) + x_2^i, \epsilon] - g_2[\bar{x}_1, \epsilon \varphi_1(\bar{x}_1), \epsilon]
\end{cases} \tag{89}
\]

By equating the terms of order zero and one with respect to \( \epsilon \), one has the same set provided by the previous approach, e.g. equations (67)-(68) and (74)-(75) for \( X_{i0} \) and \( X_{i1} \) respectively, where the non-homogeneous term in (75) is turned to

\[
\tilde{B}_0'(...) = [2\dot{x}_1(0)\tau + 6\varphi_1(\bar{x}_1(0)) - 2(a + c)]X_{20} + X_{20}^2.
\]

It follows that the initial condition for (85) must be

\[
\bar{x}_1(0) = b + \frac{c}{2} - X_{10}(0) - \epsilon X_{11}(0) = b + \frac{c}{2} + \epsilon I(\infty)
\]

and it can now be used to find the unexpanded outer component of the slow variable, by integration of the differential equation (85).

In conclusion, in terms of the original density variables \( n_1, n_2 \) the \( \epsilon \)-order approximation achieved by using the compressed expansions algorithm is

\[
n_1^{(c)}(t, \epsilon) \simeq \bar{x}_1(t) - \frac{1}{2} X_{20} \left( \frac{t}{\epsilon} \right) + \epsilon \left[ -\frac{1}{2} \varphi_1(\bar{x}_1) + X_{11} \left( \frac{t}{\epsilon} \right) - \frac{1}{2} X_{21} \left( \frac{t}{\epsilon} \right) \right] \tag{90}
\]
\[
n_2^{(c)}(t, \epsilon) \simeq X_{20} \left( \frac{t}{\epsilon} \right) + \epsilon \left[ \varphi_1(\bar{x}_1) + X_{21} \left( \frac{t}{\epsilon} \right) \right]. \tag{91}
\]

We are not reporting on the zero order approximation since it is not difficult to check that the unexpanded part \( \bar{x}_1(t) \) would coincide with the unknown \( x_{10} \) of the uncompressed procedure, and consequently we would get the same results from the two algorithms.
5 Numerical Results

The results of the approximate asymptotic solutions derived in the previous Sections are now illustrated and discussed. We consider the dynamical system (15) together with initial conditions (16) and we first compute its “exact” (numerical) solution by means of an accurate ODE solver; the density $n_0$ comes then from the first integral (3). In our numerical examples we start with the following reference numerical values

$$
\epsilon = 0.01, \quad a = 0, \quad b = 1, \quad c = 4.
$$

They have to be considered as dimensionless (for illustrative purposes only), and corresponding to arbitrary scales.

In Fig. 1.a we compare the temporal evolutions of $n_0, n_1, n_2$ obtained by the “exact” solution (solid line), by the zero-order Hilbert expansion (dotted line), and by the first-order Hilbert expansion (dashed–dotted line). The initial layer clearly shows up, and it is evident that the first-order Hilbert approximation better reproduces the “exact” behaviour (the very slight differences can be hardly recognized in the graph). We recall that, as already seen, the zero-order Hilbert expansion coincides analytically with the zero-order compressed expansion and with the zero-order solution of the fast–slow variables method, as well as, at first order, the Hilbert approximation and the fast–slow variables method give exactly the same analytical results. The widely used stationary-state approximation has been compared with the outer solution of the first-order Hilbert expansion in Fig. 1.b, where the temporal evolution of the densities $n_i$ is shown. The initial data are the same as for the outer solution in the Hilbert expansion, namely

$$
n_1(0) = n_{10}(0) + \epsilon n_{11}(0)
$$

where $n_{10}(0)$ and $n_{11}(0)$ are given by (34) and (49). Similar results could be obtained by choosing initial data in such a way that the least square error between the “exact” and the stationary-state solutions is minimal. The solid line represents again the reference “exact” numerical solution, whereas the stationary-state approximation and the outer solution, which overlap almost entirely, are given by the dotted and the dashed-dotted lines respectively. We can notice that, apart from the initial layer of thickness $O(\epsilon)$, the stationary-state approximation provides an accurate description of the evolution in the bulk region.

In Fig. 2.a we report the results as in Fig. 1.a obtained by changing the initial data. A different trend with respect to the reference case can be observed in the evolution of the three number densities, and a wide range of behaviours could be obtained by playing with initial data. Of course, the initial layer effect tends to disappear when the initial condition approaches the quasi steady–state condition (9), as already pointed out in [6]. Indeed, it was already observed in (36), (37) that the zero order inner solution vanishes for $c = 0$. The effect of varying $\epsilon$ is depicted in Fig. 2.b, where we plot the results obtained for $\epsilon = 0.05$ when we start with the reference initial data. As expected, a larger initial
layer shows up, and the zero- and even first-order Hilbert approximations lead to worse results than in case $\epsilon = 0.01$.

The first-order compressed expansion gives rise to solutions which differs, in principle, from the ones obtained by the first-order Hilbert approximation, but the discrepancies are not quantitatively appreciable in the graphs $(t, n_i)$. In Fig. 3.a we then show the temporal trend (in logarithmic scale) of the error vectors, defined as the pointwise euclidean norm of the vector $(n_0 - n_0^{ex}, n_1 - n_1^{ex}, n_2 - n_2^{ex})$, where $n_i^{ex}$ stands for the “exact” numerical values. We compare there the errors for the two values of $\epsilon$ used above versus time. The solid lines are relevant to the error in the first-order Hilbert expansion, whereas the dotted lines represent the error in the first-order compressed expansion. As we can see, the two methods do not show significant discrepancies in the results, although they come from two different asymptotic strategies. The compressed algorithm enhances a bit the accuracy in the bulk region. Fig. 3.b shows instead the behaviour of the errors (with respect to the “exact” solution again) in the stationary-state approximation (solid line) and in the first-order Hilbert expansion (dotted line), with exclusion of the very initial region, where the former exhibits very high deviations. It is worth noticing that in the steady-state approximation the error tends to vanish for $t$ large enough, since no truncation occurs in the fixed point of the problem with respect to the exact one.

To summarize the results, we report finally in Table 1 the values of the density $n_1$ computed at time instant $t = 0.01$, $t = 0.001$ by using both the ODE solver and the different asymptotic approximations described above. The values marked by $*$ are not significant since they are relevant to the stationary-state approximation out of its region of validity, namely in the initial layer.

<table>
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<th>$\epsilon$</th>
<th>$n_1$</th>
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<th>$n_1^{(1)}$</th>
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**Table 1.** Computed values of density $n_1$ obtained by zero- ($n_1^{(0)}$) and first order ($n_1^{(1)}$) Hilbert expansion, first-order compressed method ($n_1^{(c)}$) and stationary-state approximation ($n_1^{(s)}$) at two different time instants $t = 0.01$ and $t = 0.001$. 
Figure 1: Reference case $\epsilon = 0.01$. (a) Exact solution (solid line), zero-order (dotted line) and first-order (dashed–dotted line) Hilbert expansion; (b) Stationary-state approximation (dotted line), outer expansion (dashed–dotted line) and exact solution (solid line).

Figure 2: (a) Exact solution and Hilbert expansions obtained for different initial data $(a = 0, b = 2.5, c = 2.5)$ and the same $\epsilon = 0.01$. (b) Exact solution (solid line), zero-order (dotted line) and first-order (dashed–dotted line) Hilbert expansion obtained for $\epsilon = 0.05$ and initial data as in Fig. 1.
Figure 3: (a) Comparison of the error in the first–order Hilbert expansion (solid line) and in the first–order compressed expansion (dotted line) obtained for $\epsilon = 0.01$ and $\epsilon = 0.05$ respectively (logarithmic scale). (b) Error in the stationary-state approximation (solid line) and in the Hilbert first-order expansion (dotted line) (case $\epsilon = 0.01$).

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References


