

# DERIVATION OF THE NEUTRON DIFFUSION EQUATION

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## ABSTRACT

We discuss the diffusion equation as an asymptotic limit of the neutron transport equation for large scattering cross sections. We show that the classical asymptotic expansion procedure does not lead to the diffusion equation and present two modified approaches to overcome this difficulty. The effect of the initial layer is also discussed.

## Introduction

In the early years of this century there existed two completely independent descriptions of fluids.

In the fluid dynamics theory, linked to such names as Euler, Navier and Stokes, fluid is treated as a continuous medium described in terms of local density, velocity and energy which satisfy partial differential equations. Fluid dynamical approach has proved to be extremely successful in practical applications and up to this day is a basic tool for predicting the behaviour of fluids.

With the advent of the molecular hypothesis and after Boltzmann had formulated his famous equation, the kinetic theory appeared as an alternative description of fluids. It treated fluid as a collection of particles in terms of a one-particle distribution function satisfying an integro-differential equation.

At this stage there was a great deal of uneasiness among the physicists who could not see any link between the two theories. It took a mathematician, David Hilbert, to supply such a link. In 1912 he published a monograph on integral equations in which he introduced a perturbation procedure for the Boltzmann equation to illustrate the Fredholm alternative. To the astonishment of contemporary physicists he was able to show that the well known Euler equations describing an inviscid fluid can be obtained as an asymptotic limit of the Boltzmann kinetic equation if the collision frequency is very large or, in other words, the system tends rapidly to the local thermal equilibrium.

Soon afterwards, Chapman and then, independently, Enskog, introduced a modified asymptotic expansion which lead to the Navier-Stokes equation describing viscous fluids. Since then it has been generally accepted that any kinetic system in which the approach to the local thermal equilibrium is sufficiently rapid, can be adequately described by the first five moments of the distribution function, that is, density, three components of velocity and energy.

In the real world the majority of fluids are not far away from the state of local thermal equilibrium and the standard tool for physicists and engineers solving practical problems for fluids are the (nonlinear) partial differential equations of fluid dynamics. Only in exceptional cases the more complicated description offered by the Boltzmann kinetic equation is to be used.

In general the fluid-dynamical and kinetic equations are nonlinear due to the binary collisions between particles or collective interactions in media such as liquids and plasmas. In some instances, however, the density of particles under consideration is so low that only the interactions with the host medium are to be taken into account and the equations become linear. In such cases the kinetic description is given by the so-called transport equation and the fluid-dynamical description by the diffusion equation.

By far the most important and most widely developed field of application of the transport theory is the description of the behaviour of neutrons in a nuclear fission reactor. First attempts in this direction were made already in the 1930's but the real development started during the second world war in connection with the Manhattan project.

Following the general pattern of the statistical mechanics the neutron transport and diffusion equations were introduced independently of each other and derived from the first principles (see, for instance, the famous monograph of Glasstone and Edlund [1]). It was then a common wisdom that diffusion theory was valid in case of small absorption and far away from the boundaries. The link between the two descriptions of a neutron gas was being obtained by an heuristic argument which consisted of expanding the neutron distribution function into Legendre polynomials and assuming that the gradient of the second moment as well as the time derivative of the neutron current can be neglected. An alternative procedure described in detail in the bible of neutron transport theoreticians, the monograph of Davidson [2], consists of considering exact solutions to the transport equation and showing their asymptotic parts to satisfy the diffusion equation.

The early attempts to treat the diffusion equation as an asymptotic limit of the neutron transport equation were hampered by the fact that the classical asymptotic

procedure of the type used by Hilbert for the Boltzmann equation does not give satisfactory results. The breakthrough was achieved by Larsen and Keller [3] who proposed a new time scale which allowed them to derive the diffusion equation by an heuristic argument. Using the same approach Bardos, Santos and Sentis [4] have proved rigorously that the diffusion equation is an asymptotic limit of the transport equation when the scattering mean free path tends to zero.

Recently, the authors [5, 6] proposed a different approach to the asymptotic analysis of the neutron transport equation based upon the adaptation of the Chapman-Enskog procedure.

In this paper we describe the three different asymptotic procedures and show in which sense the diffusion equation can be treated as an asymptotic limit of the transport equation. We present here only the heuristic argument, the rigorous treatment can be found in [5].

## Asymptotic analysis of the neutron transport equation

For the sake of simplicity we will consider one-velocity neutrons in plane geometry. Then the neutron distribution function  $\psi$  depends on space variable  $x$ , the angular variable  $\mu$  and time  $t$ . If  $\psi$  is expanded into normalised Legendre polynomials so that

$$\psi(x, \mu, t) = \sum_{m=0}^{\infty} u^m(x, t) P_m(\mu) \quad (1)$$

where

$$P_0(\mu) = \frac{1}{\sqrt{2}}, \quad P_1(\mu) = \sqrt{\frac{3}{2}}\mu,$$

$$\mu P_m(\mu) = \frac{m+1}{\sqrt{2m+3}\sqrt{2m+1}} P_{m+1}(\mu) + \frac{m}{\sqrt{2m+1}\sqrt{2m-1}} P_{m-1}(\mu), \quad m = 1, 2, \dots \quad (2)$$

then the neutron transport equation is equivalent to the infinite system (which Weinberg and Wigner [7] called the second form of the transport equation)

$$\begin{aligned} \partial_t u^0 + \frac{1}{\sqrt{3}} \partial_x u^1 + \sigma_a u^0 &= 0, \\ \partial_t u^m + \frac{m}{\sqrt{2m-1}\sqrt{2m+1}} \partial_x u^{m-1} + \\ + \frac{m+1}{\sqrt{2m+1}\sqrt{2m+3}} \partial_x u^{m+1} + \sigma_a u^m + \sigma_s(1-b_m)u^m &= 0, \quad m = 1, 2, \dots \end{aligned} \quad (3)$$

Here  $\partial_t = \frac{\partial}{\partial t}$ ,  $\partial_x = \frac{\partial}{\partial x}$ ,  $\sigma_a$  and  $\sigma_s$  are the absorption and scattering cross sections and  $b_m$  describe the anisotropic scattering with  $b_1$  equal to the average cosine of the

scattering angle. The coefficients  $\sigma_a, \sigma_s$  and  $b_m$  may depend on  $x$  and  $b_m(x) \leq \beta_m < 1$  for all  $x$ .

Here we are interested in time evolution of neutrons so we will assume that the system is infinite and no boundary condition for (3) is needed. Alternatively [5, 6] we could take periodic boundary conditions.

As the initial condition we take

$$u^m(x, 0) = \alpha_m(x), \quad m = 0, 1, 2, \dots \quad (4)$$

where  $\alpha_m(x)$  are given.

Now we make the assumption that the system described by (3) is rapidly approaching the (local) thermal equilibrium due to collisions. This means that we have to treat  $\sigma_s$  as very large or, alternatively, introduce a non-dimensional positive parameter  $\epsilon$  whose main task is to label terms of various orders of magnitude and write (3) in the form

$$\begin{aligned} \partial_t u^0 + \frac{1}{\sqrt{3}} \partial_x u^0 + \sigma_a u^0 &= 0, \\ \epsilon \left[ \partial_t u^m + \frac{m}{\sqrt{2m-1}\sqrt{2m+1}} \partial_x u^{m-1} + \frac{m+1}{\sqrt{2m+1}\sqrt{2m+3}} \partial_x u^{m+1} + \sigma_a u^m \right] \\ &+ \sigma_s(1-b_m)u^m = 0, \quad m = 1, 2, \dots \end{aligned} \quad (5)$$

This is a singularly perturbed problem and we expect that the approximate solution will consist of the bulk solution and of the initial layer solution which decays exponentially over the time interval of order of  $\epsilon$ .

In the classical approach which coincides with that of Hilbert the bulk solution is assumed to be of the form

$$u^m = u_0^m + \epsilon u_1^m + \epsilon^2 u_2^m + \dots, \quad m = 0, 1, 2, \dots \quad (6)$$

This is inserted into (5) and terms of the same order in  $\epsilon$  are collected. As a result one obtains the system of equations for the first two moments:

$$\begin{aligned} \epsilon^0 : \quad \partial_t u_0^0 + \frac{1}{\sqrt{3}} \partial_x u_0^0 + \sigma_a u_0^0 &= 0, \\ u_0^1 &= 0, \\ \epsilon^1 : \quad \partial_t u_1^0 + \frac{1}{\sqrt{3}} \partial_x u_1^0 + \sigma_a u_1^0 &= 0, \\ u_1^1 &= -\frac{\lambda_{tr}}{\sqrt{3}} \partial_x u_0^0, \\ \epsilon^2 : \quad \partial_t u_2^0 + \frac{1}{\sqrt{3}} \partial_x u_2^0 + \sigma_a u_2^0 &= 0, \\ u_2^1 &= -\frac{\lambda_{tr}}{\sqrt{3}} \partial_x u_1^0 + \frac{\lambda_{tr}^2}{\sqrt{3}} (\partial_t + \sigma_a) \partial_x u_0^0, \end{aligned} \quad (7)$$

where  $1/\lambda_{tr} = \sigma_s(1 - b_1)$ .

Eliminating  $u_1^1$  and  $u_2^1$  we obtain

$$\begin{aligned} \epsilon^0 &: \partial_t u_0^0 + \sigma_a u_0^0 = 0, \\ \epsilon^1 &: \partial_t u_1^0 + \sigma_a u_1^0 - \frac{1}{3} \partial_x (\lambda_{tr} \partial_x u_0^0) = 0, \\ \epsilon^2 &: \partial_t u_2^0 + \sigma_a u_2^0 - \frac{1}{3} (\lambda_{tr} \partial_x u_1^0) \\ &\quad + \frac{1}{3} \partial_x [\lambda_{tr}^2 (\partial_t + \sigma_a) \partial_x u_0^0] = 0. \end{aligned} \tag{8}$$

We see that at each level of approximation we have a rather trivial ordinary differential equation with the inhomogeneous term of increasing complexity but no diffusion equation.

To overcome this difficulty Larsen and Keller [3] proposed to relabel the terms in (5) by introducing the new time variable  $\theta = \epsilon t$  as it had been done previously by Kurtz [8] for the Carleman model of the Boltzmann equation. The system (5) will now have the form

$$\begin{aligned} \epsilon \partial_\theta u^0 + \frac{1}{\sqrt{3}} \partial_x u^1 + \epsilon \sigma_a u^0 &= 0, \\ \epsilon^2 [\partial_t u^m + \sigma_a u^m] + \epsilon \left[ \frac{m}{\sqrt{2m-1}\sqrt{2m+1}} \partial_x u^{m-1} + \frac{m+1}{\sqrt{2m+1}\sqrt{2m+3}} \partial_x u^{m+1} \right] \\ + \sigma_s(1 - b_m) u^m &= 0, \quad m = 1, 2, \dots \end{aligned} \tag{9}$$

In writing (9) we have to assume additionally that the absorption is very small when compared with streaming.

We expand now  $u^m$  in powers of  $\epsilon$  as in (6), substitute the expansion into (9) and compare terms of the same order in  $\epsilon$  to obtain

$$\begin{aligned} \epsilon^0 &: u_0^1 = 0, \\ \epsilon^1 &: \partial_\theta u_0^0 + \frac{1}{\sqrt{3}} \partial_x u_1^1 + \sigma_a u_0^0 = 0, \\ &\quad u_1^1 = -\frac{\lambda_{tr}}{\sqrt{3}} \partial_x u_0^0, \\ \epsilon^2 &: \partial_\theta u_1^0 + \frac{1}{\sqrt{3}} \partial_x u_2^1 + \sigma_a u_1^0 = 0, \\ &\quad u_2^1 = -\frac{\lambda_{tr}}{\sqrt{3}} \partial_x u_1^0. \end{aligned} \tag{10}$$

Eliminating  $u_1^1$  and  $u_2^1$  we see that both  $u_0^0$  and  $u_1^0$  satisfy the same diffusion equation. Introducing

$$u^{0(1)} = u_0^0 + \epsilon u_1^0 \tag{11}$$

which represents the  $O(\epsilon^2)$  approximation to the neutron density and returning to the original time variable we see that it satisfies the diffusion equation

$$\partial_t u^{0(1)} - \epsilon \partial_x (D \partial_x u^{0(1)}) + \sigma_a u^{0(1)} = 0 \quad (12)$$

where the diffusion constant  $D = \epsilon \lambda_{tr}/3$  is proportional to  $\epsilon$  and so is the absorption term.

In [5, 6] the authors proposed an alternative derivation of the diffusion equation using the asymptotic procedure of Chapman-Enskog in the version proposed by Mika [9]. The basic assumptions of that approach are:

- (i) the neutron density  $u^0$  remains unexpanded at each level of approximation,
- (ii) the time derivatives of higher moments  $u^m$ ,  $m \geq 1$ , are expressed in terms of spatial derivatives of  $u^0$ .

To obtain the  $O(\epsilon^2)$  approximation  $u^{0(1)}$  to the neutron density we substitute  $u_0^1 + \epsilon u_1^1$  into (5). Then we have

$$\partial_t u^{0(1)} + \frac{1}{\sqrt{3}} \partial_x (u_0^1 + \epsilon u_1^1) + \sigma_a u^{0(1)} = 0. \quad (13)$$

As in previous cases  $u_0^1 = 0$  and

$$u_1^1 = -\frac{\lambda_{tr}}{\sqrt{3}} \partial_x y^{0(1)} \quad (14)$$

so that (13) gives the diffusion equation

$$\partial_t u^{0(1)} - \epsilon \partial_x (D \partial_x u^{0(1)}) + \sigma_a u^{0(1)} = 0 \quad (15)$$

which differs from (12) only in that  $\sigma_a$  is not multiplied by  $\epsilon$ .

## Initial layer solution and the effective initial condition for the diffusion equation

The diffusion equation (12) (or (15)) is supposed to describe the neutron density up to terms of order of  $\epsilon^2$  except for the initial layer. However, even if we are not interested in what is actually happening near  $t = 0$ , to maintain the  $O(\epsilon^2)$  approximation we have to modify the straightforward initial condition for  $u^0$  as given in (4).

The initial layer is analysed by introducing the stretched time  $\tau = t/\epsilon$  into the system of equations (5) and then using the standard approach expanding all moments into powers of  $\epsilon$ . The details can be found in [5]. Here we will merely quote the final result.

The effective initial condition to be used for (12) or (15) is

$$u^{0(1)}(0, x) = \alpha_0(x) - \epsilon \sqrt{\frac{3}{2}} \partial_x [D(x) \alpha_1(x)]. \quad (16)$$

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