

The diffusion approximation in neutron transport theory – asymptotic expansions

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1 Introduction

intro

- Motion of neutrons through a material medium is usually described by the Boltzmann transport equations. This is a linear integrodifferential equation for the neutron distribution, with appropriate initial and boundary conditions.
- A common approximation is diffusion theory. This is a linear equation based on Fick's law for the neutron flux. It yields good working results for most practical situations, but tends to be based on seemingly ad-hoc assumptions.
- Objectives are
 1. Derive the diffusion equation systematically from the transport equation.
 2. Determine appropriate boundary conditions for it.
- Main references:
 - K.M. Case, Elementary solutions of the transport equation and their applications, *Annals Phys.* **9** (1960), 1–23.
 - K.M. Case and P.F. Zweifel, *Linear transport theory*, Addison-Wesley, Reading, Mass., (1967).
 - G.J. Habetler and B.J. Matkowsky, Uniform asymptotic expansions in transport theory with small mean free paths, and the diffusion approximation, *J. Math. Phys.* **16** (1975), 846–854.

2 Problem formulation

We closely follow here the notation of Prinja and Larsen [7], when appropriate. Let $N(\mathbf{r}, \boldsymbol{\Omega}, t)$ denote the (angular) neutron density (number per unit volume) at spatial location \mathbf{r} , velocity direction $\boldsymbol{\Omega}$ and time t . We only consider neutrons of the same

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energy i.e. the so-called one-speed or monoenergetic case. Let $V \subset D$ be an arbitrary fixed volume within the domain $D \subset \mathbb{R}^3$. The statement for conservation of neutrons is

$$\frac{d}{dt} \int_V N dV = - \int_{\partial V} \mathbf{H} \cdot \mathbf{n} dS + \int_V q dV \quad (1) \quad \boxed{\text{eq:cons1}}$$

where \mathbf{H} is the flux of neutrons i.e. numbers crossing a unit cross-section per unit time, \mathbf{n} is the unit outward normal to the boundary ∂V , q is the neutron source (sink). Using the divergence theorem gives

$$\int_V \left(\frac{\partial N}{\partial t} + \nabla \cdot \mathbf{H} - q \right) dV = 0. \quad (2) \quad \boxed{\text{eq:cons2}}$$

Since V is arbitrary and the integrand is assumed continuous, we may deduce the point form ¹

$$\frac{\partial N}{\partial t} + \nabla \cdot \mathbf{H} = q. \quad (3) \quad \boxed{\text{eq:cons3}}$$

The neutron flux is given by $\mathbf{H} = N\mathbf{v}$, where \mathbf{v} is the velocity. The velocity is assumed constant and written as $\mathbf{v} = v\boldsymbol{\Omega}$, where v is the speed (constant) and $\boldsymbol{\Omega}$ is the direction. Thus

$$\nabla \cdot \mathbf{H} = v\boldsymbol{\Omega} \cdot \nabla N \quad (4) \quad \boxed{\text{eq:flux}}$$

noting that $\nabla \cdot \mathbf{v} = 0$.

The source q is composed of several terms relating to the different types of neutron interaction as well as a genuine external neutron source $Q(\mathbf{r}, \boldsymbol{\Omega}, t)$. The types of interaction are scattering, fission and capture. Each interaction has an associated macroscopic cross-section, which is related to it's microscopic cross-section (see Appendix A). The macroscopic cross-sections of fission and capture may depend on position and are denoted by $\sigma_f(\mathbf{r})$ and $\sigma_c(\mathbf{r})$ respectively. The macroscopic cross-section of scattering may vary with position as well as orientation and is denoted by $\sigma_s(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')$. The total macroscopic cross-section $\sigma(\mathbf{r})$ is defined as

$$\sigma(\mathbf{r}) = \sigma_f(\mathbf{r}) + \sigma_c(\mathbf{r}) + \frac{1}{4\pi} \int_{\mathbb{S}^2} \sigma_s(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') dS(\boldsymbol{\Omega}'). \quad (5) \quad \boxed{\text{eq:sigt}}$$

As neutrons are lost through the total cross-section as well as gained through scattering and fission, we take

$$q = -v\sigma(\mathbf{r}) N(\mathbf{r}, \boldsymbol{\Omega}, t) + \frac{1}{4\pi} \int_{\mathbb{S}^2} v\sigma_s(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') N(\mathbf{r}, \boldsymbol{\Omega}', t) dS(\boldsymbol{\Omega}') + \frac{\nu(\mathbf{r})}{4\pi} v\sigma_f(\mathbf{r}) \int_{\mathbb{S}^2} N(\mathbf{r}, \boldsymbol{\Omega}', t) dS(\boldsymbol{\Omega}') + Q(\mathbf{r}, t), \quad (6) \quad \boxed{\text{eq:q}}$$

¹Equation (3) is a conservation statement that also holds more generally in other application contexts such as heat as well as mass transfer, see for example, section 5.1 in Fowler [4]. Interpreting N as temperature (technically heat) or concentration, then the well known heat equation follows using Fourier's law for the heat flux or the diffusion equation if Fick's law is used for the concentration flux.

where ν denotes the number of new neutrons from fission. Introducing the angular flux $\psi(\mathbf{r}, \boldsymbol{\Omega}, t) = \nu N(\mathbf{r}, \boldsymbol{\Omega}, t)$, then using (4) and (6) in (3) gives as the governing equation

$$\begin{aligned} \frac{1}{v} \frac{\partial \psi(\mathbf{r}, \boldsymbol{\Omega}, t)}{\partial t} + \boldsymbol{\Omega} \cdot \nabla \psi(\mathbf{r}, \boldsymbol{\Omega}, t) + \sigma(\mathbf{r}) \psi(\mathbf{r}, \boldsymbol{\Omega}, t) &= \frac{1}{4\pi} \int_{\mathbb{S}^2} \sigma_s(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') \psi(\mathbf{r}, \boldsymbol{\Omega}', t) dS(\boldsymbol{\Omega}') \\ &+ \frac{\nu}{4\pi} \sigma_f(\mathbf{r}) \int_{\mathbb{S}^2} \psi(\mathbf{r}, \boldsymbol{\Omega}', t) dS(\boldsymbol{\Omega}') + Q(\mathbf{r}, t). \end{aligned} \quad (7) \quad \boxed{\text{eq:ge}}$$

This equation is the fundamental transport equation for neutrons. If the scattering is assumed to be isotropic, so that $\sigma_s(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') = \sigma_s(\mathbf{r})$, then (7) simplifies to

$$\begin{aligned} \frac{1}{v} \frac{\partial \psi(\mathbf{r}, \boldsymbol{\Omega}, t)}{\partial t} + \boldsymbol{\Omega} \cdot \nabla \psi(\mathbf{r}, \boldsymbol{\Omega}, t) + \sigma(\mathbf{r}) \psi(\mathbf{r}, \boldsymbol{\Omega}, t) &= \frac{\sigma(\mathbf{r})c(\mathbf{r})}{4\pi} \int_{\mathbb{S}^2} \psi(\mathbf{r}, \boldsymbol{\Omega}', t) dS(\boldsymbol{\Omega}') \\ &+ Q(\mathbf{r}, t). \end{aligned} \quad (8) \quad \boxed{\text{eq:ge2}}$$

Here $c(\mathbf{r})$ is defined by

$$c(\mathbf{r}) = \frac{\sigma_s(\mathbf{r}) + \nu \sigma_f(\mathbf{r})}{\sigma(\mathbf{r})}$$

and represents the mean number of secondary neutrons produced per collision.

3 The 1-D problem and non-dimensionalisation

Here we derive the 1-D problem following [2]. We consider 1D slab geometry, so that the neutron flux ψ only depends on the position coordinate x and the direction coordinate $\Omega_x = \boldsymbol{\Omega} \cdot \mathbf{i} = \cos \theta = \mu$ ($\theta \in [0, \pi]$ being the polar angle). This reduces (8) to

$$\frac{1}{v} \frac{\partial \psi(x, \mu, t)}{\partial t} + \mu \frac{\partial \psi(x, \mu, t)}{\partial x} + \sigma(x) \psi(x, \mu, t) = \frac{\sigma(x)c(x)}{2} \int_{-1}^1 \psi(x, \mu', t) d\mu' + Q(x, t). \quad (9) \quad \boxed{\text{eq:ge1d}}$$

It is common to introduce the change of independent variable

$$x' = \int \sigma(x) dx, \quad (10) \quad \boxed{\text{eq:xp}}$$

where x' is termed the optical thickness. It is dimensionless and when combined with a scaling of the neutron source $Q(x, t) = \sigma(x)Q'(x', t)$ removes the cross-section function $\sigma(x)$ from all of the terms except for the time derivative term. However, for clarity of our nondimensionalisation below, we refrain from introducing this variable at this stage.

We consider the equation (9) on the interval $0 < x < d$ and $-1 \leq \mu \leq 1$, subject to boundary conditions

$$\begin{aligned} \text{on } x = 0: & \quad \psi = f_1(\mu, t) \quad \text{for } \mu > 0, \\ \text{on } x = d: & \quad \psi = f_2(\mu, t) \quad \text{for } \mu < 0, \end{aligned} \quad (11)$$

and the initial condition

$$\text{at } t = 0: \quad \psi = g(x, \mu) \quad \text{for } 0 \leq x \leq d, -1 \leq \mu \leq 1. \quad (12) \quad \boxed{\text{eq:ic}}$$

Here f_1, f_2 and g are prescribed functions, which may be assumed bounded and piecewise continuous.

We nondimensionalise as follows

$$x = d\bar{x}, \quad t = \frac{d}{v}\bar{t}, \quad \psi = \psi_0\bar{\psi}, \quad Q = \psi_0\sigma(x)\bar{Q}, \quad (13) \quad \boxed{\text{eq:nd1}}$$

using the geometry and neutron speed for characteristic length and time scales. The representative neutron density ψ_0 may be furnished from either the boundary conditions or the initial condition, which we conveniently write as

$$f_1 = \psi_0\bar{f}_1, \quad f_2 = \psi_0\bar{f}_2, \quad g = \psi_0\bar{g}. \quad (14) \quad \boxed{\text{eq:nd2}}$$

The variable μ is already dimensionless. The cross-section function is written as $\sigma = \sigma_0\bar{\sigma}(\bar{x})$, with the constant σ_0 being a representative value and introduce the dimensionless parameter

$$\epsilon = \frac{1}{\sigma_0 d}. \quad (15) \quad \boxed{\text{eq:ndp}}$$

This parameter may be interpreted as the ratio of mean free length $1/\sigma_0$ to the typical physical length of the domain. Using (13)–(15) in (9)–(12), we obtain for $\bar{\psi}(\bar{x}, \bar{t})$ the dimensionless problem

$$\frac{\epsilon}{\bar{\sigma}(\bar{x})} \frac{\partial \bar{\psi}}{\partial \bar{t}} + \frac{\epsilon \mu}{\bar{\sigma}(\bar{x})} \frac{\partial \bar{\psi}(\bar{x}, \mu, \bar{t})}{\partial \bar{x}} + \bar{\psi}(\bar{x}, \mu, \bar{t}) = \frac{c(\bar{x})}{2} \int_{-1}^1 \bar{\psi}(\bar{x}, \mu', \bar{t}) d\mu' + \bar{Q}(\bar{x}, \bar{t}), \quad (16) \quad \boxed{\text{eq:ndge}}$$

in $0 < \bar{x} < 1, -1 \leq \mu \leq 1$, with

$$\text{on } \bar{x} = 0: \quad \bar{\psi} = \bar{f}_1(\mu, \bar{t}) \quad \text{for } \mu > 0, \quad (17) \quad \boxed{\text{eq:ndbc1}}$$

$$\text{on } \bar{x} = 1: \quad \bar{\psi} = \bar{f}_2(\mu, \bar{t}) \quad \text{for } \mu < 0, \quad (18) \quad \boxed{\text{eq:ndbc2}}$$

$$\text{at } \bar{t} = 0: \quad \bar{\psi} = \bar{g}(\bar{x}, \mu) \quad \text{for } 0 \leq \bar{x} \leq 1, -1 \leq \mu \leq 1. \quad (19) \quad \boxed{\text{eq:ndic}}$$

Some remarks follow:

- It is noteworthy that nondimensionalisation has significantly reduced the number of parameters in the problem. The dimensional problem (9)–(12) has the four dimensional parameters (d, v, ψ_0, σ_0) , whilst (16)–(19) contains only the dimensionless parameter (or group) ϵ . The solution is thus controlled by the single dimensionless parameter ϵ , classifying solutions relative to which is much easier than the original four dimensional parameter space. Estimates of the size of ϵ (see Appendix A) are in the range

$$\epsilon \sim 10^{-9} - 10^{-3}. \quad (20)$$

This suggests considering the asymptotic limit $\epsilon \rightarrow 0$ for the system (16)–(19), which we address in the next section. It is worth remarking that numerical

solution of (16)–(19) runs into convergence difficulties at around $\epsilon \approx 10^{-5}$ to 10^{-6} . The asymptotic solution that we construct in section 4 becomes a better approximation as ϵ becomes smaller. Thus the asymptotic solution provides a viable alternative approximate solution in a parameter range that the numerical approaches encounter difficulties. As such, asymptotic and numerical approaches complement each other and the use of both allows accurate approximate solutions to be obtained over a wide (often full) parameter range.

- We could introduce the change of spatial variable

$$\xi = \int_0^{\bar{x}} \bar{\sigma}(s) ds \quad (21) \quad \boxed{\text{eq:xi}}$$

with $\xi_0 = \int_0^1 \bar{\sigma}(s) ds$, so that $\bar{\sigma}$ may be absorbed into the spatial derivative term i.e. $\frac{1}{\bar{\sigma}} \frac{\partial \bar{\psi}}{\partial \bar{x}} = \frac{\partial \bar{\psi}}{\partial \xi}$. Equation (16) is now posed on $0 < \xi < \xi_0$. The variable ξ is related to the optical thickness x' in (10) by $\xi = \epsilon x'$ with $\xi_0 = \epsilon d'$, where $d' = \int_0^d \sigma(s') ds'$ is the optical thickness of the physical length d of the domain. In the time-independent case this allows $\bar{\sigma}$ to be removed from the problem.

- For convenience we subsequently drop bars in (16)–(19).

4 Matched asymptotic expansions

sec:asy

We use the method of matched asymptotic expansions to determine the behaviour of the system (16)–(19) in the limit $\epsilon \rightarrow 0$. An introduction to the technique may be found in Bender and Orszag [1] and Hinch [5]. The key observation is that the problem with $\epsilon = 0$ is fundamentally different from that when $\epsilon > 0$, in that the both derivative terms are lost. As a result neither the boundary nor initial conditions can be imposed when $\epsilon = 0$. This suggests that the limit $\epsilon \rightarrow 0$ is singular. It turns out that the $\epsilon = 0$ problem will hold within the interior of the domain $0 < x < 1$, whilst in narrow regions near the spatial boundaries at $x = 0$ and $x = 1$, we will need to pull back the lost spatial derivative term. The convention is to term the region interior to the domain the outer region, whilst the narrow regions at the domain boundaries are termed inner regions or boundary layers. The approach is much like a jigsaw, where balances are found in different spatial (and time) regions and these then have to be pieced together to form the solution. The formal process of piecing the regions together is termed matching. The analysis below illustrates the method.

4.1 The outer region $0 < x < 1$

We begin by posing the regular expansion

$$\psi = \psi_0(x, \mu, t) + \epsilon \psi_1(x, \mu, t) + \epsilon^2 \psi_2(x, \mu, t) + \dots \quad \text{as } \epsilon \rightarrow 0. \quad (22) \quad \boxed{\text{eq:outer1}}$$

This series in powers of the small parameter ϵ is suggested directly from the governing equation (16) and is termed a Poincare expansion. For generality, we also expand

the mean secondary neutron function $c(x)$ and source $Q(x, t)$ in powers of ϵ , namely

$$c(x) = c_0(x) + \epsilon c_1(x) + \epsilon^2 c_2(x) + \dots \quad (23) \quad \text{eq:outer2}$$

$$Q(x, t) = Q_0(x, t) + \epsilon Q_1(x, t) + \epsilon^2 Q_2(x, t) + \dots \quad (24) \quad \text{eq:outer3}$$

since our objective is to understand when (16) yields a diffusion equation for ψ . It is also not clear at this stage if we are on the correct time scale and so we introduce the time scaling

$$t = \frac{\epsilon}{\delta} \tau \quad (25) \quad \text{eq:outer4}$$

with new time variable τ . For generality we take

$$\delta = K_0 + K_1 \epsilon + K_2 \epsilon^2 + \dots \quad (26) \quad \text{eq:outer5}$$

and the K_i are constants. Substituting (22)–(26) into (16) and equating like powers of ϵ gives a series of subproblems.

$$\text{At } O(\epsilon^0): \quad \frac{K_0}{\sigma(x)} \frac{\partial \psi_0}{\partial \tau} + \psi_0 = \frac{c_0(x)}{2} \int_{-1}^1 \psi_0(x, \mu', t) d\mu' + Q_0(x, t). \quad (27) \quad \text{eq:outep0}$$

Since μ does not occur explicitly in this equation, we have that

$$\psi_0 = \psi_0(x, \tau) \quad (28) \quad \text{eq:outpsi0}$$

i.e. ψ_0 is a function on x and τ only. Consequently (27) reduces to

$$\frac{K_0}{\sigma(x)} \frac{\partial \psi_0}{\partial \tau} + (1 - c_0(x)) \psi_0 = Q_0(x, \tau).$$

This equation allows the imposition of the initial condition (due to the presence of the time derivative) and is a valid equation for ψ_0 . However it is not a diffusion equation but rather a source dominated equation that can accommodate $c_0(x) \neq 1$. We note that if the coefficients in this equation vanish then ψ_0 will be undetermined at this order in ϵ , allowing it to satisfy a possibly different equation. Thus we take

$$K_0 = 0, \quad c_0 = 0 \quad \text{and} \quad Q_0 = 0. \quad (29)$$

$$\begin{aligned} \text{At } O(\epsilon): \quad \frac{K_1}{\sigma(x)} \frac{\partial \psi_0}{\partial \tau} + \frac{\mu}{\sigma(x)} \frac{\partial \psi_0}{\partial x} + \psi_1 &= \frac{c_0(x)}{2} \int_{-1}^1 \psi_1(x, \mu', \tau) d\mu' \\ &+ \frac{c_1(x)}{2} \int_{-1}^1 \psi_0(x, \tau) d\mu' + Q_1(x, \tau). \end{aligned} \quad (30) \quad \text{eq:outep1}$$

Thus $\psi_1(x, \mu, \tau)$ is at most linear in μ . Writing

$$\psi_1 = \psi_{10}(x, \tau) + \mu \psi_{11}(x, \tau) \quad (31) \quad \text{eq:outpsi1}$$

and using $c_0 = 1$, (30) gives

$$\frac{K_1}{\sigma(x)} \frac{\partial \psi_0}{\partial \tau} = c_1(x) \psi_0 + Q_1(x, \tau), \quad (32) \quad \text{eq:outep1a}$$

$$\frac{1}{\sigma(x)} \frac{\partial \psi_0}{\partial x} + \psi_{11} = 0, \quad (33) \quad \text{eq:outep1b}$$

on equating powers of μ . Again, (32) does not yield a diffusion equation for ψ_0 which remains undetermined (together with ψ_{10}) if

$$K_1 = 0, \quad c_1 = 0 \quad \text{and} \quad Q_1 = 0. \quad (34)$$

$$\begin{aligned} \text{At } O(\epsilon^2): \quad \frac{K_2}{\sigma(x)} \frac{\partial \psi_0}{\partial \tau} + \frac{\mu}{\sigma(x)} \frac{\partial \psi_1}{\partial x} + \psi_2 &= \frac{1}{2} \int_{-1}^1 \psi_2(x, \mu', \tau) d\mu' \\ &+ \frac{c_2(x)}{2} \int_{-1}^1 \psi_0(x, \tau) d\mu' + Q_2(x, \tau). \end{aligned} \quad (35) \quad \boxed{\text{eq:outep2}}$$

Thus $\psi_2(x, \mu, \tau)$ is at most quadratic in μ . Writing

$$\psi_2 = \psi_{20}(x, \tau) + \mu \psi_{21}(x, \tau) + \mu^2 \psi_{22}(x, \tau), \quad (36) \quad \boxed{\text{eq:outpsi2}}$$

and using with (28), (31) and (36) in (35) gives

$$\frac{K_2}{\sigma(x)} \frac{\partial \psi_0}{\partial \tau} = \frac{1}{3} \psi_{22} + c_2(x) \psi_0 + Q_2(x, \tau), \quad (37) \quad \boxed{\text{eq:outep2a}}$$

$$\frac{1}{\sigma(x)} \frac{\partial \psi_{10}}{\partial x} + \psi_{21} = 0, \quad (38) \quad \boxed{\text{eq:outep2b}}$$

$$\frac{1}{\sigma(x)} \frac{\partial \psi_{11}}{\partial x} + \psi_{22} = 0, \quad (39) \quad \boxed{\text{eq:outep2c}}$$

on equating powers of μ . Using (33) and (39) in (37) now yields

$$\frac{K_2}{\sigma(x)} \frac{\partial \psi_0}{\partial \tau} = \frac{1}{3\sigma(x)} \frac{\partial}{\partial x} \left(\frac{1}{\sigma(x)} \frac{\partial \psi_0}{\partial x} \right) + c_2(x) \psi_0 + Q_2, \quad (40) \quad \boxed{\text{eq:psi0diff}}$$

which is a diffusion equation for ψ_0 . Thus the timescale to obtain this diffusion equation is $t = O(1/\epsilon)$ and the source needs to be $O(\epsilon^2)$ for its effects not to dominate. From now on, we adopt this time scale with $\delta = K_2 \epsilon^2$, setting $K_i = 0$ for $i \geq 3$.

$$\begin{aligned} \text{At } O(\epsilon^3): \quad \frac{K_2}{\sigma(x)} \frac{\partial \psi_1}{\partial \tau} + \frac{\mu}{\sigma(x)} \frac{\partial \psi_2}{\partial x} + \psi_3 &= \frac{1}{2} \int_{-1}^1 \psi_3(x, \mu', \tau) d\mu' \\ &+ \frac{c_2(x)}{2} \int_{-1}^1 \psi_1(x, \mu', \tau) d\mu' + \frac{c_3(x)}{2} \int_{-1}^1 \psi_0(x, \tau) d\mu' + Q_3(x, \tau). \end{aligned} \quad (41) \quad \boxed{\text{eq:outep3}}$$

Thus $\psi_3(x, \mu, \tau)$ is at most a cubic in μ . Writing

$$\psi_3 = \psi_{30}(x, \tau) + \mu \psi_{31}(x, \tau) + \mu^2 \psi_{32}(x, \tau) + \mu^3 \psi_{33}(x, \tau), \quad (42) \quad \boxed{\text{eq:outpsi3}}$$

and using with (28), (31), (36) and (42) in (41) gives

$$\frac{K_2}{\sigma(x)} \frac{\partial \psi_{10}}{\partial \tau} = \frac{1}{3} \psi_{32} + c_2(x) \psi_{10} + c_3(x) \psi_0 + Q_3(x, \tau), \quad (43) \quad \text{eq:outep3a}$$

$$\frac{K_2}{\sigma(x)} \frac{\partial \psi_{11}}{\partial \tau} + \frac{1}{\sigma(x)} \frac{\partial \psi_{20}}{\partial x} + \psi_{31} = 0, \quad (44) \quad \text{eq:outep3b}$$

$$\frac{1}{\sigma(x)} \frac{\partial \psi_{21}}{\partial x} + \psi_{32} = 0, \quad (45) \quad \text{eq:outep3c}$$

$$\frac{1}{\sigma(x)} \frac{\partial \psi_{22}}{\partial x} + \psi_{33} = 0, \quad (46) \quad \text{eq:outep3d}$$

on equating powers of μ . Using (38) and (45) in (43) gives a diffusion equation for ψ_{10} , namely

$$\frac{K_2}{\sigma(x)} \frac{\partial \psi_{10}}{\partial \tau} = \frac{1}{3\sigma(x)} \frac{\partial}{\partial x} \left(\frac{1}{\sigma(x)} \frac{\partial \psi_{10}}{\partial x} \right) + c_2(x) \psi_{10} + c_3(x) \psi_0 + Q_3. \quad (47) \quad \text{eq:psi10diff}$$

Some remarks:

- Clearly we may proceed in a similar manner to higher order terms.
- The equation derived for the leading order term $\psi_0(x, \tau)$ will not be able to satisfy the boundary conditions (17) and (18) (since they involve μ , whilst ψ_0 is independent of μ). The reason for this is that the spatial derivative term in (16) is not present in (27) due to the small parameter ϵ . Consequently we need to recover the spatial derivative term in (16) in regions near the boundaries. This motivates the inner regions considered next.

4.2 The inner regions

We now consider the equation (16) in regions near to the boundaries. These will be termed inner regions or boundary layers as their width will be shown to be small relative to that of the outer region. We present the analysis for the region near $x = 0$, since that for $x = 1$ will then follow similarly.

We consider as inner variables

$$x = \epsilon y, \quad \psi = \Psi, \quad (48) \quad \text{eq:invars}$$

in terms of which, (16) becomes

$$\frac{\epsilon^2}{\sigma(\epsilon y)} \frac{\partial \Psi}{\partial \tau} + \frac{\mu}{\sigma(\epsilon y)} \frac{\partial \Psi(y, \mu, \tau)}{\partial y} + \Psi(y, \mu, \tau) = \frac{c(\epsilon y)}{2} \int_{-1}^1 \Psi(y, \mu', \tau) d\mu' + Q(\epsilon y, \tau). \quad (49) \quad \text{eq:inge1}$$

Here we have adopted the time scale identified by the outer expansion, namely $t = \tau/\epsilon$ (taking $K_2 = 1$). We assume that σ and Q have no spatial variation² in this region so that for small ϵ (keeping y fixed)

$$\sigma(\epsilon y) = \sigma(0), \quad Q(\epsilon y, \tau) = \epsilon^2 Q_2(0, \tau),$$

²If $\sigma(x)$ varies near the boundaries then it is advantageous to perform the change of variable (21).

where we set subsequent terms in the source expansion in (24) to zero for convenience. Also, for small ϵ with y fixed we have

$$\begin{aligned} c(\epsilon y) &= 1 + \epsilon^2 c_2(\epsilon y) + \epsilon^3 c_3(\epsilon y) + O(\epsilon^4) \\ &= 1 + \epsilon^2 c_2(0) + \epsilon^3 (c_3(0) + y c_2'(0)) + O(\epsilon^4), \end{aligned} \quad (50) \quad \text{eq:inc}$$

so that we may introduce

$$\hat{c}(y) = c(\epsilon y) = 1 + \epsilon^2 \hat{c}_2(y) + \epsilon^3 \hat{c}_3(y) + O(\epsilon^4) \quad (51) \quad \text{eq:chat}$$

with the $\hat{c}_i(y)$ as given in (50). Thus (49) takes the form

$$\frac{\epsilon^2}{\sigma(0)} \frac{\partial \Psi}{\partial \tau} + \frac{\mu}{\sigma(0)} \frac{\partial \Psi(y, \mu, \tau)}{\partial y} + \Psi(y, \mu, \tau) = \frac{\hat{c}(y)}{2} \int_{-1}^1 \Psi(y, \mu', \tau) d\mu' + \epsilon^2 Q_2(0, \tau). \quad (52) \quad \text{eq:inge2}$$

We consider this equation on the domain³ $0 < y < \infty$, $-1 \leq \mu \leq 1$. The boundary condition (17) becomes

$$\text{on } y = 0: \quad \Psi = f_1(\mu, \tau) \text{ for } \mu > 0, \quad (53) \quad \text{eq:inbc1}$$

We pose the expansion

$$\Psi = \Psi_0(y, \mu, \tau) + \epsilon \Psi_1(y, \mu, \tau) + \epsilon^2 \Psi_2(y, \mu, \tau) + \dots \quad \text{as } \epsilon \rightarrow 0. \quad (54) \quad \text{eq:inexp}$$

Substituting into (52) and using (51) gives a sequence of problems at each order in ϵ .

$$\text{At } O(\epsilon^0): \quad \frac{\mu}{\sigma(0)} \frac{\partial \Psi_0}{\partial y} + \Psi_0 = \frac{1}{2} \int_{-1}^1 \Psi_0(y, \mu', \tau) d\mu'. \quad (55) \quad \text{eq:inexp0}$$

$$\text{At } O(\epsilon): \quad \frac{\mu}{\sigma(0)} \frac{\partial \Psi_1}{\partial y} + \Psi_1 = \frac{1}{2} \int_{-1}^1 \Psi_1(y, \mu', \tau) d\mu'. \quad (56) \quad \text{eq:inexp1}$$

$$\begin{aligned} \text{At } O(\epsilon^2): \quad \frac{1}{\sigma(0)} \frac{\partial \Psi_0}{\partial \tau} + \frac{\mu}{\sigma(0)} \frac{\partial \Psi_2}{\partial y} + \Psi_2 &= \frac{1}{2} \int_{-1}^1 \Psi_2(y, \mu', \tau) d\mu' \\ &+ \frac{\hat{c}_2(y)}{2} \int_{-1}^1 \Psi_0(y, \mu', \tau) d\mu' + Q_2(0, \tau). \end{aligned} \quad (57) \quad \text{eq:inexp2}$$

The time derivative and source term do not enter the leading order problem for Ψ_0 nor the first order problem for Ψ_1 , but rather the second order problem for Ψ_2 . Substituting (54) into the boundary condition (53) gives

$$\text{At } O(\epsilon^0): \quad \Psi_0(0, \mu, \tau) = f_1(\mu, \tau). \quad (58) \quad \text{eq:inbcep0}$$

$$\text{At } O(\epsilon^1): \quad \Psi_1(0, \mu, \tau) = 0. \quad (59) \quad \text{eq:inbcep1}$$

$$\text{At } O(\epsilon^2): \quad \Psi_2(0, \mu, \tau) = 0. \quad (60) \quad \text{eq:inbcep2}$$

³The reason for y being on the semi-infinite interval is that the outer region is where $x = O(1)$. Hence $y = O(1/\epsilon)$ which tends to infinity as $\epsilon \rightarrow 0$.

The leading order term, Ψ_0 , satisfies a constant coefficient half-space problem. The equation (55) possess a general solution in the form

$$\Psi_0(y, \mu, \tau) = a_0(\tau) + b_0(\tau)(\sigma(0)y - \mu) + \int_{-1}^1 A_0(\nu, \tau) \phi_\nu(\mu) e^{-y\sigma(0)/\nu} d\nu \quad (61) \quad \text{eq:Psi0}$$

where

$$\phi_\nu(\mu) = \frac{\nu}{2} P \frac{1}{\nu - \mu} + \lambda(\nu) \delta(\nu - \mu), \quad \lambda(\nu) = 1 - \nu \tanh^{-1} \nu. \quad (62) \quad \text{eq:phi}$$

The representation (61) is an eigenfunction expansion, where P denotes the Cauchy principle value and δ the Dirac delta function. The solutions 1 and $(\sigma(0)y - \mu)$ are classical solutions and correspond to the discrete spectrum of the transport operator, whilst the functions $\phi_\nu(\mu) e^{-y/\nu}$ are a one parameter family of singular or distributional solutions corresponding to the continuous spectrum. These are derived and discussed further in Appendix B. Here, $a_0(\tau)$, $b_0(\tau)$, $A_0(\mu, \tau)$ are arbitrary functions of τ (and also μ in the case of A_0) and are to be determined from the boundary condition at $y = 0$ and the matching condition as $y \rightarrow \infty$.

We perform matching of the outer and inner solutions in the next section. However, it is worth noting that the leading order outer solution contains no growing exponentials, so matching with the leading order inner solution requires that

$$A_0(\nu, \tau) = 0 \quad \text{for } \nu < 0. \quad (63) \quad \text{eq:A0a}$$

This restricts the continuous eigenfunctions to the half range $0 \leq \mu \leq 1$. A half-range completeness theorem is stated in Case [2] or section 4.8 of Case and Zweifel [3]. The boundary condition (58) gives

$$f_1(\mu, \tau) = a_0(\tau) - b_0(\tau)\mu + \int_0^1 A_0(\nu, \tau) \phi_\nu(\mu) d\nu, \quad \mu > 0. \quad (64) \quad \text{eq:inbc0}$$

The necessary orthogonality conditions to extract the coefficients a_0, b_0, A_0 are

$$\int_0^1 \phi_\nu(\mu) \gamma(\mu) d\mu = 0 \quad (65) \quad \text{eq:oc1}$$

and

$$\int_0^1 \phi_\nu(\mu) \phi_{\nu'}(\mu) \gamma(\mu) d\mu = \frac{\gamma(\nu)}{\nu} N(\nu) \delta(\nu - \nu'), \quad (66) \quad \text{eq:oc2}$$

where

$$\gamma(\mu) = \frac{3\mu}{2X(-\mu)}, \quad N(\nu) = \nu \left(\lambda(\nu)^2 + \frac{\pi^2 \nu^2}{4} \right). \quad (67) \quad \text{eq:gamma}$$

The function $X(z)$ is defined as

$$X(z) = \frac{1}{1-z} \exp \left(\frac{1}{\pi} \int_0^1 \frac{1}{(\mu' - z)} \tan^{-1} \left[\frac{\pi \mu'}{2\lambda(\mu')} \right] d\mu' \right),$$

whilst $\lambda(\nu)$ is given in (62). Multiplying (64) respectively by the weight function $\gamma(\mu)$ and then $\phi_{\nu'}(\mu)\gamma(\mu)$ gives

$$\int_0^1 f_1(\mu, \tau) \gamma(\mu) d\mu = a_0(\tau) \gamma_0 - b_0(\tau) \gamma_1,$$

and

$$\int_0^1 f_1(\mu, \tau) \phi_{\nu'}(\mu) \gamma(\mu) d\mu = \frac{\nu b_0(\tau) \gamma_0}{\nu'} + \frac{A_0(\nu')}{\nu'} \gamma(\nu') N(\nu'),$$

where

$$\gamma_i = \int_0^1 \mu^i \gamma(\mu) d\mu \quad \text{for } i = 0, 1.$$

Consequently

$$a_0(\tau) = \frac{\gamma_1}{\gamma_0} b_0(\tau) + \frac{1}{\gamma_0} \int_0^1 f_1(\mu, \tau) \gamma(\mu) d\mu, \quad (68) \quad \boxed{\text{eq:a0}}$$

$$A_0(\nu, \tau) = -\frac{\nu^2 \gamma_0 b_0(\tau)}{2\gamma(\nu) N(\nu)} + \frac{\nu}{\gamma(\nu) N(\nu)} \int_0^1 f_1(\mu, \tau) \phi_{\nu}(\mu) \gamma(\mu) d\mu. \quad (69) \quad \boxed{\text{eq:A0}}$$

The function $b_0(\tau)$ remains to be determined through matching to the outer solution.

In a similar manner, the solution to the first order problem (56) with (59) is

$$\Psi_1(y, \mu, \tau) = a_1(\tau) + b_1(\tau)(\sigma(0)y - \mu) + \int_0^1 A_1(\mu, \tau) \phi_{\nu}(\mu) e^{-y\sigma(0)/\nu} d\nu, \quad (70) \quad \boxed{\text{eq:Psi1}}$$

with

$$a_1(\tau) = \frac{\gamma_1}{\gamma_0} b_1(\tau), \quad (71)$$

$$A_1(\nu, \tau) = -\frac{\nu^2 \gamma_0 b_1(\tau)}{2\gamma(\nu) N(\nu)}, \quad (72)$$

which may be deduced from (68) and (69) on taking $f_1(\mu, \tau) = 0$.

4.3 Matching

The process of matching requires the existence of an overlap domain in which the outer and inner expansions are valid. Then by comparing the expansions within the overlap region and requiring them to be the same, we can obtain the matching conditions. The overlap region has both x small and y large i.e. $\epsilon \ll x = \epsilon y \ll 1$. This process is distinct from patching, which simply seeks to make two functions and their derivatives agree at a single point. There are several ways to perform matching, the two most common approaches being Van Dyke's matching rule and intermediate variable. Here we use Van Dyke's matching rule.

First we write the outer expansion (22) in inner variables (48):

$$\begin{aligned} \Psi &= \psi_0(\epsilon y, \mu, \tau) + \epsilon \psi_1(\epsilon y, \mu, \tau) + \epsilon^2 \psi_2(\epsilon y, \mu, \tau) + \dots \\ &= \psi_0(0, \tau) + \epsilon \left[y \frac{\partial \psi_0(0, \mu, \tau)}{\partial x} + \psi_1(0, \mu, \tau) \right] \\ &\quad + \epsilon^2 \left[\frac{y^2}{2} \frac{\partial^2 \psi_0(0, \mu, \tau)}{\partial x^2} + y \frac{\partial \psi_1(0, \mu, \tau)}{\partial x} + \psi_2(0, \mu, \tau) \right] + \dots \end{aligned} \quad (73) \quad \boxed{\text{eq:outlim}}$$

We compare this with the outer limit of the inner expansion:

$$\Psi = \Psi_0(y, \mu, \tau) + \epsilon \Psi_1(y, \mu, \tau) + \epsilon^2 \Psi_2(y, \mu, \tau) + \dots \quad \text{as } y \rightarrow \infty. \quad (74) \quad \text{eq:inlim}$$

Thus

$$\text{At } O(\epsilon^0): \quad \lim_{y \rightarrow \infty} \Psi_0(y, \mu, \tau) = \psi_0(0, \tau). \quad (75) \quad \text{eq:match0}$$

$$\text{At } O(\epsilon^1): \quad \lim_{y \rightarrow \infty} \Psi_1(y, \mu, \tau) = y \frac{\partial \psi_0(0, \mu, \tau)}{\partial x} + \psi_1(0, \mu, \tau). \quad (76) \quad \text{eq:match1}$$

Now, (61), (70) and (31) give

$$\begin{aligned} \Psi_0(y, \mu, \tau) &= b_0(\tau)\sigma(0)y + (a_0(\tau) - b_0(\tau)\mu) + o(1) && \text{as } y \rightarrow \infty, \\ \Psi_1(y, \mu, \tau) &= b_1(\tau)\sigma(0)y + (a_1(\tau) - b_1(\tau)\mu) + o(1) && \text{as } y \rightarrow \infty, \\ \psi_1(0, \mu, \tau) &= \psi_{10}(0, \tau) + \mu\psi_{11}(0, \tau), \end{aligned}$$

and using in (75)–(76) we obtain

$$\begin{aligned} b_0(\tau) &= 0, \quad a_0(\tau) = \psi_0(0, \tau), \\ b_1(\tau) &= \frac{1}{\sigma(0)} \frac{\partial \psi_0(0, \tau)}{\partial x} = -\psi_{11}(0, \tau), \quad a_1(\tau) = \psi_{10}(0, \tau). \end{aligned} \quad (77) \quad \text{eq:matchcoeffs}$$

Thus the boundary conditions for the outer functions $\psi_0(x, \tau)$ and $\psi_{10}(x, \tau)$ are

$$\psi_0(0, \tau) = \int_0^1 f_1(\mu, \tau) \gamma(\mu) d\mu, \quad \psi_{10}(0, \tau) = \frac{\gamma_1}{\sigma(0)} \frac{\partial \psi_0(0, \tau)}{\partial x}, \quad (78) \quad \text{eq:outerbc0}$$

where we have used that $\gamma_0 = 1$ and we note that $\gamma_1 \approx 0.7104$ (see Case and Zweifel [3]). In a completely analogous way, the boundary conditions at $x = 1$ would be

$$\psi_0(1, \tau) = \int_0^1 f_2(\mu, \tau) \gamma(\mu) d\mu, \quad \psi_{10}(1, \tau) = -\frac{\gamma_1}{\sigma(1)} \frac{\partial \psi_0(1, \tau)}{\partial x}. \quad (79) \quad \text{eq:outerbc1}$$

In summary, we have derived the following boundary value problems for the first two terms in the outer expansion. The leading order term $\psi_0(x, \tau)$ satisfies

$$\frac{K_2}{\sigma(x)} \frac{\partial \psi_0}{\partial \tau} = \frac{1}{3\sigma(x)} \frac{\partial}{\partial x} \left(\frac{1}{\sigma(x)} \frac{\partial \psi_0}{\partial x} \right) + c_2(x)\psi_0 + Q_2 \quad \text{in } 0 < x < 1, \tau > 0, \quad (80) \quad \text{eq:psi0diffb}$$

with boundary conditions

$$\psi_0(0, \tau) = \int_0^1 f_1(\mu, \tau) \gamma(\mu) d\mu, \quad \psi_0(1, \tau) = \int_0^1 f_2(\mu, \tau) \gamma(\mu) d\mu. \quad (81) \quad \text{eq:psi0bc}$$

We note that these boundary conditions are the weighted average of the boundary functions wrt μ with the weight function being the orthogonality weight function $\gamma(\mu)$. The correction to this diffusion problem is given by the component $\psi_{10}(x, \tau)$ of the first order term which satisfies

$$\frac{K_2}{\sigma(x)} \frac{\partial \psi_{10}}{\partial \tau} = \frac{1}{3\sigma(x)} \frac{\partial}{\partial x} \left(\frac{1}{\sigma(x)} \frac{\partial \psi_{10}}{\partial x} \right) + c_2(x)\psi_{10} + c_3(x)\psi_0 + Q_3 \quad \text{in } 0 < x < 1, \tau > 0, \quad (82) \quad \text{eq:psi10diffb}$$

with boundary conditions

$$\psi_{10}(0, \tau) = \frac{\gamma_1}{\sigma(0)} \frac{\partial \psi_0(0, \tau)}{\partial x}, \quad \psi_{10}(1, \tau) = -\frac{\gamma_1}{\sigma(1)} \frac{\partial \psi_0(1, \tau)}{\partial x}. \quad (83) \quad \text{eq:psi10bc}$$

Both of these problems requires suitable initial conditions to complete their full statement. For similar reasons for the appearance of the spatial boundary layers, a temporal layer is required in order to accommodate the initial condition (19). We don't pursue this here, but is left as an exercise.

4.4 Uniform expansions and extrapolated end point conditions

A uniform expansion over the whole x interval can be constructed by using the outer expansion together with the inner expansions at both boundaries. These are simply added with the common behaviour in the overlap regions subtracted. Let us denote N terms of the outer expansion (22) by ψ_N^{outer} and of the inner expansion (54) at $x = 0$ be Ψ_N^{0in} with a similar expansion for the boundary layer at $x = 1$. Then an N term uniform expansion ψ_N^{unif} is given by

$$\psi_N^{unif} = \psi_N^{outer} + \Psi_N^{0in} - \Psi_N^{0overlap} + \Psi_N^{1in} - \Psi_N^{1overlap}. \quad (84) \quad \text{eq:unif}$$

The overlap expansions are precisely (73) or equivalently (74). For example,

$$\psi_1^{unif} = \psi_0(x, \tau) + \int_0^1 A_0(\nu, \tau) \phi_\nu(\mu) e^{-y\sigma(0)/\nu} d\nu + \int_0^1 B_0(\nu, \tau) \phi_\nu(\mu) e^{-(1-y)\sigma(1)/\nu} d\nu, \quad (85)$$

$$\begin{aligned} \psi_2^{unif} = \psi_1^{unif} + \epsilon \left[\psi_{10}(x, \tau) + \mu \psi_{11}(x, \tau) + \int_0^1 A_1(\nu, \tau) \phi_\nu(\mu) e^{-y\sigma(0)/\nu} d\nu \right. \\ \left. + \int_0^1 B_1(\nu, \tau) \phi_\nu(\mu) e^{-(1-y)\sigma(1)/\nu} d\nu \right], \quad (86) \end{aligned}$$

where

$$\begin{aligned} B_0(\nu, \tau) &= \frac{\nu}{\gamma(\nu)N(\nu)} \int_0^1 f_2(\mu, \tau) \phi_\nu(\mu) \gamma(\mu) d\mu, \\ B_1(\nu, \tau) &= \frac{\nu^2}{2\gamma(\nu)N(\nu)\sigma(1)} \frac{\partial \psi_0(1, \tau)}{\partial x}, \end{aligned}$$

are analogous expansion functions to A_0, A_1 in the boundary layer at $x = 1$. These uniform expansions are formed by additive composition. An alternative is multiplicative composition (see Van Dyke [8]).

Another modification is that of the so called extrapolated end point condition. The outer solution is technically not valid within a region of order ϵ of the boundaries. We are thus at liberty to modify the location of our end points for the outer solution to within a distance of ϵ . We demonstrate this with the $x = 0$ boundary. Following Habetler and Matkowsky [6] let us consider the flux $\hat{\psi}(x, \tau)$ defined by

$$\hat{\psi}(x, \tau) = \int_{-1}^1 \psi(x, \mu', \tau) d\mu'. \quad (87) \quad \text{eq:nflux}$$

Using the outer expansion (22) with (28) and (31) we obtain

$$\begin{aligned}\hat{\psi}(x, \tau) &= \int_{-1}^1 (\psi_0(x, \tau) + \epsilon[\psi_{10}(x, \tau) + \mu\psi_{11}(x, \tau)] + O(\epsilon^2)) d\mu' \\ &= \psi_0(x, \tau) + \epsilon\psi_{10}(x, \tau) + O(\epsilon^2).\end{aligned}\tag{88} \quad \text{eq:psihatexp}$$

Let us write

$$\hat{\psi}_1(x, \tau) = \psi_0(x, \tau) + \epsilon\psi_{10}(x, \tau),$$

which we note satisfies the diffusion equation

$$\frac{K_2}{\sigma(x)} \frac{\partial \hat{\psi}_1}{\partial \tau} = \frac{1}{3\sigma(x)} \frac{\partial}{\partial x} \left(\frac{1}{\sigma(x)} \frac{\partial \hat{\psi}_1}{\partial x} \right) + \hat{c}(x)\hat{\psi}_1 + \hat{Q},\tag{89} \quad \text{eq:psi1hat}$$

where $\hat{c}(x) = c_2(x) + \epsilon c_3(x)$, $\hat{Q} = Q_2 + \epsilon Q_3$ and we ignore terms of $O(\epsilon^2)$ in the product $\hat{c}(x)\hat{\psi}_1$. For the boundary conditions satisfied by $\hat{\psi}_1$, we expand (88) about an arbitrary point $x = \epsilon y_0$ close to the $x = 0$ boundary,

$$\begin{aligned}\hat{\psi}(\epsilon y_0, \tau) &= \psi_0(\epsilon y_0, \tau) + \epsilon\psi_{10}(\epsilon y_0, \tau) + O(\epsilon^2) \\ &= \psi_0(0, \tau) + \epsilon \left[y_0 \frac{\partial \psi_0(0, \tau)}{\partial x} + \psi_{10}(0, \tau) \right] + O(\epsilon^2) \\ &= \psi_0(0, \tau) + \epsilon \left[y_0 + \frac{\gamma_1}{\sigma(0)} \right] \frac{\partial \psi_0(0, \tau)}{\partial x} + O(\epsilon^2),\end{aligned}\tag{90} \quad \text{eq:psihatbc}$$

using the ψ_{10} boundary condition in (78). Since $\frac{\partial \psi_0(0, \tau)}{\partial x}$ is not known (but only determined after solving for ψ_0), it is convenient to take

$$y_0 = -\frac{\gamma_1}{\sigma(0)}.\tag{91} \quad \text{eq:y0}$$

Then

$$\hat{\psi}_1(\epsilon y_0, \tau) = \psi_0(0, \tau) = \int_0^1 f_1(\mu, \tau) d\mu\tag{92} \quad \text{eq:hatpsibc2}$$

is the boundary condition with (89) now posed over $\epsilon y_0 < x < 1 - \epsilon y_1$, with $y_1 = -\gamma_1/\sigma(1)$. The important observation is that this problem for $\hat{\psi}_1$ gives a two-term accurate solution for the outer expansion. Clearly, we may proceed to higher order terms and corrections to y_0 and y_1 can be found.

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Appendix A. Estimates of the macro cross-sections

appa

	Thermal cross section (barn)			Fast cross section (barn)		
	Scattering	Capture	Fission	Scattering	Capture	Fission
U-235	10	99	583	4	0.09	1
U-238	9	2	2×10^{-5}	5	0.07	0.3
Pu-239	8	269	748	5	0.05	2

Table 1: Typical micro cross-sections $\hat{\sigma}$ for fuels used in nuclear reactors. Unit of 1 barn = 10^{-28} m² or 10^{-24} cm².

table1

- The mean free path λ of a particle is the average length between two interactions. It is given by $1/\sigma$, where σ is the macroscopic cross section (units of cm⁻¹).
- The macroscopic cross σ section is related to the microscopic cross section $\hat{\sigma}$ by

$$\sigma = N\hat{\sigma}, \tag{1}$$

eq:micmac

where N is the atom density (atoms per unit volume). N may be calculated from

$$N = \frac{\rho N_A}{M},$$

where $N_A = 6.02310^{23}$ is Avogadro's number, ρ is the density (g/cm³) and M is the gram atomic weight.

- Estimates of the microscopic cross sections for common fuels are given in Table 1, with Table 2 recording their properties and estimates of the atom density. Table 3 gives estimates of the macroscopic cross sections using (1).

	density ρ g/cm ³	M gram atomic weight	N atom density atoms/cm ³
U-235	19	235.04	4.87×10^{22}
U-238	19	238.03	4.81×10^{22}
Pu-239	19.8	244	4.89×10^{22}

Table 2: Typical micro cross-sections $\hat{\sigma}$ for fuels used in nuclear reactors. Unit of 1 barn = 10^{-28} m² or 10^{-24} cm².

table2

	Thermal cross section (cm ⁻¹)			Fast cross section (cm ⁻¹)		
	Scattering	Capture	Fission	Scattering	Capture	Fission
U-235	4.9×10^{-1}	4.8	2.8×10^1	1.95×10^{-1}	4.4×10^{-3}	4.9×10^{-2}
U-238	4.3×10^{-1}	9.6×10^{-2}	9.6×10^{-7}	2.4×10^{-1}	3.4×10^{-3}	1.4×10^{-2}
Pu-239	7.8×10^{-1}	1.3×10^1	3.7×10^1	2.4×10^{-1}	2.4×10^{-3}	9.8×10^{-2}

Table 3: Typical macro cross-sections σ for fuels used in nuclear reactors.

table3

- If the typical length of the reactor is taken as $d = 100$ cm then estimates of $\epsilon = 1/(\sigma d)$ from the values in Table 3 are $O(10^{-4})$ using the largest macro cross sections.

Appendix B. Separable solutions of the time-independent transport equation

appb

We consider the steady transport equation with constant coefficients and no source in the form

$$\mu \frac{\partial \psi(x, \mu)}{\partial x} + \psi(x, \mu) = \frac{c}{2} \int_{-1}^1 \psi(x, \mu') d\mu', \quad (1) \quad \text{eq:sepg}$$

for $0 < x < \infty$ and $-1 \leq \mu \leq 1$ with c here taken to be constant. Seeking separable solutions in the form $\psi(x, \mu) = F(x)G(\mu)$ gives

$$\frac{F'(x)}{F(x)} = -\frac{1}{\nu} \quad \text{and} \quad \left(1 - \frac{\mu}{\nu}\right) G(\mu) = \frac{c}{2} \int_{-1}^1 G(\mu') d\mu',$$

where $1/\nu$ is a constant of separation. Thus

$$F(x) = e^{-x/\nu}$$

to within a multiplicative constant and for convenience we normalise such that

$$\int_{-1}^1 G(\mu') d\mu' = 1. \quad (2) \quad \text{eq:norm}$$

Writing $G(\mu) = \phi_\nu(\mu)$ we thus have separable solutions in the form

$$\psi = e^{-x/\nu} \phi_\nu(\mu), \quad (3)$$

where $\phi_\nu(\mu)$ satisfies

$$(\nu - \mu)\phi_\nu(\mu) = \frac{c}{2}\nu \quad \text{with} \quad \int_{-1}^1 \phi_\nu(\mu') d\mu' = 1. \quad (4)$$

Assuming $|\nu| > 1$ then we have solutions in the form

$$\phi_{\pm\nu_0}(\mu) = \frac{c}{2} \frac{(\pm\nu_0)}{(\pm\nu_0) - \mu}, \quad (5) \quad \boxed{\text{eq:dmodes}}$$

where $\nu = \pm\nu_0$ are the two roots of the transcendental equation

$$1 = c\nu \tanh^{-1}(1/\nu), \quad (6) \quad \boxed{\text{eq:trans}}$$

which follows from use of the normalisation condition. These are the discrete solution modes of the equation. However, if $|\nu| < 1$ then there are distributional or singular solutions of the form

$$\phi_\nu(\mu) = \frac{c}{2} P \frac{\nu}{\nu - \mu} + \lambda(\nu)\delta(\nu - \mu), \quad \lambda(\nu) = 1 - c\nu \tanh^{-1} \nu, \quad (7)$$

where P denotes the Cauchy principle value, which is to be understood when integrating the expression in the normalisation condition which now has a singular integrand in the interval of integration. These give a continuous set of solution modes.

The general solution to (1) by linear superposition of the discrete and continuous modes may be written in the form

$$\psi(x, \mu) = a_{0+}\phi_{+\nu_0}(\mu)e^{-x/\nu_0} + a_{0-}\phi_{-\nu_0}(\mu)e^{x/\nu_0} + \int_{-1}^1 A_0(\nu)\phi_\nu(\mu)e^{-x/\nu} d\nu, \quad (8) \quad \boxed{\text{eq:gensol}}$$

for arbitrary constants $a_{0\pm}$ and an arbitrary function $A_0(\nu)$. Full $-1 \leq \mu \leq 1$ and half-range $0 \leq \mu \leq 1$ completeness theorems are stated in Case [2] or Case and Zweifel [3], along with the appropriate orthogonality conditions.

We make the following remarks on the roots of the transcendental equation (6):

- If $c < 1$ then there are two real roots $\pm\nu_0$ on the real axis.
- If $c > 1$ then there are two complex roots $\pm\nu_0$ on the imaginary axis.
- If $c = 1$ then the two roots coalesce at ∞ .

It is the case $c = 1$ we wish to make some further comments on, since it occurs in the inner region problem. The solution for the two discrete modes may be written as

$$\psi(x, \mu) = \frac{A}{2} \left(\frac{\nu_0}{\nu_0 - \mu} \right) e^{-x/\nu_0} + \frac{B}{2} \left(\frac{\nu_0}{\nu_0 + \mu} \right) e^{x/\nu_0} \quad (9)$$

with arbitrary constants A, B . Expanding for large ν_0 (with x fixed) gives

$$\begin{aligned}
\psi(x, \mu) &= \frac{A}{2} \left(1 + \frac{\mu}{\nu_0} + \frac{\mu^2}{2\nu_0^2} + \dots \right) \left(1 - \frac{x}{\nu_0} + \frac{x^2}{2\nu_0^2} - \dots \right) \\
&\quad + \frac{B}{2} \left(1 - \frac{\mu}{\nu_0} + \frac{\mu^2}{2\nu_0^2} - \dots \right) \left(1 + \frac{x}{\nu_0} + \frac{x^2}{2\nu_0^2} + \dots \right) \\
&= \frac{(A+B)}{2} \left(1 + \frac{(x-\mu)^2}{2\nu_0^2} + O(1/\nu_0^4) \right) + \frac{(B-A)}{2} \left(\frac{(x-\mu)}{\nu_0} + O(1/\nu_0^3) \right).
\end{aligned} \tag{10}$$

Writing $B + A = 2a_0$ and $B - A = 2b_0\nu_0$, in the limit $\nu_0 \rightarrow \infty$, we obtain

$$\psi(x, \mu) = a_0 + b_0(x - \mu), \tag{11}$$

which derives the so called classical solutions.