NON-LTE Line Radiative Transfer Quasi-stationary Approximation

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In this paper, we prove existence and uniqueness of solutions to the coupling between the radiative transfer equation and equations for the population of atoms in a certain state. We also prove the validity of the quasi-static approximation in this context.

Keywords: Radiative transfer, quasi-static approximation

1. Introduction

We consider a coupling between a radiating field and a plasma. The radiation is described by the following transport equation

$$\frac{1}{c}\partial_t f + v \cdot \nabla_x f = \eta - \chi f, \tag{1}$$

where the constant c is the speed of light, $v \in \mathbb{S}^2$ is the direction of propagation of photons, η is the emission coefficient (or emissivity) of matter, χ is the absorption coefficient (or extinction coefficient) of matter, and the unknown is the specific intensity $f := f(t, x, v, \nu)$ which is a function of time $t \in \mathbb{R}^+$, space position $x \in X \subset \mathbb{R}^3$, velocity direction $v \in \mathbb{S}^2$, and frequency $\nu \in \mathbb{R}^+$.

If we consider the coefficients η and χ as given, the transfer equation (1) is linear and its solution can be written explicitly by integrating along the characteristics. These coefficients depend however in reality upon the internal excitation and ionization states of the plasma. These states are fixed in part by radiative processes that populate and depopulate atomic levels. For the line radiative transfer (bound-bound transitions without ionization), they depend on the Einstein coefficients, the spontaneous emission probability A_{ji} (with $i, j \in \{1, .., K\}$, $i < j$), the absorption probability B_{ij} and the induced (stimulated) emission probability B_{ji}, and can be written as

$$\eta = \sum_i \sum_{j>i} n_j A_{ji} h\nu \phi_{ij}(\nu), \tag{2}$$

$$\chi = \sum_i \sum_{j>i} \left(n_i B_{ij} - n_j B_{ji}\right) h\nu \phi_{ij}(\nu), \tag{3}$$

where n_i (respectively n_j) denotes the population density at the atomic level $i = 1, .., K$ (respectively j), and $\phi_{ij}(\nu)$ represents the line profile for these transitions (it can for example be approximated by a Gaussian function of ν centered around the frequency ν_{ij} of the transition). Finally, h is the Planck constant.

The population density n_i at level i satisfies the following rate equation, in a static medium,

$$\frac{\partial n_i}{\partial t} = \sum_{j \neq i} n_j P_{ji} - n_i \sum_{j \neq i} P_{ij}, \tag{4}$$

where P_{ij} denotes the total (radiative plus collisional) transition rate from level i to level j. Note that the total population of atoms $n := \sum_{i=1}^{K} n_i$ is clearly conserved along time.

Bound-bound transitions (line transitions) between the lower energy level i and the upper energy level j may occur as radiative excitation, spontaneous radiative de-excitation, induced radiative de-excitation, collisional excitation and collisional de-excitation. Let us denote C_{ij} (respectively C_{ji}) the rate of collisional excitation (respectively the rate of collisional de-excitation). In (4), the total excitation rate P_{ij} and the total de-excitation rate P_{ji} can be written as

$$P_{ij} = B_{ij}\rho_{ij} + C_{ij}, \qquad P_{ji} = A_{ji} + B_{ji}\rho_{ij} + C_{ji}, \tag{5}$$

where ρ_{ij} is the integrated mean intensity over the line profile $\phi_{ij}(\nu)$:

$$\rho_{ij}(t, x) = \int_{\mathbb{R}^+} \int_{\mathbb{S}^2} f(t, x, v, \nu)\, \phi_{ij}(\nu)\, \mathrm{d}v \mathrm{d}\nu, \tag{6}$$

with $\mathrm{d}v$ denoting the normalized Lebesgue measure on $\mathbb{S}^2$. For the physical background underlying eq. (1) – (6), we refer to to[9] §85,[10] §2.6.

In general, the radiation field and the internal state of the matter must be determined simultaneously and self-consistently. In many situtions, the characteristic time of the excitation and de-excitation processes of the matter is much smaller than the characteristic time of the evolution of the radiative field. After adimensionalizing the time variable in eq. (1) and (4), it is therefore possible to introduce a parameter $\epsilon > 0$ such that our coupled system becomes

$$\begin{cases} \frac{1}{c}\partial_t f^\epsilon + v\cdot\nabla_x f^\epsilon \\ \qquad = \sum_i \sum_{j>i} n_j^\epsilon A_{ji} h\nu\phi_{ij}(\nu) - \sum_i\sum_{j>i} \left(n_i^\epsilon B_{ij} - n_j^\epsilon B_{ji}\right) h\nu\phi_{ij}(\nu) f^\epsilon, \\ \epsilon \frac{\partial n_i^\epsilon}{\partial t} = \sum_{j\neq i} n_j^\epsilon P_{ji} - \sum_{j\neq i} n_i^\epsilon P_{ij}. \end{cases} \tag{7}$$

We consider the system (7) in the case when the position variable x varies in a bounded (regular, open) domain $X \subset \mathbb{R}^3$. We add therefore the initial condition

$$f^\epsilon(0,x,v,\nu) = f_0(x,v,\nu), \tag{8}$$

and the incoming boundary condition

$$f^\epsilon|_{\mathbb{R}^+\times(\partial X\times\mathbb{S}^2)_-\times\mathbb{R}^+} = g(t,x,v,\nu), \tag{9}$$

where $(\partial X\times\mathbb{S}^2)_- := \left\{(x,v)\in\partial X\times\mathbb{S}^2 : \Gamma_x\cdot v<0\right\}$, with Γ_x denoting the outward normal to X at the point $x\in\partial X$. Finally, the initial population densities $n_i^\epsilon(0,x)$ are given by

$$\forall i = 1,..,K, \qquad n_i^\epsilon(0,x) = n_{i0}(x) \geq 0. \tag{10}$$

We are interested in the existence of solutions f^ϵ, $(n_i^\epsilon)_{i=1,..,K}$, to (5) – (10) (when $\epsilon > 0$ is fixed), and in the behavior of the solutions f^ϵ, n_i^ϵ, as $\epsilon\to 0$ (quasi-stationary approximation).

In the sequel, we shall consider the following assumption on the data:

Assumption A: The initial condition f_0 and the boundary condition g satisfy

$$0\leq f_0 \in L^\infty(X\times\mathbb{S}^2\times\mathbb{R}^+), \qquad 0\leq g\in L^\infty(\mathbb{R}^+\times(\partial X\times\mathbb{S}^2)_-\times\mathbb{R}^+), \tag{11}$$

and the initial occupation numbers n_{i0} are such that $n(x) = \sum_{i=1}^K n_{i0}(x) \in L^\infty(X)$.

The Einstein Coefficients A_{ji}, B_{ij} and B_{ji} are (strictly positive) constants, and the collisional coefficients C_{ij} and C_{ji} are (nonnegative) functions of the position $x\in X$ verifying

$$\delta_* \leq C_{ij}(x),\ C_{ji}(x) \leq \delta^*, \tag{12}$$

for some δ_*, $\delta^* > 0$.

Finally, the line profile ϕ_{ij} is integrable on $\mathbb{R}^+$ and satisfies, for some $\delta > 0$,

$$\forall \nu \in \mathbb{R}^+, \qquad 0 \leq \phi_{ij}(\nu) h\nu \leq \delta. \tag{13}$$

Our main result is stated as

Theorem 1.1. *Let assumption A on the data be satisfied. Then, for any given $T > 0$, there exists a unique nonnegative solution f^ϵ, $(n_i^\epsilon)_{i=1,..,K}$, to* (5) – (10)*, which belongs to $L^\infty([0,T] \times X \times \mathbb{S}^2 \times \mathbb{R}^+) \times (L^\infty([0,T] \times X))^K$. Furthermore, as $\epsilon \to 0$, this solution converges in $L^\infty([0,T] \times X \times \mathbb{S}^2 \times \mathbb{R}^+) \times (L^\infty([0,T] \times X))^K$ weak * to f, $(n_i)_{i=1,..,K}$, unique nonnegative solution in $L^\infty([0,T] \times X \times \mathbb{S}^2 \times \mathbb{R}^+) \times (L^\infty([0,T] \times X))^K$ to the system*

$$\begin{cases} \dfrac{1}{c}\partial_t f + v \cdot \nabla_x f \\ \qquad\qquad = \displaystyle\sum_i \sum_{j>i} n_j A_{ji} h\nu \phi_{ij}(\nu) - \sum_i \sum_{j>i} (n_i B_{ij} - n_j B_{ji})\, h\nu \phi_{ij}(\nu) f, \\ 0 = \displaystyle\sum_{j \neq i} n_j P_{ji} - \sum_{j \neq i} n_i P_{ij}, \\ f(0,x,v,\nu) = f_0(x,v,\nu), \qquad f|_{\mathbb{R}^+ \times (\partial X \times \mathbb{S}^2)_- \times \mathbb{R}^+}(t,x,v,\nu) = g(t,x,v,\nu), \end{cases} \tag{14}$$

where P_{ji}, P_{ij} are given by formulas (5), (6).

Most of the rest of the paper is devoted to the proof of Theorem 1.1. Existence and uniqueness of a solution to (5) – (10) (for a given ϵ) are proven in section 2. At the end of this section, we also show a result of existence and uniqueness for the limiting system (5), (6), (14).

Then, in section 3, we prove the validity of the quasi-stationary approximation, that is the convergence of solutions of (5) – (10) when $\epsilon \to 0$ toward solutions of (5), (6), (14).

Finally, we present a numerical test in order to illustrate this convergence in section 4.

In all the sequel, we shall restrict ourselves in the proof, for the sake of simplicity, to a two-level molecular model (that is, $K = 2$). The proof in the general case is identical.

In this paper we limit our discussion to the bound-bound transitions, we refer for details on the bound-free transitions or the free-free transitions to,[9,10] or the papers.[2,3,5]

We refer to[1] for the existence theory of the radiative transfer equation for a 'grey' model, by using the compactness result introduced in,[6,7] that is, the averaging lemma.

In,[4,11] the authors studied some numerical methods for the line radiative transfer, and the comparison was given between a number of independent computer programs for radiative transfer in molecular rotational lines. Our numerical tests are inspired from the data introduced in.[4,11]

2. Proof of existence and uniqueness to system $(5)-(10)$ for a given ϵ

We begin with a classical explicit resolution of the linear kinetic equation.

Lemma 2.1. *Let X be a bounded regular open set in $\mathbb{R}^3$. We consider the following system:*

$$\left\{\begin{aligned} \frac{1}{c}\partial_t f + v\cdot\nabla_x f &= \eta - \chi f, \\ f(0,x,v,\nu) &= f_0(x,v,\nu) \geq 0, \\ f|_{\mathbb{R}^+\times(\partial X\times\mathbb{S}^2)_-\times\mathbb{R}^+}(t,x,v,\nu) &= g(t,x,v,\nu) \geq 0, \end{aligned}\right. \tag{15}$$

where the initial data f_0, the boundary data g, and the coefficients η, χ are bounded.

Then, for any given $T>0$, there exists a constant $\delta(T)>0$ (depending only on T and the L^∞ norms of η, χ, f_0 and g) such that

$$\forall (t,x,v,\nu)\in[0,T]\times X\times\mathbb{S}^2\times\mathbb{R}^+, \qquad 0\leq f(t,x,v,\nu)\leq\delta(T). \tag{16}$$

Proof of Lemma 2.1.

Let us denote $Q=\{(t,x)|t\in\mathbb{R}^+, x\in X\}$, and denote by Σ the boundary of Q. The boundary Σ has thus two parts:

$$\Sigma=\Sigma_1\bigcup\Sigma_2=\{(0,x)|x\in X\}\bigcup\left\{(t,x)|t\in\mathbb{R}^+, x\in\partial X\right\}.$$

Let us fix a point $M^*=(t^*,x^*)$ in Q, and introduce a characteristic line through M^* as

$$t\longmapsto x(t)=x^*-c\ v(t^*-t). \tag{17}$$

We look for the intersection of this characteristic line with Σ, the boundary of Q. There are two cases: either the line remains in Q and intersects Σ_1, (that is, the plane $t=0$) at the point $x(0)=x_0=x^*-c\ v\ t^*$, or the line intersects $\Sigma_2=\{(t,x)|x\in\partial X, t>0\}$ at some point $(t_0,x(t_0))$ with $0\leq t_0<t^*$.

In both cases, it is possible to write f explicitly in terms of f_0, g, χ and η using the characteristic lines (17) and Duhamel's formula. The estimate is obtained by taking L^∞ norms in this explicit formulation of f. We refer to[8] for details. □

Proof of Theorem 1.1: We begin by proving the existence of solutions to system (5) – (10) (when ϵ is fixed) thanks to an iterative procedure. In order to keep notations tractable, we denote f instead of f^ϵ and n_i instead of n_i^ϵ.

This procedure is defined in this way:

For $t \geq 0$, we set

$$f^0(t,x,v,\nu) = f_0(x,v,\nu), \quad n_i^0(t,x) = n_{i0}(x),\ i = 1,2;$$

For $k = 0,1,2,...$, we assume that (f^k, n_1^k, n_2^k) are defined. We define $f^{k+1}, n_1^{k+1}, n_2^{k+1}$ by

$$\begin{cases} \dfrac{1}{c}\partial_t f^{k+1} + v \cdot \nabla_x f^{k+1} = \left(n_2^k A_{21} - (n_1^k B_{12} - n_2^k B_{21}) f^{k+1}\right) \phi_{12}(\nu) h\nu, \\ f^{k+1}(0,x,v,\nu) = f_0(x,v,\nu), \\ f^{k+1}|_{\mathbb{R}^+ \times (\partial X \times \mathbb{S}^2)_- \times \mathbb{R}^+}(t,x,v,\nu) = g(t,x,v,\nu), \end{cases} \tag{18}$$

and

$$\begin{cases} \epsilon \partial_t n_1^{k+1} = n_2^{k+1} A_{21} + (n_2^{k+1} B_{21} - n_1^{k+1} B_{12}) \rho^{k+1} + (n_2^{k+1} C_{21} - n_1^{k+1} C_{12}), \\ \epsilon \partial_t n_2^{k+1} = -\left[n_2^{k+1} A_{21} + (n_2^{k+1} B_{21} - n_1^{k+1} B_{12}) \rho^{k+1} + (n_2^{k+1} C_{21} - n_1^{k+1} C_{12})\right], \\ n_i^{k+1}(0,x) = n_{i0}(x),\ i = 1,2. \end{cases} \tag{19}$$

Note that n_1^{k+1} and n_2^{k+1} can be written explicitly in terms of f^{k+1} in eq. (19) thanks to Duhamel's formula.

Using Lemma 2.1 and the nonnegativity of the initial population densities n_{i0} (and of f_0), we see that $(f^{k+1}, n_1^{k+1}, n_2^{k+1})$ are well-defined, and that

$$\forall k \in \mathbb{N},\ i = 1,2, \qquad n_i^k \geq 0, \qquad n_1^k + n_2^k = n_{10} + n_{20} = n.$$

Moreover, still thanks to lemma 2.1, we see that f^k satisfies $0 \leq f^k(t,x,v,\nu) \leq \delta(T)$, for all $(t,x,v,\nu) \in [0,T] \times X \times \mathbb{S}^2 \times \mathbb{R}^+$.

Using the equation satisfied by $f^{k+1} - f^k$ and the characteristics, it is possible to show that (when $t \in [0,T]$)

$$\left\| f^{k+1} - f^k \right\|_{L^\infty_{x,v,\nu}}(t) \leq \xi_1(T) \int_0^t \left\| \left(n_1^k - n_1^{k-1}\right)(s) \right\|_{L^\infty_x} \mathrm{d}s, \tag{20}$$

for some constant $\xi_1(T) \geq 0$.

Using then the equation satisfied by $n_1^{k+1} - n_1^k$, it is possible to show that (when $t \in [0,T]$)

$$\|n_1^{k+1} - n_1^k\|_{L^\infty_x}(t) \leq \frac{\xi_2(T)}{\epsilon} \sup_{s\in[0,t]} \left\| \left(f^{k+1} - f^k\right)(s) \right\|_{L^\infty_{x,v,\nu}}, \qquad (21)$$

for some constant $\xi_2(T) \geq 0$. The proof of estimates (20) and (21) is detailed in.[8]

Using (20) and (21), a classical induction argument shows that for all $k \in \mathbb{N},\ p \in \mathbb{N}^*$,

$$\|n_1^{k+p} - n_1^k\|_{L^\infty([0,T]\times X)} \leq Cst \sum_{l=k}^{k+p-1} \frac{(\xi_1(T)\,\xi_2(T)/\epsilon)^l}{l!}.$$

Thus we obtain that $(n_1^k)_k$ is a Cauchy sequence in $L^\infty([0,T]\times X)$. The same holds of course for $(n_2^k)_k$. Then, using estimate (20), we see that $(f^k)_k$ is also a Cauchy sequence in $L^\infty([0,T]\times X\times \mathbb{S}^2\times\mathbb{R}^+)$. We can therefore pass to the limit in (the Duhamel formulations of) equations (18) and (19), and obtain a bounded solution f, n_1, n_2 to the coupled system (5) – (10).

Uniqueness is obtained by simply considering two solutions (f, n_1, n_2) and $(\overline{f}, \overline{n}_1, \overline{n}_2)$ to (5) – (10) with the same initial and boundary conditions, and by using estimates (20), (21) (with f, $\overline{f}$ instead of f^{k+1}, f^k, and the same for the populations). This ends the proof of the first part of theorem 1.1.

We conclude this section by observing that when we replace (19) by

$$\begin{cases} n_1^{k+1} = \dfrac{A_{21} + B_{21}\rho^{k+1} + C_{21}}{A_{21} + (B_{21}+B_{12})\rho^{k+1} + C_{12} + C_{21}}\, n, \\ n_2^{k+1} = \dfrac{B_{12}\rho^{k+1} + C_{12}}{A_{21} + (B_{21}+B_{12})\rho^{k+1} + C_{12} + C_{21}}\, n, \end{cases} \qquad (22)$$

the inductive procedure (18), (22) together with estimate (20) enables to build a solution to system (5), (6), (14). Uniqueness for this system is also a consequence of estimate (20). We refer to[8] for details.

3. Quasi-stationary approximation, convergence

In this section, we prove the second part of Theorem 1.1, that is the convergence of the solution f^ϵ, $(n_i^\epsilon)_{i=1,2}$ toward the solution f, $(n_i)_{i=1,2}$ of the limiting system (5), (6), (14).

We already know that for $i = 1, 2$, $0 \leq n_i^\epsilon(t,x) \leq ||n||_{L^\infty}$. As a consequence of lemma 2.1 and this estimate, we obtain that $(f^\epsilon)_\epsilon$ is bounded in

$L^\infty([0,T]\times X\times\mathbb{S}^2\times\mathbb{R}^+)$, so that $\int_{\mathbb{R}^+} f^\epsilon(t,x,v,\nu)\,\phi_{12}(\nu)\,\mathrm{d}\nu$ is bounded in $L^\infty([0,T]\times X\times\mathbb{S}^2)$. Furthermore, this quantity solves the following system:

$$\begin{cases} \dfrac{1}{c}\partial_t \displaystyle\int_{\mathbb{R}^+} f^\epsilon\phi_{12}(\nu)\mathrm{d}\nu + v\cdot\nabla_x \int_{\mathbb{R}^+} f^\epsilon\phi_{12}(\nu)\mathrm{d}\nu \\ \qquad = n_2^\epsilon A_{21}\displaystyle\int_{\mathbb{R}^+}\phi_{12}^2(\nu)h\nu\mathrm{d}\nu - (n_1^\epsilon B_{12}-n_2^\epsilon B_{21})\int_{\mathbb{R}^+} f^\epsilon\phi_{12}^2(\nu)h\nu\mathrm{d}\nu, \\ \left(\displaystyle\int_{\mathbb{R}^+} f^\epsilon\phi_{12}(\nu)\mathrm{d}\nu\right)(0,x,v) = \int_{\mathbb{R}^+} f_0(x,v,\nu)\phi_{12}(\nu)\mathrm{d}\nu, \\ \left(\displaystyle\int_{\mathbb{R}^+} f^\epsilon\phi_{12}(\nu)\mathrm{d}\nu\right)\Big|_{\mathbb{R}^+\times(\partial X\times\mathbb{S}^2)_-} = \int_{\mathbb{R}^+} g(t,x,v,\nu)\phi_{12}(\nu)\mathrm{d}\nu. \end{cases}$$

Using the L^∞ bounds of f^ϵ, n_i^ϵ and the properties of ϕ_{12}, we see that

$$(\frac{1}{c}\partial_t + v\cdot\nabla_x)\int_{\mathbb{R}^+} f^\epsilon\phi_{12}(\nu)\mathrm{d}\nu$$

is bounded in $L^\infty([0,T]\times X\times\mathbb{S}^2)$. Thanks to an averaging lemma ([6,7]), we obtain that the family $\int_{\mathbb{R}^+}\int_{\mathbb{S}^2} f^\epsilon(t,x,v,\nu)\phi(\nu)\mathrm{d}v\mathrm{d}\nu = \rho^\epsilon(t,x)$ is strongly compact in $L^2([0,T]\times X)$. This ensures that ρ^ϵ converges (up to a subsequence) a.e.

Thus (still up to a subsequence), we can assume that

$$\begin{aligned} &n_i^\epsilon \rightharpoonup n_i \text{ weakly}^* \text{ in } L^\infty([0,T]\times X), \qquad i=1,2; \\ &f^\epsilon \rightharpoonup f \text{ weakly}^* \text{ in } L^\infty([0,T]\times X\times\mathbb{S}^2\times\mathbb{R}^+); \\ &\rho^\epsilon \to \rho \text{ strongly in } L^1([0,T]\times X), \end{aligned}$$

where

$$\rho = \int_{\mathbb{R}^+}\int_{\mathbb{S}^2} f\phi_{12}(\nu)\mathrm{d}v\mathrm{d}\nu.$$

The sequence $n_i^\epsilon\rho^\epsilon$ converges therefore to $n_i\rho$ weakly in $L^1([0,T]\times X)$.

It remains also to pass to the limit in the quantity $n_i^\epsilon\, f^\epsilon\,\phi_{12}(\nu)\,h\nu$. This is done by observing that for any test function $\psi_1(v)\,\psi_2(\nu)$ (with $\psi_1,\psi_2\in\mathcal{D}$), the quantity

$$\int_{\mathbb{R}^+}\int_{\mathbb{S}^2} f^\epsilon(t,x,v,\nu)\,\phi_{12}(\nu)\,h\nu\,\psi_1(v)\,\psi_2(\nu)\,\mathrm{d}v\mathrm{d}\nu$$

converges for a.e. t,x. This is due to the fact that the quantity $\int_{\mathbb{R}^+} f^\epsilon(t,x,v,\nu)\,\phi_{12}(\nu)\,h\nu\,\psi_2(\nu)\,\mathrm{d}\nu$ satisfies a kinetic equation (like $\int_{\mathbb{R}^+} f^\epsilon(t,x,v,\nu)\,\phi_{12}(\nu)\,\mathrm{d}\nu$), so that it is possible to use an averaging lemma.

Finally, when ϵ tend to 0, the solution to (5) – (10) converges up to extraction to a solution of (5), (6), (14).

Thanks to the result of uniqueness for (5), (6), (14) obtained in the previous section, the convergence is in fact not restricted to a subsequence. This ends the proof of Theorem 1.1.

We notice that in the limiting equation, no initial data are needed for the populations n_1, n_2. As a consequence, an initial layer appears if the initial data of the problem for a given $\epsilon > 0$ are not compatible with the limiting equation.

4. Numerical simulation

We introduce a numerical test in order to see how the quasi-static approximation is valid in practice. This test is inspired from the problem that was introduced in.[4,11] It consists in a 3D computation with two populations of atoms ($K = 2$), and no initial layer. For a detailed description of the data, we refer to.[8]

The rate equations of the atomic populations are discretized with usual methods for the ODEs, while for solving the kinetic equation, we use a particle method.

In order to verify the convergence of solutions, we compute the (relative) difference between n_1^ϵ and n_1, (solution of the limiting system) i.e

$$\frac{|n_1^\epsilon(t,x) - n_1(t,x)|}{n_1(t,x)}, \tag{23}$$

obtained at a given time for different values of ϵ. This quantity is presented as a function of $|x|$, for a given direction of the space variable.

The validity of the quasi-static approximation is observed on our simulation, see fig. 1. In practice, the value of ϵ is usually extremely small (smaller than in the simulations presented here).

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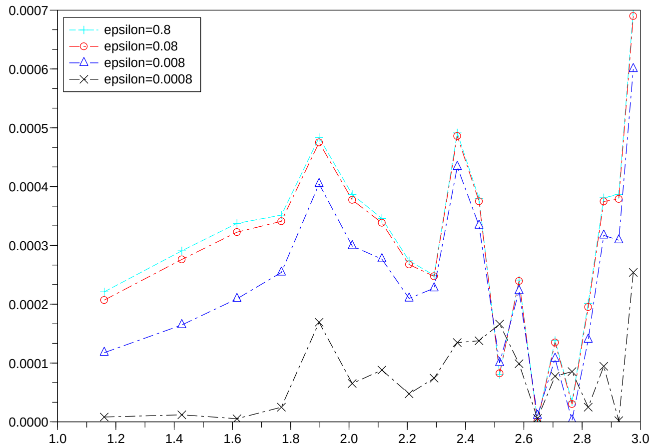

Fig. 1. $|n_1^\epsilon - n_1|/n_1$ in terms of $|x|$

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