12 Month Research Report

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as part of a Ph. D. sponsored by AMEC

at the University of Bath

Contents

Chapter 1

Introduction

1.1 The Neutron Transport Equation

An important problem in applied nuclear physics is that of efficiently solving the neutron transport equation. This equation governs the behaviour of neutrons within a nuclear fission reaction by specifying a quantity known as the *neutron flux*, which we denote $\psi(\mathbf{r}, \Omega, E)$, where $\mathbf{r} \in V \subset \mathbb{R}^3$ is the neutron's location in a 3D coordinate system, $\Omega \in \mathbb{S}^2$ is its direction of travel, and $E \in \mathbb{R}^+$ is the neutron's kinetic energy. The quantity $\psi(\mathbf{r}, \Omega, E)$ is then the number of neutrons passing through a unit space at $\mathbf{r}$ in direction Ω with energy E per unit time. The transport equation describes the behaviour of the neutron flux based upon the probabilities of various neutron interactions (or collisions) occurring, and based on the characteristics of a *neutron source*. Throughout this document we will be considering only steady-state versions of the neutron transport equation, so there will be no time dependence.

When modelling a nuclear reactor, it is generally specified that neutrons can undergo three types of interaction: they can cause *fission*, can be *scattered* or they can be *captured*. Neutron-neutron interactions are not often considered due to the small size of a neutron, and thus the comparative improbability of these events. We consider the three interactions in order.

First of all, a neutron could collide with some *fissile material* and undergo a *fission event*. Fissile material is material which, upon collision with a low-energy (*slow* or *thermal*) neutron, can capture it and then undergo a fission event [20]. This releases a number of new neutrons, specified by $\nu(E) \in \mathbb{R}^+$ for a collision caused by a neutron with energy E. These are released over a spectrum of different energies specified by $\chi(E) \in \mathbb{R}^+$, where $\chi(E)\mathrm{d}E$ is the probability that a neutron produced during fission will have an energy within $\mathrm{d}E$ of E [15]. The neutrons produced by the fission may be travelling in any direction with no bias (i.e. they are *isotropic* in angle). This is a *fission collision* and the probability of such a collision occurring is denoted by the variable $\sigma_f(\mathbf{r}, E) \in \mathbb{R}^+$, known as the *fission cross-section*.

Next, upon collision with a nucleus, a neutron could be deflected and so end up travelling in a different direction with different energy. In this case the neutron is said to have been *scattered* and the probability of such an event occurring is denoted by the variable $\sigma_s(\mathbf{r}, \Omega', \Omega, E', E) \in \mathbb{R}^+$, known as the *scatter cross-section*. Here the neutron is scattered from travelling with energy E' in direction Ω' to travelling with energy E in direction Ω.

Lastly, upon collision with a nucleus a neutron could be *captured* and so no longer be considered within the ongoing reaction. The probability of such an event occurring is denoted by the variable $\sigma_c(\mathbf{r}, E) \in \mathbb{R}^+$ and is known as the *capture cross-section*. If we denote by $\sigma_t(\mathbf{r}, E) \in \mathbb{R}^+$ a quantity known as the *total cross-section*, defined to be the probability of any collision occurring to neutrons at position $\mathbf{r}$ with energy E, then the following relation holds

$$\sigma_t(\mathbf{r}, E) = \sigma_f(\mathbf{r}, E) + \frac{1}{4\pi}\int_{\mathbb{R}^+}\int_{\mathbb{S}^2} \sigma_s(\mathbf{r}, \Omega', \hat{\Omega}, E', \hat{E})\, \mathrm{d}\hat{\Omega}\, \mathrm{d}\hat{E} + \sigma_c(\mathbf{r}, E). \tag{1.1}$$

We will also define for convenience $\sigma_a(\mathbf{r}, E) \equiv \sigma_c(\mathbf{r}, E) + \sigma_f(\mathbf{r}, E)$. This is called the *absorption* cross-section, and represents all collisions which result in the neutron being absorbed.

It is important to note that since $\psi(\mathbf{r}, \Omega, E)$ only considers specific angles and energies, after each of the three collision types the neutron is no longer travelling in the same direction with the the same energy, and so is no longer a part of that specific neutron flux. The *neutron source* term will be denoted by $Q(\mathbf{r}, \Omega, E)$ and is a non-fission source term of neutrons from position $\mathbf{r}$, in direction Ω and energy E.

Using this notation we can now state the 3D steady-state neutron transport equation as follows

$$\begin{aligned} \Omega \cdot \nabla\psi(\mathbf{r}, \Omega, E) = &-\sigma_t(\mathbf{r}, E)\psi(\mathbf{r}, \Omega, E) \\ &+ \frac{1}{4\pi}\int_{\mathbb{R}^+}\int_{\mathbb{S}^2} \sigma_s(\mathbf{r}, \Omega', \Omega, E', E)\psi(\mathbf{r}, \Omega', E')\, \mathrm{d}\Omega'\, \mathrm{d}E' \\ &+ \frac{\chi(E)}{4\pi}\int_{\mathbb{R}^+} \nu(\mathbf{r}, E')\sigma_f(\mathbf{r}, E')\int_{\mathbb{S}^2} \psi(\mathbf{r}, \Omega', E')\, \mathrm{d}\Omega'\, \mathrm{d}E' \\ &+ Q(\mathbf{r}, \Omega, E). \end{aligned} \tag{1.2}$$

The term on the left of (1.2) and the first term on the right represent neutron loss from the system, while the other three terms represent neutron gain. We will now briefly talk through their physical meanings. First of all the term on the left represents neutron loss due to streaming, while the first term on the right removes those neutrons that undergo any type of collision. The second term on the right adds in those neutrons

which have been scattered from other energies and/or directions (E' and Ω') into the considered energy and direction (E and Ω), and so are now to be considered a part of the flux. The third term adds neutrons that have been produced by nuclear fission, travelling in the correct direction with the correct energy. Finally $Q(\mathbf{r}, \Omega, E)$ adds in neutrons produced by the non-fission source.

1.1.1 Simplifying Assumptions

Throughout this report several physical assumptions will be made in order to reduce the transport equation into a form that is simpler to analyse. It has already been mentioned that we are considering the steady-state form of the neutron transport equation, which is why no time dependence was introduced in the previous section. We will further assume that all neutrons are travelling with the same energy, thus removing this dependence from all areas of consideration. This is not a realistic assumption since in reality the energy a particle has dramatically affects the cross-sections. In fact, the variation of the cross-sections with respect to a neutron's energy is so complex that it cannot be calculated or accurately modelled at each point, so instead a range of energy 'intervals' are considered (see [15], [19]). In this regard, we will be using just one interval in our model. This is often referred to as working in the *monoenergetic* case.

As well as this we will assume that scattering collisions and the non-fission source term are isotropic in angle. By this we mean that the direction a neutron is travelling

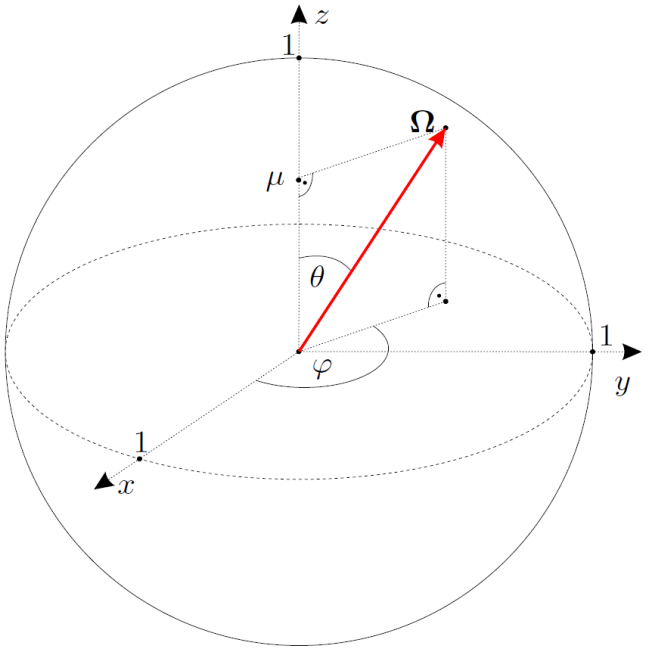

Figure 1-1: *Standard polar coordinates on $\mathbb{S}^2$, showing the contribution of Ω in the z-direction. Taken from [19].*

after it has been scattered is independent of its direction of travel prior to the collision, and that all possible directions are equally likely. This reduces the dependencies of the various cross-sections and the non-fission source to just the spatial variable. Lastly, we will be considering the one-dimensional form of the transport equation using slab geometry. To satisfy this our spatial variable will become $x \in [a, b] \subset \mathbb{R}$ instead of $\mathbf{r}$. Also, considering standard polar coordinates on $\mathbb{S}^2$, we denote by μ the contribution of Ω in the spatial z-direction (see figure 1-1) [6]. Then μ parametrises the unit 'sphere' in 1D via $\mu = \cos(\theta)$ for $\theta \in [0, \pi]$, so $\mu \in [-1, 1]$.

Under these assumptions, the transport equation (1.2) becomes

$$\mu \frac{\partial}{\partial x}\psi(x, \mu) + \sigma_t(x)\psi(x, \mu) = \frac{\sigma_s(x)}{2}\int_{-1}^{1} \psi(x, \mu)\, \mathrm{d}\mu + Q(x). \tag{1.3}$$

In this we have also not included the term relating to fission interactions. This may appear to be a big assumption to make, however the fission term can be thought to have been included implicitly in the scatter term. Hence our later analysis will apply to both the with fission and without fission cases.

Boundary Conditions

As with any equation governing a physical system, (1.3) can only be solved when combined with some relevant boundary conditions. We will consider two types of condition in this section: *vacuum* boundary conditions and *reflecting* boundary conditions.

First of all, vacuum conditions are used to enforce a requirement for zero incoming neutron flux over the boundary of the spatial domain. This means that the only source of neutrons under consideration is from within the reactor itself. These conditions are specified as follows.

$$\begin{aligned} \psi(a, \mu) &= 0 \quad \text{for } \mu > 0, \\ \psi(b, \mu) &= 0 \quad \text{for } \mu < 0. \end{aligned} \tag{1.4}$$

So we have that at the left-most end of the domain ($x = a$), the flux in the inward direction (positive μ) is zero, and vice versa for the right-most end ($x = b$).

Next, reflecting boundary conditions say that the incoming flux and outgoing flux at the boundary of the spatial domain are equal. These conditions are specified as follows.

$$\begin{aligned} \psi(a, -\mu) &= \psi(a, \mu), \\ \psi(b, -\mu) &= \psi(b, \mu). \end{aligned} \tag{1.5}$$

This ensures that the boundary flux in an outgoing angle equals that of the opposing incoming angle at each end of the domain. This effectively prevents neutrons from escaping the system. In more complicated geometries, these can be used to model

infinite arrays of a certain region. This is done by defining one copy of the region, and then applying reflecting conditions around the boundary. This implicitly assumes an average flux of zero over boundaries between the regions, however still creates a good representation of the set up.

1.2 Solution Methods

In this section we will talk about the different types of methods that are used to solve the transport equation in modelling nuclear fission reactors. Broadly these methods can be broken down into two genres: *deterministic* methods and *Monte Carlo* (stochastic) methods. Monte Carlo methods are discussed widely in the literature (see [15] Chapter 7, [7] Chapter 9) and are currently used to model reactor criticality. These methods have an advantage in that the complexity of the domain does not dramatically affect the solve time, so they are often used to model complex geometrical set-ups (see [15] Chapter 7 for a discussion, and figure 1-2 for a representation of a complex geometry). We will touch briefly upon some theory related to Monte Carlo later in Section 2.7, but will not explain how these methods are used to any depth. The majority of our analysis will be focussed around deterministic methods.

Deterministic methods are those that will always produce the same output for a given input. These methods discretise the transport equation and form a system of coupled algebraic equations which can then be solved. This can involve using iterative methods (provided they don't contain calls to random variables), such as *Krylov* methods (see [10], [17], [18]) that are to be one of the focus points of our research (see

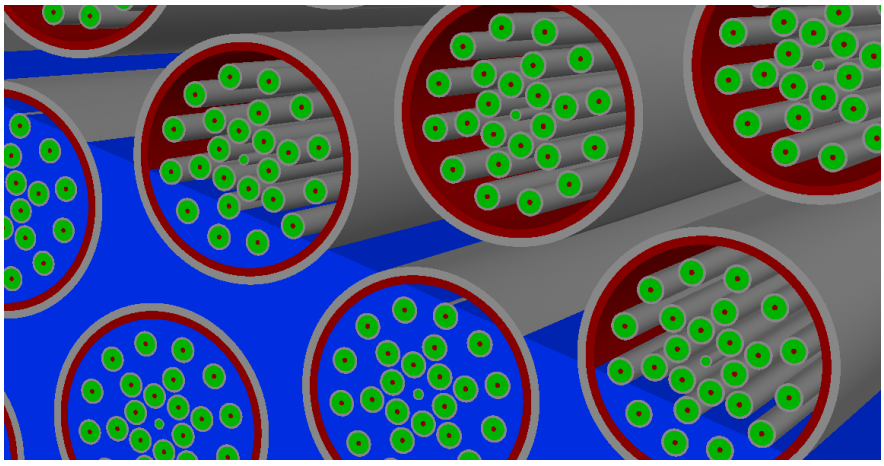

Figure 1-2: *An example of a complicated reactor domain partially filled with water for which Monte Carlo methods may be used to determine criticality. This figure is intended only to represent part of a possible complicated fuel pin array, and not to represent any real-world reactor. It was produced using a development version of VisualWorkshop3a, which is part of the ANSWERS® Software Service provided by AMEC.*

Section 1.3). Deterministic approaches include methods like *discrete ordinates* (the S_N-method), *spherical harmonics* (the P_N-method) and *diffusion theory*.

1.2.1 Discrete Ordinates

The discrete ordinates method works by sampling the angular variable, μ, at a number of discrete points, and then replacing the integrals over μ in (1.3) (or (1.2)) by weighted quadrature summations. The quadrature points and weights should be chosen so that the neutron flux in both the positive and negative directions are given equal importance. After this the spatial derivatives will be discretised via some finite difference or finite element method, allowing a numerical solution method to be applied. This method is often called the S_N-method, and further information on it can be found in [21] Chapter 4, [15] Chapters 3 and 4, [20] Chapter 9, and [8] Chapter 9 among others.

1.2.2 Spherical Harmonics

The spherical harmonics method for solving the neutron transport equation works by expanding the angular component of the neutron flux in terms of Legendre polynomials. By truncating this expansion and applying the orthogonality property of Legendre polynomials, a finite system of semidiscrete equations is obtained. Discretising the spatial variable using finite difference methods or finite element methods once again allows for the application of a suitable solver. This method is often called the P_N-method, and further information can be found in [4] Chapter 3 or [15] Chapter 3.

1.2.3 Diffusion Theory

Diffusion theory states that the solution to the transport equation can be approximated by a diffusion equation of the form

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{3\sigma_t(x)}\frac{\mathrm{d}}{\mathrm{d}x}\phi(x)\right)+\sigma_a(x)\phi(x)=Q(x), \tag{1.6}$$

where

$$\phi(x)\equiv\frac{1}{2}\int_{-1}^{1}\psi(x,\mu)\,\mathrm{d}\mu,$$

is known as the *scalar flux* (this will be introduced again in Section 2.2). To make this approximation several assumptions, given in [14], are made. Firstly that the physical medium is several *mean free paths* thick, where a mean free path is the average distance travelled by a neutron between successive collisions. Secondly that the probability of a neutron collision resulting in a scatter is far higher than it resulting in an absorption, i.e. $\sigma_a \ll \sigma_s$. Lastly, that the neutron flux, cross-sections and source are continuous, and vary by only a 'small amount' in space over the distance of a mean free path. We will

clarify these further and understand their consequences in Section 2.4. Unfortunately the third of these assumptions does not hold near boundaries, but the approximation can actually still give accurate predictions by working on a homogenised domain where the cross-sections are averaged spatially (see [20] Chapter 3, p.47).

Extension of this theory into an iterative acceleration scheme, known as *diffusion synthetic acceleration*, or DSA, will be addressed in Section 2.6. Good information on DSA can be found in [1] Chapters 1 and 2, and we will reference other relevant papers in Section 2.6.

1.3 Research Aims

In this section we will state and then justify the current aims of our research, and then later talk about to what extent these have been achieved. The current aims are:

1. To investigate Krylov methods for use in solving the neutron transport equation.
2. To investigate preconditioners (in particular utilising the diffusion approximation) to speed up Krylov solves.

Iterative solves are used in current industrial deterministic software for solving criticality problems including the neutron transport problem. One example is in the WIMS code (part of the ANSWERS® Software Service provided by AMEC) where the deterministic methods mentioned in section 1.2 can be used (i.e. S_N, P_N and diffusion theory) as well as the method of characteristics, alongside iterative solvers. They are still a very relevant part of the industry and as such any improvements in efficiency (and so accuracy) of solves can only be beneficial for both energy and environmental concerns alike. Firstly for reducing associated risks, and secondly for continuing to satisfy growing energy demands [20](Preface). Krylov methods are well understood mathematically (see [17] and [18]) and make good intuitive sense (see [10]). Currently the dominant iterative scheme used in nuclear modelling software is simple iteration (I do not have a reference for this, however information on simple iteration can be found in [6], [8], [19], and many others) which we will introduce in Section 2.3. Because of this a move to Krylov based methods could be advantageous.

Preconditioning a system involves transforming it (via some process or operator known as a *preconditioner*) into a form more easily solved using numerical methods. The key to this is that the cost of preconditioning should not outweigh the benefits. Preconditioning is a frequently used process, backed up with a wealth of mathematical knowledge and understanding (see [8] and [17], or [1] for a transport specific text). In particular the case of preconditioning Krylov subspace methods has been considered in detail in [18] Chapter 9 and in [5].

In the neutron transport literature it is accepted that the diffusion equation can be a good approximation of the neutron transport equation under some circumstances (see in particular [20] Chapter 3, [1], [4], [21]). We will use an argument involving the P_N-equations (mentioned above) to obtain an approximate diffusion form of the transport equation in Section 2.4, along with relevant boundary conditions. This diffusion approximation has been used to construct an acceleration scheme known as *diffusion synthetic acceleration*, which works in parallel with another iterative scheme and uses diffusion solves to update the approximate solution at each iteration. See [1] Chapters 2 and 3, and [3] for analysis; see [2] and [12] for application. Acceleration schemes can be shown to be equivalent to preconditioning methods ([8] and [1] Chapter 1 for discussion) and we are hoping to formulate diffusion synthetic acceleration as a preconditioner to a Krylov solver. If we are successful, this would allow us to utilise the existing vast knowledge about preconditioning Krylov methods mentioned earlier.

A lot of effort has been put into overcoming instability issues inherent in discretising the transport and diffusion equations (see [2] for the recognised solution, [12] for some follow up work), and this has led to a good understanding of how to guarantee stability in the scheme. However there have been fewer thorough attempts to analyse the scheme mathematically with the aim of fully understanding what causes errors and justifying methods of minimising them (one discussion is in [3]. This paper looks very relevant though I do not understand it to any depth yet). We have put some effort into obtaining an error bound for the diffusion approximation of the transport equation and a summary of this is given in Section 2.5, though it is currently inconclusive.

There is an understanding that transport theory transitions into diffusion theory as the scattering cross-section converges to the total cross-section [14]. This can be shown by obtaining the diffusion equation from the transport equation using an asymptotic argument given in [9], [13] and [14]. We will give an asymptotic derivation of the continuous diffusion approximation in Section 2.4 and demonstrate this transition in the scattering limit.

As mentioned in Section 1.2, we will briefly touch upon Monte Carlo methods in Section 2.7 of this report. In that section we will prove a result related to the convergence of Neumann series obtained from a form of the transport equation. This result is essentially equivalent to one given in Section 2.3 but is nonetheless interesting and relevant to the application of Monte Carlo methods. We will also talk about possible extensions to this theory to make it more physically relevant.

Chapter 2

Theory

2.1 Overview

In this chapter we will cover in as much detail as possible what we have done so far. We will aim to highlight where assumptions were made or where there are gaps in our understanding, and if appropriate indicate how we are trying to remove or resolve these respectively.

In Section 2.2 we will start by recapping the neutron transport equation in 1D as introduced in Chapter 1 along with a further assumption that we are working over a homogeneous spatial medium. We will also recap the associated boundary conditions, and will introduce operators to simplify notation. In Section 2.3 we will look at the 'bread and butter' iterative technique known as *source iteration* for solving the transport equation. We will also prove that source iteration is a contraction. Section 2.4 will move on from here to look at the diffusion approximation to the transport equation and will show how it can be derived in two ways. Firstly using Legendre polynomials, and then using an asymptotic approach. We will also derive the relevant associated boundary conditions from those given in Section 2.2 for the first method, and explain some difficulties in doing this in the asymptotic case. Since this is just an approximation to the transport equation, Section 2.5 will look at bounding the associated error. This is incomplete right now, however we will talk about some directions that may enable progress. After that, Section 2.6 will look at how the diffusion approximation may be used as part of a two-step iterative scheme known as *diffusion synthetic acceleration* to solve the neutron transport problem. We will define this scheme, as well as explaining what we know of its stability and convergence properties. Lastly Section 2.7 will investigate the convergencce of a Neumann series relevant to Monte Carlo solution methods. We will also mention extensions to this work that would improve its physical relevance.

2.2 The Neutron Transport Equation

The 1D steady-state monoenergetic transport equation with isotropic scattering was defined in (1.3). If we assume that we are working over a homogeneous spatial domain, then all cross-sections become constant. Under this assumption, (1.3) becomes

$$\mu\frac{\partial}{\partial x}\psi(x,\mu)+\sigma_t\psi(x,\mu)=\frac{\sigma_s}{2}\int_{-1}^{1}\psi(x,\mu)\,\mathrm{d}\mu+Q(x). \tag{2.1}$$

This equation defines the neutron flux, $\psi(x,\mu)$, where we shall take $x\in[a,b]$ and $\mu\in[-1,1]$ in the homogeneous case. To specify a solution we will impose either vacuum boundary conditions,

$$\begin{aligned}\psi(a,\mu)&=0 \quad \text{for } \mu>0,\\ \psi(b,\mu)&=0 \quad \text{for } \mu<0,\end{aligned} \tag{2.2}$$

or reflecting boundary conditions,

$$\begin{aligned}\psi(a,-\mu)&=\psi(a,\mu),\\ \psi(b,-\mu)&=\psi(b,\mu).\end{aligned} \tag{2.3}$$

There are other possibilities and combinations of boundary conditions, however we will only mention these two.

To specify precisely where we are working, we introduce the following space

$$L^2\left(V,L^1(S)\right)\equiv\left\{\psi:V\times S\to\mathbb{R}\ :\ \int_V\|\psi(x,\cdot)\|^2_{L^1(S)}\ \mathrm{d}x<\infty\right\},$$

where

$$\|\psi\|_{L^2(V,L^1(S))}=\int_V\|\psi(x,\cdot)\|^2_{L^1(S)}\ \mathrm{d}x,$$

with $\|\psi(x,\cdot)\|_{L^1(S)}=\int_S|\psi(x,\mu)|\ \mathrm{d}\mu$, the usual L^1-norm. Using this we can specify that in solving (2.1) we are looking for $\psi\in L^2\left([a,b],L^1[-1,1]\right)$ that satisfies our chosen boundary conditions.

Operator Notation

To simplify the notation in (2.1) we can introduce two *operators*, $\mathcal{T}$ and $\mathcal{S}$, that represent the transport and scatter parts of (2.1) respectively. These are defined as follows

$$\begin{aligned}\mathcal{T}(\cdot)&\equiv\frac{\partial}{\partial x}(\cdot)+\sigma_t(\cdot),\\ \mathcal{S}(\cdot)&\equiv\frac{\sigma_s}{2}\int_{-1}^{1}(\cdot)\,\mathrm{d}\mu.\end{aligned} \tag{2.4}$$

These allow for (2.1) to be written in operator form as

$$(\mathcal{T} - \mathcal{S})\psi = Q. \tag{2.5}$$

It will be useful in the following section if we take this a little further. First we can define

$$\mathcal{P}(\cdot) = \frac{1}{2}\int_{-1}^{1} (\cdot)\, \mathrm{d}\mu, \tag{2.6}$$

and use this to define another quantity, $\phi(x) \in L^2[a,b]$, known as the *scalar flux* as

$$\phi(x) \equiv \mathcal{P}\psi(x,\mu). \tag{2.7}$$

Using this notation we can give the following two results that are proved in [19] (Lemma 2.3 and Theorem 2.9 respectively).

Lemma 2.1:
If $\psi(x,\mu) \in L^2\left([a,b], L^1[-1,1]\right)$ *satisfies*

$$\mathcal{T}\psi(x,\mu) = g(x), \tag{2.8}$$

then

$$\phi(x) = \left(\mathcal{K}_{\sigma_t} g\right)(x) \equiv \left(\mathcal{P}\mathcal{T}^{-1} g\right)(x), \tag{2.9}$$

where $\mathcal{T}^{-1}$ *is defined in [19] (equation (2.14)) and [16] (equation (2.2)).*

Theorem 2.2:
If $\mathcal{K}_{\sigma_t}$ *is the operator defined in Lemma 2.1 then*

$$\|\mathcal{K}_{\sigma_t}\|_{\mathscr{L}(L^2[a,b])} \leq \frac{1}{\sigma_t}. \tag{2.10}$$

Here, $\|\cdot\|_{\mathscr{L}(L^2[a,b])}$ is the standard operator norm defined as

$$\|\mathcal{K}_{\sigma_t}\|_{\mathscr{L}(L^2[a,b])} \equiv \sup\left\{ \frac{\|\mathcal{K}_{\sigma_t} g\|_{L^2[a,b]}}{\|g\|_{L^2[a,b]}} \;:\; g \in L^2[a,b], g \neq 0 \right\} \tag{2.11}$$

Using these results let us state and prove the following that will become useful in the next section when we are looking at the convergence of source iteration.

Lemma 2.3:
If $\mathcal{K}_{\sigma_t}$ is the operator defined in Lemma 2.1 and $\psi(x,\mu) \in L^2\left([a,b], L^1[-1,1]\right)$ satisfies (2.8), then

$$\|\phi\|_{L^2[a,b]} \leq \frac{1}{\sigma_t} \|g\|_{L^2[a,b]}, \tag{2.12}$$

where $\phi(x) = \mathcal{P}\psi(x,\mu)$.

Proof.
The operator norm definition give

$$\frac{\|\mathcal{K}_{\sigma_t} g\|_{L^2[a,b]}}{\|g\|_{L^2[a,b]}} \leq \|\mathcal{K}_{\sigma_t}\|_{\mathscr{L}(L^2[a,b])} \leq \frac{1}{\sigma_t}. \tag{2.13}$$

Since $\psi(x,\mu) \in L^2\left([a,b], L^1[-1,1]\right)$ satisfies (2.8), we know from Lemma 2.1 that $\phi(x) = \left(\mathcal{K}_{\sigma_t} g\right)(x)$. Thus we have

$$\frac{\|\phi\|_{L^2[a,b]}}{\|g\|_{L^2[a,b]}} \leq \frac{1}{\sigma_t}. \tag{2.14}$$

Multiplying through by $\|g\|_{L^2[a,b]}$ yields the result.

□

2.3 Source Iteration

One possible method for solving the transport equation is known as *source iteration*, and we will now work through this basic iterative method and prove some convergence results about it. Firstly, let us rewrite (2.5) in the following form

$$\begin{aligned} \mathcal{T}\psi(x,\mu) &= \mathcal{S}\psi(x,\mu) + Q(x), \\ &= \sigma_s \phi(x) + Q(x). \end{aligned} \tag{2.15}$$

From here, source iteration can be defined as

1. Start with some initial $\phi^{(0)}$,
2. solve
$$\mathcal{T}\psi^{(i+1)}(x,\mu) = \sigma_s \phi^{(i)}(x) + Q(x). \tag{2.16}$$
for $\psi^{(i+1)}$,
3. integrate to find $\phi^{(i+1)} = \mathcal{P}\psi^{(i+1)}$, and repeat from step 2.

The obvious follow up question is under what conditions does this converge? To discover this we first obtain an equation for the error in this scheme by subtracting (2.16) from (2.15), leaving

$$\mathcal{T}e^{(i+1)}(x,\mu) = \sigma_s E^{(i)}(x), \tag{2.17}$$

where

$$\begin{aligned} e^{(i)}(x,\mu) &\equiv \left(\psi - \psi^{(i)}\right)(x,\mu), \\ E^{(i)}(x) &\equiv \left(\phi - \phi^{(i)}\right)(x), \end{aligned} \tag{2.18}$$

with $E^{(i)}(x) = \mathcal{P}e^{(i)}(x,\mu)$ as you would expect. We can prove the following convergence result

Lemma 2.4:
Under the definitions in (2.18)*, the following bound holds*

$$\left\|E^{(i+1)}\right\|_{L^2[a,b]} \leq \frac{\sigma_s}{\sigma_t}\left\|E^{(i)}\right\|_{L^2[a,b]}. \tag{2.19}$$

Proof.
Combining (2.17) with Lemma 2.3 we get immediately

$$\left\|E^{(i+1)}\right\|_{L^2[a,b]} \leq \frac{1}{\sigma_t}\left\|\sigma_s E^{(i)}\right\|_{L^2[a,b]} = \frac{\sigma_s}{\sigma_t}\left\|E^{(i)}\right\|_{L^2[a,b]}. \tag{2.20}$$

□

Since $\sigma_s < \sigma_t$, Lemma 2.4 implies that source iteration is a contraction.

2.4 The Diffusion Approximation

In this section we will look at using the diffusion equation (defined in Section 1.2.3) to approximate the transport equation. First of all we will work from the standard transport equation given in Section 2.2 and derive the diffusion equation by expanding the flux in terms of Legendre polynomials. Secondly we will define an asymptotic version of the neutron transport equation, and use an asymptotic expansion of the flux to derive the diffusion approximation. In the first case we will also give a full derivation of the associated boundary conditions, however in the second case we have not yet achieved this and so will instead explain what the difficulty is.

2.4.1 The P_N Derivation

Consider again the operator form (2.5) that we restate here as

$$\mathcal{T}\psi(x,\mu) = \mathcal{S}\psi(x,\mu) + Q(x), \tag{2.21}$$

and define the following

$$\begin{aligned}\phi_n(x) &= \langle \psi(x,\cdot), P_n(\cdot)\rangle \\ &= \tfrac{1}{2}\int_{-1}^{1} \psi(x,\mu)P_n(\mu)\,\mathrm{d}\mu,\end{aligned} \tag{2.22}$$

where the $P_n(\mu)$ are Legendre polynomials, defined via Rodrigues' formula as

$$\begin{aligned}P_0(\mu) &= 1, \\ P_n(\mu) &= \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}\mu^n}(\mu^2-1)^n, \quad n = 1, 2, \ldots.\end{aligned} \tag{2.23}$$

Now, taking inner products of both sides of (2.21) against P_0 and P_1 respectively gives

$$\frac{\mathrm{d}}{\mathrm{d}x}\phi_1(x) + \sigma_t\phi_0(x) = \mathcal{S}\psi(x,\mu) + Q(x), \tag{2.24}$$

and

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\int_{-1}^{1}\mu^2\psi(x,\mu)\,\mathrm{d}\mu + \sigma_t\phi_1(x) = 0. \tag{2.25}$$

If we expand $\psi(x,\mu)$ in terms of Legendre polynomials we get

$$\begin{aligned}\psi(x,\mu) &= \sum_{n=0}^{\infty}\frac{\langle\psi(x,\mu),P_n(\mu)\rangle}{\langle P_n(\mu),P_n(\mu)\rangle}P_n(\mu), \\ &= \sum_{n=0}^{\infty}(2n+1)\phi_n(x)P_n(\mu).\end{aligned} \tag{2.26}$$

Truncating at $n = 1$ yields the following expression

$$\psi(x,\mu) = \phi_0(x) + 3\mu\phi_1(x) + r(x,\mu), \tag{2.27}$$

where $r(x,\mu)$ is a residual term containing the rest of the summation. Substituting (2.27) into (2.25) and evaluating the integrals results in

$$\frac{1}{3}\phi_0' + \sigma_t\phi_1 = -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\int_{-1}^{1}\mu^2 r\,\mathrm{d}\mu, \tag{2.28}$$

with $\phi_0'(x)$ denoting $\frac{\mathrm{d}}{\mathrm{d}x}\phi_0(x)$. We have dropped the dependencies at this step to make the derivation clearer. Also, using (2.27) in (2.24) we find

$$\begin{aligned}\phi_1' + \sigma_t\phi_0 &= \mathcal{S}\left(\phi_0 + 3\mu\phi_1 + r\right) + Q, \\ &= \sigma_s\phi_0 + Q + \mathcal{S}r, \\ \Rightarrow \quad \phi_1' + \sigma_a\phi_0 &= Q + \mathcal{S}r.\end{aligned} \tag{2.29}$$

If we again define the operator, $\mathcal{P}$, to be

$$\mathcal{P}(\cdot) \equiv \frac{1}{2}\int_{-1}^{1}(\cdot)\,\mathrm{d}\mu, \tag{2.30}$$

and note that this gives us $\mathcal{S} \equiv \sigma_s \mathcal{P}$, then combining (2.28) and (2.29) together we get

$$-\left(\frac{1}{3\sigma_t}\phi_0'\right)' + \sigma_a \phi_0 = Q + \left(\sigma_s \mathcal{P}(r) + \frac{1}{\sigma_t}\mathcal{P}(\mu^2 r'')\right). \tag{2.31}$$

An approximation $\tilde{\phi}_0(x)$ of $\phi_0(x)$ can be obtained by setting $r(x,\mu) = 0$ and solving the resulting form of (2.31)

$$-\left(\frac{1}{3\sigma_t}\tilde{\phi}_0'(x)\right)' + \sigma_a \tilde{\phi}_0(x) = Q(x), \tag{2.32}$$

This is a form of the diffusion equation and, as mentioned in Section 1.2.3, under certain conditions it provides a good approximation to the transport equation (2.21).

For (2.32) to be solvable, we need to specify boundary conditions. As in Section 2.2 we will now give two types of condition: vacuum and reflecting.

Vacuum Boundary Conditions

Firstly we look at vacuum conditions, which impose the condition of zero incoming flux at either end of the domain. Bell and Glasstone, [4], Section 2.5d, give a good discussion of the difficulties associated with defining this type of condition for a P_N approximation with finite N. For $N = 1$ (which we implicitly applied to obtain (2.27)) Marshak conditions are used as they include this feature and they are given by

$$\int_0^1 \mu\psi(a,\mu)\,\mathrm{d}\mu = \int_0^1 \mu\psi(b,-\mu)\,\mathrm{d}\mu = 0. \tag{2.33}$$

From (2.27), taking $r(x,\mu) = 0$ leaves the approximation

$$\psi(x,\mu) \approx \phi_0(x) + 3\mu\phi_1(x), \tag{2.34}$$

which when combined with (2.33) give

$$\begin{aligned} \int_0^1 \mu\left[\phi_0(a) + 3\mu\phi_1(a)\right]\,\mathrm{d}\mu &\approx 0, \\ \int_{-1}^0 \mu\left[\phi_0(b) + 3\mu\phi_1(b)\right]\,\mathrm{d}\mu &\approx 0. \end{aligned} \tag{2.35}$$

Integrating directly results in

$$\begin{aligned} \phi_1(a) + \frac{1}{2}\phi_0(a) &\approx 0, \\ \phi_1(b) - \frac{1}{2}\phi_0(b) &\approx 0. \end{aligned} \tag{2.36}$$

Now (2.28) when $r(x,\mu) = 0$ says that

$$\frac{1}{3}\phi_0'(x) + \sigma_t\phi_1(x) = 0, \tag{2.37}$$

which when combined with (2.36) finally yields

$$\begin{aligned} \phi_0(a) - \frac{2}{3\sigma_1}\phi_0'(a) &\approx 0, \\ \phi_0(b) + \frac{2}{3\sigma_1}\phi_0'(b) &\approx 0. \end{aligned} \tag{2.38}$$

These represent vacuum boundary conditions at either end of the spatial domain for the diffusion approximation (2.32).

Reflecting Boundary Conditions

We now proceed to find formulae representing reflecting boundary conditions at either end of the domain. Reflecting boundary conditions specify that the neutron flux is an even function of μ at the boundaries, i.e.

$$\begin{aligned} \psi(a,\mu) &= \psi(a,-\mu), \\ \psi(b,\mu) &= \psi(b,-\mu). \end{aligned} \tag{2.39}$$

Legendre polynomials (defined by (2.23)) satisfy the relations

$$\begin{aligned} P_n(\mu) &= P_n(-\mu) \qquad \text{for } n \text{ even}, \\ -P_n(\mu) &= P_n(-\mu) \qquad \text{for } n \text{ odd}. \end{aligned} \tag{2.40}$$

Writing (2.39) using the expansion (2.26) truncated at N gives us

$$\sum_{n=0}^{N} (2n+1)\,\phi_n(x)P_n(\mu) = \sum_{n=0}^{N} (2n+1)\,\phi_n(x)P_n(-\mu). \tag{2.41}$$

Now using the relations (2.40) it is implied that the desired relation (2.39) will hold if we impose that

$$\left.\begin{aligned} \phi_n(a) &= 0, \\ \phi_n(b) &= 0, \end{aligned}\right\} \qquad \text{for } n \text{ odd}. \tag{2.42}$$

This means $\phi_1(x) = 0$ for both $x = a$ and $x = b$, so by (2.37)

$$\begin{aligned} 0 = \phi_1(a) &= -\frac{1}{3\sigma_t}\phi_0'(a), \\ 0 = \phi_1(b) &= -\frac{1}{3\sigma_t}\phi_0'(b), \end{aligned} \tag{2.43}$$

which when rearranged yields

$$\begin{aligned} \phi_0'(a) &= 0, \\ \phi_0'(b) &= 0. \end{aligned} \tag{2.44}$$

These represent reflecting boundary conditions at either end of the spatial domain for the diffusion approximation (2.32).

2.4.2 The Asymptotic Derivation

In this section we will again derive the diffusion approximation to the transport equation, however we will use an asymptotic expansion method to achieve this. We will require some new concepts and consequently some new notation. Firstly, let us state the neutron transport equation in a dimensional form

$$\mu \frac{\partial}{\partial z}\tilde{\psi}(z,\mu) + \sigma_t \tilde{\psi}(z,\mu) = \frac{\sigma_s}{2}\int_{-1}^{1} \tilde{\psi}(z,\mu)\, \mathrm{d}\mu + \tilde{q}(z), \tag{2.45}$$

where the $\tilde{}$ notation specifies that a quantity is dimensional, and $z \in [X_{min}, X_{max}] \subset \mathbb{R}$ is the dimensional spatial variable. Note also that the cross-sections satisfy the relation

$$\sigma_t = \sigma_a + \sigma_s. \tag{2.46}$$

We now define a distance known as a *scale length*, denoted ρ, to be a typical distance over which $\tilde{\psi}$ and $\tilde{q}$ vary by at most an $O(1)$ amount. For a good discussion on how to choose such a value, see [14], p.288. Using this length we can introduce

$$x \equiv \frac{z}{\rho}, \quad \psi(x,\mu) \equiv \tilde{\psi}(z,\rho), \tag{2.47}$$

as dimensionless variables. Using these, (2.45) becomes

$$\mu \frac{\partial}{\partial x}\psi(x,\mu) + \rho\sigma_t \psi(x,\mu) = \frac{\rho\sigma_s}{2}\int_{-1}^{1} \psi(x,\mu)\, \mathrm{d}\mu + \rho\tilde{q}(z), \tag{2.48}$$

Another length we need is called a *mean free path*. Typically this is equal to the reciprocal of the average length of the total cross-section, i.e. if we denote the average length of the total cross-section by $\langle\sigma_t\rangle$, then $\langle\sigma_t\rangle^{-1}$ is a typical mean free path. However, since we are working over a homogeneous domain the cross-sections are constants, thus $\langle\sigma_t\rangle = \sigma_t$. Using this length, we now define

$$\epsilon \equiv \frac{\langle\sigma_t\rangle^{-1}}{\rho} = \frac{\text{typical mean free path}}{\text{scale length}}, \tag{2.49}$$

and so

$$\rho\sigma_t = \frac{1}{\epsilon}. \tag{2.50}$$

At this point, we shall assume that the problem we are working of is *diffusive*. This is defined concisely in [14], p.284, as a regime that satisfies the following three assumptions:

1. The physical medium is several mean free paths thick. This is often referred to as being *optically thick*.
2. Neutron collisions are scattering-dominated, i.e. $\sigma_a \ll \sigma_s$.
3. The neutron flux, cross-sections and source are continuous, and vary by only a small amount in space over the distance of a mean free path.

To clarify, by "a small amount" we mean an amount significantly smaller than an $O(1)$ amount. Since we are working with constant cross-sections they immediately satisfy assumption 3. We also know that the neutron flux and source can vary by an $O(1)$ amount over a scale length. Therefore assumption 3 implies there must be many mean free paths in a scale length, and so

$$\epsilon \ll 1. \tag{2.51}$$

We can now further say that in order for the medium to be optically thick, it must be about as big (or bigger) than a scale length. This just leaves assumption 2, which requires that σ_a be small in relation to σ_s. To enforce this we set the condition that

$$\sigma_a = \frac{\epsilon}{\rho} \ll 1. \tag{2.52}$$

We impose a similar scaling to the dimensional source term, and define

$$\rho\tilde{q}(z) = \epsilon q(x). \tag{2.53}$$

While this scaling is not necessary, it is useful as it forces the cross sections and source terms to be of a comparable size.

Now combining (2.48), (2.50), (2.52) and (2.53) we obtain a fully nondimensional version of the transport equation, given by

$$\mu\frac{\partial}{\partial x}\psi + \frac{1}{\epsilon}\psi = \frac{1}{2}\left[\frac{1}{\epsilon} - \epsilon\right]\int_{-1}^{1}\psi \,\mathrm{d}\mu + \epsilon q, \tag{2.54}$$

where all functions are in terms of x, not z. The term $\frac{1}{\epsilon} - \epsilon$ arises since

$$\begin{aligned}\rho\sigma_s &= \rho\sigma_t - \rho\sigma_a, \\ &= \frac{1}{\epsilon} - \epsilon.\end{aligned} \tag{2.55}$$

Let us now introduce the following asymptotic expansion of ψ in terms of ϵ

$$\psi(x,\mu) \sim \sum_{k=0}^{\infty} \epsilon^k \psi^{(k)}(x,\mu). \tag{2.56}$$

Substituting this into (2.54) leaves

$$\mu \sum_{k=0}^{\infty} \epsilon^k \frac{\partial}{\partial x}\psi^{(k)} + \frac{1}{\epsilon}\sum_{k=0}^{\infty} \epsilon^k \psi^{(k)} = \frac{1}{2}\left[\frac{1}{\epsilon} - \epsilon\right] \int_{-1}^{1} \sum_{k=0}^{\infty} \epsilon^k \psi^{(k)} \, \mathrm{d}\mu + \epsilon q, \tag{2.57}$$

and the coefficients of the first three powers of ϵ in (2.57) are

$$\begin{aligned}
\epsilon^{-1} : \quad & \psi^{(0)} = \frac{1}{2}\int_{-1}^{1} \psi^{(0)} \, \mathrm{d}\mu, \\
\epsilon^{0} \quad : \quad & \mu\frac{\partial}{\partial x}\psi^{(0)} + \psi^{(1)} = \frac{1}{2}\int_{-1}^{1} \psi^{(1)} \, \mathrm{d}\mu, \\
\epsilon^{1} \quad : \quad & \mu\frac{\partial}{\partial x}\psi^{(1)} + \psi^{(2)} = \frac{1}{2}\int_{-1}^{1} \psi^{(2)} \, \mathrm{d}\mu - \frac{1}{2}\int_{-1}^{1} \psi^{(0)} \, \mathrm{d}\mu + q.
\end{aligned} \tag{2.58}$$

By defining

$$\phi^{(i)}(x) \equiv \frac{1}{2}\int_{-1}^{1} \psi^{(i)}(x,\mu) \, \mathrm{d}\mu, \tag{2.59}$$

the coefficient of ϵ^{-1} gives us that

$$\psi^{(0)}(x,\mu) = \phi^{(0)}(x). \tag{2.60}$$

We will refer back to this particular equation again at the end of this section. Using this with the coefficient of ϵ^0 we then get

$$\begin{aligned}
\mu\frac{\mathrm{d}}{\mathrm{d}x}\phi^{(0)} + \psi^{(1)} &= \frac{1}{2}\int_{-1}^{1} \psi^{(1)} \, \mathrm{d}\mu, \\
&\equiv \phi^{(1)}.
\end{aligned} \tag{2.61}$$

Now combining (2.61) and (2.60) with the coefficient of ϵ^1 we obtain

$$\mu\frac{\mathrm{d}}{\mathrm{d}x}\left(\phi^{(1)} - \mu\frac{\mathrm{d}}{\mathrm{d}x}\phi^{(0)}\right) + \left(\psi^{(2)} - \phi^{(2)}\right) + \phi^{(0)} = q. \tag{2.62}$$

Integrating both sides of this with respect to μ and scaling by $\frac{1}{2}$ leaves

$$\frac{1}{2}\int_{-1}^{1} \mu\frac{\mathrm{d}}{\mathrm{d}x}\phi^{(1)} \, \mathrm{d}\mu - \frac{1}{2}\int_{-1}^{1} \mu^2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi^{(0)} \, \mathrm{d}\mu + \left(\frac{1}{2}\int_{-1}^{1} \psi^{(2)} \, \mathrm{d}\mu - \phi^{(2)}\right) + \phi^{(0)} = q, \tag{2.63}$$

which reduces to

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{3}\frac{\mathrm{d}}{\mathrm{d}x}\phi^{(0)}(x)\right)+\phi^{(0)}(x)=q. \tag{2.64}$$

This is the non-dimensional form of the diffusion approximation in a homogeneous medium.

It is important to note at this point that upon inspection of the asymptotically expanded flux equation, (2.56), and the equations resulting from the coefficient of ϵ^{-1}, (2.60), we can deduce that

$$\lim_{\epsilon\to 0}\psi=\psi^{(0)}=\phi^{(0)}. \tag{2.65}$$

This implies that as $\epsilon\to 0$, transport theory transitions into diffusion theory. This lends credence to the use of the diffusion equation as an approximation to the transport equation. It also suggests that it will be a 'better' approximation when ϵ is close to zero. Equations (2.50) and (2.55) imply that this happens when σ_s is close to σ_t. This can also be seen as fulfilling condition 2 for the regime to be diffusive. We will return to this in Section 2.5, where we will attempt to clarify what is meant by 'better'.

Boundary Conditions

Obtaining good boundary conditions for the asymptotically derived diffusion equation has proved harder than for the Legendre polynomial version. Repeating a method used in [13], we attempted to derive boundary conditions by splitting the flux into three parts: the interior part and two boundary parts. This can be written as follows

$$\psi(x,\mu)=\psi_I(x,\mu)+\psi_{LB}(x_{LB},\mu)+\psi_{RB}(x_{RB},\mu). \tag{2.66}$$

Here, ψ_I satisfies the transport equation away from boundaries, and so acts like a particular integral. Conversely ψ_{LB} and ψ_{RB} decay rapidly away from the left and right boundaries respectively, but at the boundaries they force ψ to satisfy the required conditions. In this way, $\psi_{LB}+\psi_{RB}$ acts quite like a complementary function. The rapid decay is obtained by setting

$$\begin{aligned} x_{LB}&\equiv\frac{(x-a)}{\epsilon}-a,\\ x_{RB}&\equiv b-\frac{(b-x)}{\epsilon}, \end{aligned} \tag{2.67}$$

so that for example when $x=a$ we have $x_{LB}=0$, but for $x>a$, x_{LB} rapidly increases. Having ψ_{LB} and ψ_{RB} decay at the extremes of their spatial ranges completes the requirement.

From here, $\psi=\psi_I+\psi_{LB}+\psi_{RB}$ is substituted into the asymptotic transport equation, and the resulting form is split into three equations: one for ψ_I and the other

two for ψ_{LB} and ψ_{RB}. The ψ_I form leads to the diffusion approximation as given above, whereas the other forms should lead to relevant boundary conditions. The issue with this approach is that it requires integral equations for ψ_{LB} and ψ_{RB} to be solved, which do not have a simple solutions. It is possible that reasonable approximate solutions exist that would lead to suitable boundary conditions, however currently these are not known.

Other methods, such as the boundary layer analysis carried out in [9], could prove more successful, however more investigation into obtaining these boundary conditions is definitely needed.

2.5 The Diffusion Error

In this section we will prove a norm bound on the error incurred by the diffusion approximation, as derived in Section 2.4.1. First of all we must obtain an equation that governs the error, and we do this by subtracting the equation approximating the scalar flux away from the exact equation for the flux. I.e. we subtract (2.32) away from (2.31), and obtain

$$-\frac{1}{3\sigma_t}\left(\phi_0-\tilde{\phi}_0\right)''+\sigma_a\left(\phi_0-\tilde{\phi}_0\right)=\left(\sigma_s\mathcal{P}(r)+\frac{1}{\sigma_t}\mathcal{P}(\mu^2 r'')\right), \tag{2.68}$$

where $\left(\phi_0(x)-\tilde{\phi}_0(x)\right)$ is the error in the diffusion approximation, which we would like to bound. We can write this in a simpler form as

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}-3\sigma_t\sigma_a\right)E=R, \tag{2.69}$$

where

$$\begin{aligned} E &\equiv \phi_0-\tilde{\phi}_0, \\ R &\equiv -3\sigma_t\left(\sigma_s\mathcal{P}(r)+\frac{1}{\sigma_t}\mathcal{P}(\mu^2 r'')\right). \end{aligned} \tag{2.70}$$

So to bound the error incurred by the diffusion approximation, we need to bound the norm of E. To do this we will first solve a general form of (2.69), (in Lemma 2.5), and then prove a bound on the norm of that general solution, (in Lemma 2.6).

Lemma 2.5:
The differential equation

$$\left(\frac{d^2}{dx^2}-\alpha^2\right)(E(x))=R(x), \tag{2.71}$$

with boundary conditions has a solution given by

$$E=Ae^{\alpha x}+Be^{-\alpha x}+\mathcal{L}R(x), \tag{2.72}$$

where $A, B \in \mathbb{R}$ are chosen such that the boundary conditions are satisfied, $E, R \in L^2([a,b])$, $\alpha \geq 0$ and

$$\mathcal{L}R(x) \equiv \frac{1}{2\alpha}\int_a^b e^{\alpha|x-\xi|}R(\xi)\ d\xi.$$

Proof.
The homogeneous problem is satisfied by the complementary function

$$E_{CF} = A\mathrm{e}^{\alpha x} + B\mathrm{e}^{-\alpha x}.$$

It remains to prove that a particular integral is given by

$$E_{PI} = \mathcal{L}R.$$

Firstly, from the definition of E we can extract

$$\begin{aligned} E &= \mathcal{L}R, \\ &= \frac{1}{2\alpha}\int_a^b \mathrm{e}^{\alpha|x-\xi|}R(\xi)\ \mathrm{d}\xi, \\ &= \frac{1}{2\alpha}\left[\int_a^x \mathrm{e}^{\alpha(x-\xi)}R(\xi)\ \mathrm{d}\xi + \int_x^b \mathrm{e}^{\alpha(\xi-x)}R(\xi)\ \mathrm{d}\xi\right], \\ &= \frac{1}{2\alpha}\left[\mathrm{e}^{\alpha x}\int_a^x \mathrm{e}^{-\alpha\xi}R(\xi)\ \mathrm{d}\xi + \mathrm{e}^{-\alpha x}\int_x^b \mathrm{e}^{\alpha\xi}R(\xi)\ \mathrm{d}\xi\right]. \end{aligned}$$

From this $\frac{\mathrm{d}}{\mathrm{d}x}E$, and so $\frac{\mathrm{d}^2}{\mathrm{d}x^2}E$, can be found as follows

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}x}E &= \frac{1}{2\alpha}\left[\alpha\mathrm{e}^{\alpha x}\int_a^x \mathrm{e}^{-\alpha\xi}R(\xi)\ \mathrm{d}\xi + R(x) - \alpha\mathrm{e}^{-\alpha x}\int_x^b \mathrm{e}^{\alpha\xi}R(\xi)\ \mathrm{d}\xi - R(x)\right], \\ &= \frac{1}{2}\left[\mathrm{e}^{\alpha x}\int_a^x \mathrm{e}^{-\alpha\xi}R(\xi)\ \mathrm{d}\xi - \mathrm{e}^{-\alpha x}\int_x^b \mathrm{e}^{\alpha\xi}R(\xi)\ \mathrm{d}\xi\right], \end{aligned}$$

so

$$\begin{aligned} \frac{\mathrm{d}^2}{\mathrm{d}x^2}E &= \frac{1}{2}\left[\alpha\mathrm{e}^{\alpha x}\int_a^x \mathrm{e}^{-\alpha\xi}R(\xi)\ \mathrm{d}\xi + R(x) + \alpha\mathrm{e}^{-\alpha x}\int_x^b \mathrm{e}^{\alpha\xi}R(\xi)\ \mathrm{d}\xi + R(x)\right], \\ &= \frac{1}{2}\left[\alpha\int_a^b \mathrm{e}^{\alpha|x-\xi|}R(\xi)\ \mathrm{d}\xi + 2R(x)\right]. \end{aligned}$$

Next, straight multiplication gives

$$\alpha^2 E = \frac{\alpha}{2}\int_a^b \mathrm{e}^{\alpha|x-\xi|}R(\xi)\ \mathrm{d}\xi,$$

therefore

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}E - \alpha^2 E = R, \tag{2.73}$$

as required.

□

Under zero boundary conditions, Lemma A.1 verifies that the general solution proved in Lemma 2.5 becomes

$$E(x) = \mathcal{L}R(x) - \frac{\sinh(\alpha(b-x))}{\sinh(\alpha(b-a))}\mathcal{L}R(a) - \frac{\sinh(\alpha(x-a))}{\sinh(\alpha(b-a))}\mathcal{L}R(b). \tag{2.74}$$

We will now prove a norm bound on this solution.

Lemma 2.6:
If E is the solution to (2.69) *given in* (2.74)*, then*

$$\|E\|_2 \leq \frac{1}{\alpha^2}C(\alpha,a,b)\,\|R\|_2\,, \tag{2.75}$$

where $\|\cdot\|_2 \equiv \|\cdot\|_{L^2[a,b]}$.

Proof.
From (2.74) we have

$$E(x) = \mathcal{L}R(x) - \frac{\sinh(\alpha(b-x))}{\sinh(\alpha(b-a))}\mathcal{L}R(a) - \frac{\sinh(\alpha(x-a))}{\sinh(\alpha(b-a))}\mathcal{L}R(b). \tag{2.76}$$

where

$$\mathcal{L}R(x) \equiv \frac{1}{2\alpha}\int_a^b \mathrm{e}^{\alpha|x-\xi|}R(\xi)\,\mathrm{d}\xi.$$

Taking the norm of (2.76) leaves

$$\|E\|_2 \leq \underbrace{\|\mathcal{L}R\|_2}_{(\dagger)} + \underbrace{|\mathcal{L}R(a)|\left\|\frac{\sinh(\alpha(b-\cdot))}{\sinh(\alpha(b-a))}\right\|_2}_{(\dagger\dagger)} + \underbrace{|\mathcal{L}R(b)|\left\|\frac{\sinh(\alpha(\cdot-a))}{\sinh(\alpha(b-a))}\right\|_2}_{(\dagger\dagger\dagger)}. \tag{2.77}$$

We will consider each part of the above equation in turn, starting with (†). Defining $k(x) \equiv \mathrm{e}^{\alpha|x|}$, and recalling Young's inequality for convolutions, we have

$$\begin{aligned}\|\mathcal{L}R\|_2 &= \frac{1}{2\alpha}\|R * k\|_2 \\ &\leq \frac{1}{2\alpha}\|k\|_1\,\|R\|_2\,,\end{aligned} \tag{2.78}$$

where $*$ denotes a convolution (see Definition A.2). Evaluating the integral definition gives us that

$$\|k\|_1 = \frac{1}{\alpha}\left(\mathrm{e}^{\alpha b} - \mathrm{e}^{\alpha a}\right),$$

thus

$$\|\mathcal{L}R\|_2 \leq \frac{1}{2\alpha^2}\left(\mathrm{e}^{\alpha b} - \mathrm{e}^{\alpha a}\right)\|R\|_2 . \tag{2.79}$$

Next we consider (††). First of all

$$\begin{aligned}
|\mathcal{L}R(a)| &= \left|\frac{1}{2\alpha}\int_a^b k(a-\xi)R(\xi)\,\mathrm{d}\xi\right|, \\
&= \left|\frac{1}{2\alpha}\right|\left(\left|\int_a^b k(a-\xi)R(\xi)\,\mathrm{d}\xi\right|^2\right)^{\frac{1}{2}}, \\
&\leq \left|\frac{1}{2\alpha}\right|\left(\int_a^b |k(a-\xi)|^2\,\mathrm{d}\xi\int_a^b |R(\xi)|^2\,\mathrm{d}\xi\right)^{\frac{1}{2}}, \\
&= \left|\frac{1}{2\alpha}\right|\|k(a-\cdot)\|_2\,\|R(\cdot)\|_2 .
\end{aligned}$$

Again, evaluating the integral definition of the norm gives

$$\|k(a-\cdot)\|_2 = \left(\frac{1}{2\alpha}\left(\mathrm{e}^{2\alpha(b-a)} - 1\right)\right)^{\frac{1}{2}},$$

and so we have

$$|\mathcal{L}R(a)| \leq \left|\frac{1}{2\alpha}\right|\left(\frac{1}{2\alpha}\left(\mathrm{e}^{2\alpha(b-a)} - 1\right)\right)^{\frac{1}{2}}\|R(\cdot)\|_2 . \tag{2.80}$$

Integration also yields the following

$$\begin{aligned}
\left\|\frac{\sinh\left(\alpha(b-\cdot)\right)}{\sinh\left(\alpha(b-a)\right)}\right\|_2^2 &= \frac{1}{\left(\sinh\left(\alpha(b-a)\right)\right)^2}\int_a^b \frac{1}{2}\left(\cosh\left(2\alpha\left(b-x\right)\right) - 1\right)\,\mathrm{d}x, \\
&= \frac{1}{2\left(\sinh\left(\alpha(b-a)\right)\right)^2}\left[\frac{-1}{2\alpha}\sinh\left(2\alpha\left(b-x\right)\right) - x\right]_a^b, \\
&= \frac{\sinh\left(2\alpha(b-a)\right) - 2\alpha\left(b-a\right)}{4\alpha\left(\sinh\left(\alpha(b-a)\right)\right)^2}.
\end{aligned} \tag{2.81}$$

Combining (2.80) and (2.81) gives us that

$$|\mathcal{L}R(a)|\left\|\frac{\sinh\left(\alpha(b-\cdot)\right)}{\sinh\left(\alpha(b-a)\right)}\right\|_2 \leq \frac{1}{\alpha^2}\hat{C}(\alpha,a,b)\,\|R(\cdot)\|_2 , \tag{2.82}$$

where, once simplified, $\hat{C}(\alpha, a, b)$ satisfies

$$\hat{C}(\alpha, a, b) = \frac{1}{2\sqrt{2}} \left(1 + \mathrm{e}^{2\alpha(b-a)} - 4\alpha(b-a)\right) + \frac{\sqrt{2}\alpha(b-a)}{1 - \mathrm{e}^{2\alpha(b-a)}}. \tag{2.83}$$

For († † †) we apply an equivalent chain of reasoning to obtain the bound

$$|\mathcal{L}R(b)| \left\| \frac{\sinh(\alpha(\cdot - a))}{\sinh(\alpha(b-a))} \right\|_2 \leq \frac{1}{\alpha^2} \hat{C}(\alpha, a, b) \left\| R(\cdot) \right\|_2 . \tag{2.84}$$

Lastly, combining (2.77), (2.79), (2.82) and (2.84) leaves

$$\left\| E \right\|_2 \leq \frac{1}{\alpha^2} C(\alpha, a, b) \left\| R \right\|_2 , \tag{2.85}$$

as required.

□

Whilst this does give a bound, it is not conclusive since it says that the norm of the diffusion error, E, is bounded by the norm of a function of the residual, R. It is not immediately obvious from this when the diffusion approximation is most accurate. To try to answer this question we turn again to the asymptotic approach from Section 2.4.

2.5.1 Asymptotics and the Diffusion Error

Looking to our asymptotic method again, we can try improve our understanding of the bound obtained in Lemma 2.6. In Section 2.4.2 we had that

$$\begin{aligned} \sigma_t &= O(\epsilon^{-1}), \\ \sigma_a &= O(\epsilon), \\ \sigma_s &= \left(\epsilon^{-1} - \epsilon\right) = O(\epsilon^{-1}). \end{aligned} \tag{2.86}$$

where ϵ is a small quantity defined in (2.49). Then in Section 2.5 we worked from (2.69), which was

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} - 3\sigma_t \sigma_a \right) E = R. \tag{2.87}$$

Noting that $\sigma_t \sigma_a = O(1)$, we see that the ϵ dependence of E relies upon that of R. From (2.70) we know

$$R = -3\left(\sigma_t \sigma_s \mathcal{P}(r) + \mathcal{P}(\mu^2 r'')\right). \tag{2.88}$$

We have that $\sigma_t \sigma_s = O(\epsilon^{-2})$, so for E to depend upon a positive power of ϵ, it would be required that $\mathcal{P}(r)$ be of order greater or equal to ϵ^2. Our original asymptotic expansion

of ψ was

$$\psi(x,\mu) \sim \sum_{k=0}^{\infty} \epsilon^k \psi^{(k)}(x,\mu), \tag{2.89}$$

and we later learned that $\psi^{(0)} = \phi^{(0)}$, thus we can deduce that $\phi^{(0)} = O(1)$. Drawing a parallel between this expansion and the Legendre polynomial expansion given by

$$\psi(x,\mu) = \phi_0(x) + 3\mu\phi_1(x) + r(x,\mu) \tag{2.90}$$

hints that maybe $\phi_1 = O(\epsilon)$ and $r = O(\epsilon^2)$, however no rigorous connection has been worked out yet.

This asymptotic approach seems a positive branch to pursue, since establishing a dependence of R upon ϵ would cause Lemma 2.6 to imply that the diffusion error decreases with ϵ. This could eventually help to verify the situations in which diffusion synthetic acceleration (see the next section) is beneficial.

2.6 Diffusion Synthetic Acceleration

We have seen in Sections 2.4 and 2.5 that under certain conditions a diffusion approximation can be used to find approximate solutions to the neutron transport equation. In this section we will look at using this approximation as part of an iterative scheme to speed up convergence. The scheme we will introduce is known as *diffusion synthetic acceleration*, or DSA, however first of all we must explain what is meant by *synthetic acceleration* in general.

2.6.1 Synthetic Acceleration Methods

Synthetic acceleration methods were first introduced by Kopp [11] in 1962. They build on whatever iterative scheme you are using by treating that scheme as the first step of a two-step process. In the second step, the acceleration method attempts to estimate the error from the first step, then use that to update the current approximation. We will use the example of source iteration to illustrate what we mean here, and will follow the derivation presented in [6].

Consider source iteration written as

$$\mathcal{T}\psi^{(i+\frac{1}{2})} = \mathcal{S}\psi^{(i)} + Q, \tag{2.91}$$

which is equivalent to the form in (2.16). Using some initial $\psi^{(i)}$ this gives us a $\psi^{(i+\frac{1}{2})}$, and we then try to obtain some $\psi^{(i+1)}$ which is even closer to the true solution. This is done by looking at an equation for the error in source iteration, which can be obtained

by subtracting (2.91) from an equation for the true solution, (2.5). This gives us the following

$$\begin{aligned} \mathcal{T}\left(\psi - \psi^{(i+\frac{1}{2})}\right) &= \mathcal{S}\left(\psi - \psi^{(i)}\right), \\ &= \mathcal{S}\left(\psi - \psi^{(i+\frac{1}{2})}\right) + \mathcal{S}\left(\psi^{(i+\frac{1}{2})} - \psi^{(i)}\right), \\ \Rightarrow \quad (\mathcal{T} - \mathcal{S})\left(\psi - \psi^{(i+\frac{1}{2})}\right) &= \mathcal{S}\left(\psi^{(i+\frac{1}{2})} - \psi^{(i)}\right). \end{aligned} \tag{2.92}$$

Solving this for ψ allows us to precisely define the true solution in terms of known variables. Unfortunately to achieve this we would need to be able to find $(\mathcal{T} - \mathcal{S})^{-1}$. To get around this a synthetic acceleration scheme replaces $(\mathcal{T} - \mathcal{S})^{-1}$ with some approximation, say M, that is more easily calculable. Thus the second step of our two-step process can be written as

$$\psi^{(i+1)} = \psi^{(i+\frac{1}{2})} + M\mathcal{S}\left(\psi^{(i+\frac{1}{2})} - \psi^{(i)}\right). \tag{2.93}$$

Upon convergence it can be shown that the solution obtained by this method would satisfy the original transport problem (see, for example, [6]).

Acceleration schemes such as this can be shown to be equivalent to preconditioning (see [6]) and similarly to preconditioning, the effectiveness of the method is dependent upon the choice of M. One must find a balance between an easily calculable M that is a poor approximation to $(\mathcal{T}-\mathcal{S})^{-1}$, or one that more accurately approximates $(\mathcal{T}-\mathcal{S})^{-1}$ but is tricky to calculate.

2.6.2 Diffusion Synthetic Acceleration

In diffusion synthetic acceleration the approximation to $(\mathcal{T} - \mathcal{S})^{-1}$ is achieved via the diffusion approximation defined in Section 2.4. The first step of the iteration remains the same, given by

$$\mathcal{T}\psi^{(i+\frac{1}{2})} = \mathcal{S}\psi^{(i)} + Q. \tag{2.94}$$

To proceed with utilising the diffusion approximation we require some notation for error. First,

$$e^{(i+\frac{1}{2})}(x,\mu) \equiv \psi(x,\mu) - \psi^{(i+\frac{1}{2})}(x,\mu), \tag{2.95}$$

which denotes error in the current approximation of the neutron flux, and secondly

$$E^{(i+1)}(x) \approx \frac{1}{2}\int_{-1}^{1} e^{(i+\frac{1}{2})}(x,\mu)\,\mathrm{d}\mu, \\ \left(= \phi(x) - \phi^{(i+\frac{1}{2})(x)} \right), \tag{2.96}$$

which denotes an approximation to the error in $\phi^{(i+\frac{1}{2})(x)}$. Here we have reused notation for the scalar flux defined in (2.59). Looking back to (2.92) we now have that

$$(\mathcal{T} - \mathcal{S})\left(e^{(i+\frac{1}{2})}\right) = \mathcal{S}\left(\psi^{(i+\frac{1}{2})} - \psi^{(i)}\right). \tag{2.97}$$

Therefore our work in Section 2.4 tells us that

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{3\sigma_t}\frac{\mathrm{d}}{\mathrm{d}x}E^{(i+1)}\right) + \sigma_a E^{(i+1)} = \sigma_s\left(\phi^{(i+\frac{1}{2})} - \phi^{(i)}\right). \tag{2.98}$$

This can be solved with appropriate boundary conditions given in Section 2.4, and then the two-step iteration may begin again using

$$\phi^{(i+1)} \approx \frac{1}{2}E^{(i+1)} + \phi^{(i+\frac{1}{2})}. \tag{2.99}$$

Thus between (2.94), (2.98) and (2.99) we have theoretically constructed one complete iteration of diffusion synthetic acceleration. However we have not finished the story: questions of stability, convergence, and when best to apply this method have yet to be answered. We will address these to the best of our current knowledge in the next subsection.

2.6.3 Stability and Convergence of DSA

After Kopp's initial development of synthetic acceleration schemes in [11], they remained difficult to stabilise for a long time, which limited their applicability [12]. This was finally resolved in 1977 by Alcouffe [2] who discovered that to obtain stability, the transport equation and diffusion equation must be consistently discretised. In [12], Larsen notes that this means the discretised form of the diffusion equation must be derived from the discretised form of the transport equation. A good history both before and after Alcouffe's paper is given in [12], which also extends the work of Alcouffe and others to derive unconditionally stable acceleration methods for the slab geometry transport equation. (I think further reading of these two papers in particular would help obtain a working DSA code).

Regarding the convergence of DSA, Larsen [12], p.50, mentions that two papers in 1981 found a bound on the spectral radius of the scheme introduced by Alcouffe via Fourier analysis. He notes that the reduction on error between iterations is characterised by this radius, though I am unsure precisely what the relationship would be. We are currently unaware of any papers which fully quantify or bound the error incurred

by one iteration of a DSA scheme. We have put some effort towards finding a bound on the diffusion error (as explained in Section 2.5), though this is currently inconclusive. It may therefore be beneficial to explore the route highlighted by Larsen in trying to understand the effectiveness of the scheme. We hope that such an error bound, if found, would support the assumptions made in Section 1.2.3, and possibly yield further information about conditions under which DSA could improve convergence.

2.7 Neumann Series Convergence

In this section we will prove a convergence result related to the work in Section 2.3 but from a different point of view. When tracking particles in a Monte Carlo simulation, the terms of a Neumann series expansion are used to track neutrons between successive collisions. Physically it would make sense for this series to terminate after some finite number of terms since sub-critical reactions will eventually die out unless an artificial influx of neutrons is maintained. In this section we will find the relevant Neumann series and prove that it is convergent.

As we have seen, we can write the 1D neutron transport equation with isotropic scattering in a homogeneous medium as

$$(\mathcal{T} - \mathcal{S})\,\psi = Q, \tag{2.100}$$

where $\mathcal{T}$ and $\mathcal{S}$ are the transport and scatter operators defined in (2.4), $Q(x)$ is an isotropic source of neutrons, and $\psi(x,\mu)$ denotes the neutron flux. We are again working with $x \in [a,b] \subset \mathbb{R}$ and $\mu \in [-1,1]$. We once more introduce the space

$$L^2\left(V, L^1(S)\right) \equiv \left\{ \psi : V \times S \to \mathbb{R} \ : \ \int_V \|\psi(x,\cdot)\|^2_{L^1(S)} \ \mathrm{d}x < \infty \right\}, \tag{2.101}$$

where

$$\|\psi\|_{L^2(V,L^1(S))} = \int_V \|\psi(x,\cdot)\|^2_{L^1(S)} \ \mathrm{d}x,$$

with $\|\psi(x,\cdot)\|_{L^1(S)} = \int_S |\psi(x,\mu)| \ \mathrm{d}\mu$, the usual L^1-norm. We further define an operator, $\mathcal{P}$, which we originally defined in Section 2.2. This operator averages over angle and scales, as follows

$$\mathcal{P}(\cdot) \equiv \frac{1}{2}\int_{-1}^{1} (\cdot) \ \mathrm{d}\mu.$$

Note that this allows us to break down the scatter operator into $\mathcal{S} \equiv \sigma_s \mathcal{P}$.

The existence of a unique solution to (2.100) has been proven, (see for example [19], [16]) and so we proceed from (2.100) as follows

$$\begin{aligned}\psi &= (\mathcal{T}-\mathcal{S})^{-1}Q,\\ &= \left(\mathcal{T}\left(I-\mathcal{T}^{-1}\mathcal{S}\right)\right)^{-1}Q,\\ &= \left(I-\mathcal{T}^{-1}\mathcal{S}\right)^{-1}\mathcal{T}^{-1}Q.\end{aligned}$$

From here, we can use a Neumann expansion to obtain

$$\begin{aligned}\psi &= \left(I+\mathcal{T}^{-1}\mathcal{S}+\mathcal{T}^{-1}\mathcal{S}\mathcal{T}^{-1}\mathcal{S}+\ldots\right)\mathcal{T}^{-1}Q,\\ &= \mathcal{T}^{-1}Q+\mathcal{T}^{-1}\mathcal{S}\left(\mathcal{T}^{-1}Q\right)+\mathcal{T}^{-1}\mathcal{S}\left(\mathcal{T}^{-1}\mathcal{S}\mathcal{T}^{-1}Q\right)+\ldots.\end{aligned} \tag{2.102}$$

This is a Neumann series, and is convergent provided the relevant norm of $\mathcal{T}^{-1}\mathcal{S}$ is bounded by 1. It is equivalent to the following fixed-point iteration for (2.100)

$$\psi^{(n+1)} = \mathcal{T}^{-1}Q+\mathcal{T}^{-1}\mathcal{S}\psi^{(n)}, \tag{2.103}$$

which also converges if and only if

$$\left\|\mathcal{T}^{-1}\mathcal{S}\right\|_{\mathscr{L}(L^2([a,b],L^1[-1,1]))}<1.$$

We now prove that this norm bound holds.

Lemma 2.7:
If $\mathcal{T}$ and $\mathcal{S}$ are operators defined as in (2.4)*, then*

$$\left\|\mathcal{T}^{-1}\mathcal{S}\right\|_{\mathscr{L}(L^2([a,b],L^1[-1,1]))}<1. \tag{2.104}$$

Proof.
First define

$$\phi^{(i)}(x) = \mathcal{P}(\psi^{(i)}(x,\mu)), \tag{2.105}$$

equivalently to (2.7). Looking again at (2.103) and recalling that $\mathcal{S}\equiv\sigma_s\mathcal{P}$, we can see that

$$\begin{aligned}\psi^{(n+1)} &= \mathcal{T}^{-1}Q+\sigma_s\mathcal{T}^{-1}\mathcal{P}\psi^{(n)},\\ &= \mathcal{T}^{-1}Q+\sigma_s\mathcal{T}^{-1}\phi^{(n)},\end{aligned} \tag{2.106}$$

which is just a source iteration step as defined in (2.16). In Lemma 2.4 we proved that this scheme was a contraction, and so under the governance of (2.103) we know that $\psi^{(n)}$ converges. Hence we have that

$$\left\|\mathcal{T}^{-1}\mathcal{S}\right\|_{\mathscr{L}(L^2([a,b],L^1[-1,1]))}<1, \tag{2.107}$$

as required.

□

Using this result we have that the Neumann series, (2.102), converges and so follows the physical intuition given at the start of this section.

This result, while very neat, is not of great physical relevance. This is because the Monte Carlo simulations, to which we alluded earlier, are of greatest benefit when the spatial medium is highly inhomogeneous (see [15] chapter 7). This suggests that a good line of enquiry for future work would be to replicate this result in the inhomogeneous case. This is not a trivial extension since the constant nature of the cross sections is relied upon heavily in the above proof, and so a totally different approach may be needed.

2.8 Summary

In this chapter we have defined source iteration and given a relevant convergence result. We have seen two different methods of obtaining the diffusion approximation to the transport equation, and used the asymptotic side to see a clear indication that this approximation is sensible. We have established boundary conditions for one version of the diffusion equation, and mentioned current difficulties encountered for the other. We have obtained a bound on the error incurred by the diffusion approximation, and gone some way towards interpreting it though there is still much to be done in that area. We have defined diffusion synthetic acceleration, and have explained how the effectiveness of that scheme relies upon our earlier diffusion work. Lastly we have shown that a Neumann series relevant to Monte Carlo simulations converges, and drawn a connection between this and the convergence of source iteration.

In going forward we have outlined several areas where we would like to further our knowledge. Principally these are

- to obtain sensible boundary conditions for the asymptotic form of the diffusion equation,
- to better establish the ϵ dependence of the residual term, $r(x, \mu)$, and use this to show that the diffusion error reduces with ϵ,
- to extend the work on the Neumann series convergence to the case of non-homogeneous media.

Other areas that may be worth looking at include

- understanding the Fourier analysis carried out in [12] to see whether this could help shed light on the error in DSA,
- following up on the work of [2] and writing a diffusion solver that uses a discretisation derived from a discretised transport equation.

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Appendix A

A.1 Results for Section 2.5 on the Diffusion Approximation Error

This first result finds the values of constants A and B for the general solution found in Lemma 2.5 in the case where we have zero boundary conditions.

Lemma A.1:
The differential equation

$$\left(\frac{d^2}{dx^2} - \alpha^2\right)(E(x)) = R(x), \tag{A.1}$$

with zero boundary conditions

$$E(a) = E(b) = 0, \tag{A.2}$$

has a solution given by

$$E(x) = \mathcal{L}R(x) - \frac{\sinh(\alpha(b-x))}{\sinh(\alpha(b-a))}\mathcal{L}R(a) - \frac{\sinh(\alpha(x-a))}{\sinh(\alpha(b-a))}\mathcal{L}R(b), \tag{A.3}$$

where α and $\mathcal{L}(\cdot)$ are defined as in Lemma 2.5.

Proof.
Using the exponential definition of sinh, (A.3) can be written as

$$E(x) = \mathcal{L}R(x) + \frac{\mathrm{e}^{\alpha x}\left(\mathrm{e}^{-\alpha b}\mathcal{L}R(a) - \mathrm{e}^{-\alpha a}\mathcal{L}R(b)\right)}{2\sinh(\alpha(b-a))} + \frac{\mathrm{e}^{-\alpha x}\left(\mathrm{e}^{\alpha a}\mathcal{L}R(b) - \mathrm{e}^{\alpha b}\mathcal{L}R(a)\right)}{2\sinh(\alpha(b-a))}. \tag{A.4}$$

In this form, Lemma 2.5 says that this is a general solution to (A.1), and it remains to verify that it satisfies the required zero boundary conditions.

Since $\sinh(0) = 0$, we immediately get

$$E(a) = \mathcal{L}R(a) - \frac{\sinh(\alpha(b-a))}{\sinh(\alpha(b-a))}\mathcal{L}R(a) - 0 = 0, \tag{A.5}$$

and

$$E(x) = \mathcal{L}R(b) - 0 - \frac{\sinh(\alpha(b-a))}{\sinh(\alpha(b-a))}\mathcal{L}R(b) = 0, \tag{A.6}$$

as required.

□

The following definition and result are needed in the proof of Lemma 2.6

Definition A.2 (Convolution)**:**
If f and g are functions over the domain X, then their convolution is defined as

$$(f * g)(x) \equiv \int_X g(x-\xi)f(\xi)\ d\xi.$$

Lemma A.3 (Young's Inequality for Convolutions)**:**
If f and g are functions over the same domain, then

$$\|f * g\|_r \leq \|f\|_p \|g\|_q \tag{A.7}$$

where

$$\frac{1}{p} + \frac{1}{q} = \frac{1}{r} + 1. \tag{A.8}$$