

# The Asymptotic Drift-Diffusion Limit of Thermal Neutrons

Ryan G. McClarren, Marvin L. Adams, Pablo Vacquer  
Department of Nuclear Engineering  
Texas A&M University  
College Station, Texas, United States

Clay Strack  
Department of Petroleum Engineering  
Texas A&M University  
College Station, Texas, United States

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## Abstract

It is well known that in an infinite, source-free, purely scattering medium with physically realizable cross-sections, neutrons attain a Maxwell-Boltzmann distribution characterized by the material temperature. In this work we look at how small variations to these conditions change the behavior of the thermal-neutron distribution in space and energy. Specifically, our analysis examines the influence of small amounts of absorption and a small source as well as temperature variations in the material. We restrict our study to regions away from boundary and initial layers. The result of the asymptotic analysis is that the amplitude of the neutron scalar flux satisfies a drift-diffusion equation in which the diffusion coefficient and drift velocity depend on the first-order anisotropy of the scattering kernel as well as the gradient of the material temperature. Additionally, through first order in the asymptotic expansion the neutron energy distribution is Maxwell-Boltzmann at the local material temperature.

## 1 Introduction

There are several well known asymptotic limits of the neutron transport equation. Perhaps the best-known example is the asymptotic limit of large scattering cross-sections and small absorption cross-sections. In this situation the leading-order neutron transport solution satisfies a diffusion or drift-diffusion equation [1, 2, 3]. Other transport applications have their own useful asymptotic limits. For example, the transport equations that govern charge kinetics in semiconductors limit to a drift-diffusion model in certain circumstances [4]. In this work we use an asymptotic analysis to obtain results that to our knowledge have not been previously published. In particular we study thermal neutrons in the presence of low absorption probability and small sources. We include time and energy dependence and allow material temperature to vary in space and time. The results of our analysis are that 1) the leading-order scalar-flux amplitude satisfies a drift-diffusion equation, 2) the leading-order and next-order scalar fluxes have Maxwell-Boltzmann energy distributions at the local material temperature, 3) the drift velocity is proportional to the local temperature gradient in the scattering medium, and 4) the angular flux is isotropic to leading order and linearly anisotropic to the next order. The first and fourth results have appeared in previous analyses [3], but to our knowledge the connections with the Maxwell-Boltzmann energy distribution and material temperature gradients have not been previously published.

There is a strong connection between the results we find for thermal neutrons and the equilibrium-diffusion limit for thermal radiative transfer [5]. In that limit the distribution of thermal radiation is a

Planck distribution at the local material temperature and the radiation energy density (a constant multiple of the energy-integrated scalar flux) satisfies a nonlinear diffusion equation.

In this work we consider a medium containing a small source of neutrons,<sup>1</sup> with an absorption cross section that is much smaller than the scattering cross section. One example would be a heavy-water or graphite column (often called a thermal column) mounted next to a research reactor, as shown in Fig. 1. In such an arrangement, if the reactor water temperature is above room temperature, there could be a temperature gradient in the thermal column, as well as a small amount of absorption in the column’s material. Most of the thermal neutrons in the thermal column would have originated in the reactor (meaning little or no volumetric source in the interior of the column).

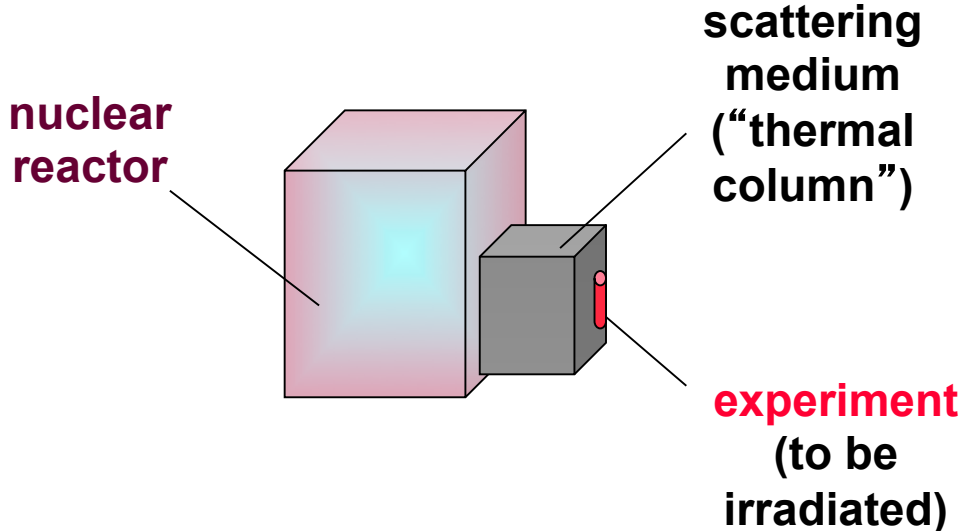


Figure 1: A thermal column mounted next to a reactor. Such thermal columns are often installed to provide thermal neutrons to irradiate experiments.

We restrict our analysis in this study to regions away from boundary and initial layers. Future work will explore appropriate boundary and initial conditions in the asymptotic limit that we study.

The outline of this paper is the following. We present our starting point, the transport equation for thermal neutrons, in Section 2. We then in Section 3 perform the asymptotic analysis and discuss the drift-diffusion model that arises. This is followed by our conclusions in Section 4. Theoretical and physical bases are presented in an appendix for some operator properties that underpin the asymptotic analysis.

## 2 Description of the Model

We begin with the transport equation for thermal neutrons:

$$\begin{aligned} \frac{1}{v} \frac{\partial \psi}{\partial t} + \hat{\Omega} \cdot \vec{\nabla} \psi + (\sigma_s(\vec{r}, E, t) + \sigma_a(\vec{r}, E, t)) \psi(\vec{r}, \hat{\Omega}, E, t) \\ = \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(\vec{r}, E', t) f(\vec{r}, E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}, t) \psi(\vec{r}, \hat{\Omega}', E', t) + q(\vec{r}, \hat{\Omega}, E, t). \end{aligned} \quad (1)$$

Our notation is standard:  $\vec{r}$  is the spatial variable,  $\hat{\Omega}$  is a unit vector in the neutron’s direction of flight,  $E$  is the neutron energy, and  $t$  is the temporal variable. The neutron speed is  $v(E)$ ,  $\psi(\vec{r}, \hat{\Omega}, E, t)$  is the neutron

<sup>1</sup>That is, we assume that the source-rate density is small relative to the collision-rate density.

angular flux,  $\sigma_s(\vec{r}, E, t)$  is the macroscopic scattering cross-section,  $\sigma_a(\vec{r}, E, t)$  is the macroscopic absorption cross-section,  $f(\vec{r}, E' \rightarrow E, \mu_0, t)$  is the double-differential scattering phase function, and  $q$  is a prescribed source of neutrons (which would typically come from downscattering of fast neutrons). We have assumed that the scattering function for a given pair of initial and final energies depends only on the scattering angle and not on the individual incident and exiting directions. That is, we assume that the medium “looks” the same to a neutron of energy  $E'$  in the lab frame, regardless of its lab-frame direction of travel. This is sometimes referred to as an “isotropic” or “rotationally invariant” medium. This assumption is valid if: 1) the bulk speed of the material in the lab frame is negligibly small relative to vibrational nucleus speeds or the speeds of the majority of the neutrons, and 2) the material does not interact differently with neutrons moving in different directions (as it might if it had non-random crystal orientations and the neutrons had large wavelengths).

We expand the scattering phase function in Legendre polynomials:

$$f(\vec{r}, E' \rightarrow E, \mu_0, t) = \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\mu_0) f_l(\vec{r}, E' \rightarrow E, t), \quad (2)$$

where

$$f_l(\vec{r}, E' \rightarrow E, t) = \int_{-1}^1 d\mu_0 P_l(\mu_0) f(\vec{r}, E' \rightarrow E, \mu_0, t). \quad (3)$$

We expand the angular flux in spherical harmonics:

$$\psi(\vec{r}, \hat{\Omega}', E', t) = \sum_{l=0}^{\infty} \sum_{m=-l}^l \phi_l^m(\vec{r}, E', t) Y_{lm}(\hat{\Omega}'), \quad (4)$$

where

$$\phi_l^m(\vec{r}, E', t) = \int_{4\pi} d\Omega Y_{lm}^*(\hat{\Omega}) \psi(\vec{r}, \hat{\Omega}, E', t), \quad (5)$$

Then, after taking advantage of the spherical-harmonics addition theorem, we obtain the transport equation with the scattering source defined in terms of Legendre scattering moments and spherical-harmonics flux moments:

$$\begin{aligned} \frac{1}{v} \frac{\partial \psi}{\partial t} + \hat{\Omega} \cdot \vec{\nabla} \psi + (\sigma_s(\vec{r}, E, t) + \sigma_a(\vec{r}, E, t)) \psi(\vec{r}, \hat{\Omega}, E, t) \\ = \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \int dE' \sigma_s(\vec{r}, E', t) f_l(\vec{r}, E' \rightarrow E, t) \phi_l^m(\vec{r}, E', t) + q(\vec{r}, \hat{\Omega}, E, t). \end{aligned} \quad (6)$$

### 3 Asymptotic Analysis

We will use a standard approach to the asymptotic analysis as shown in many other works in neutron [2, 1, 6] and radiation [5, 7] transport. To proceed with the asymptotic analysis we assume we are in a situation where:

- the scattering cross-section is large,
- the absorption cross-section is small,
- the source is small, and
- the change in time of the solution is small,
- the solution does not change much over distances of a scattering mean free path but may change significantly over distances of an absorption mean free path,

- the temperature does not change much over distances of a scattering mean free path,
- cross sections and temperatures do not change rapidly in time.

These conditions are satisfied in, for example, the thermal column experiment mentioned above. In that situation the scattering cross-section is large relative to the absorption cross section, there is at most a small thermal-neutron source inside the medium (from downscattering of fast neutrons that enter the column), and the reactor is likely operating at or near steady-state. Also to proceed we will assume that the region we are analyzing is away from any boundary and initial layers. We assume that in the interior of the medium, the spatial variation of the solution, and the material temperature, is small over a distance of a mean-free path. A large variation could potentially arise near material interfaces, for example, or anywhere the material temperature varied on a spatial scale comparable a neutron mean-free path (if such a thing were possible), but our analysis here does not address regions with such sharp spatial variations.

To express the conditions listed above we introduce a small positive parameter,  $\epsilon$ , and scale terms in Eq. (1) appropriately to obtain

$$\begin{aligned} \frac{\epsilon}{v} \frac{\partial \psi}{\partial t} + \hat{\Omega} \cdot \vec{\nabla} \psi + \left( \frac{\sigma_s(\vec{r}, E, t)}{\epsilon} + \epsilon \sigma_a(\vec{r}, E, t) \right) \psi(\vec{r}, \hat{\Omega}, E, t) \\ = \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \int dE' \frac{\sigma_s(\vec{r}, E', t)}{\epsilon} f_l(\vec{r}, E' \rightarrow E, t) \phi_l^m(\vec{r}, E', t) + \epsilon q(\vec{r}, \hat{\Omega}, E, t). \end{aligned} \quad (7)$$

Next, we formally expand the angular flux in a power series in  $\epsilon$ :

$$\psi = \sum_{l=0}^{\infty} \epsilon^l \psi^{(l)}. \quad (8)$$

We then plug this expansion into Eq. (7) and equate like powers of  $\epsilon$ .

### 3.1 The leading-order, $O(\epsilon^{-1})$ , equations

The leading-order terms in  $\epsilon$  are the  $\epsilon^{-1}$  terms; these are

$$\sigma_s(\vec{r}, E, t) \psi^{(0)}(\vec{r}, \hat{\Omega}, E, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \int dE' \sigma_s(\vec{r}, E', t) f_l(\vec{r}, E' \rightarrow E, t) \phi_l^m(\vec{r}, E', t). \quad (9)$$

This is a steady-transport equation for a source-free, absorption-free infinite medium. One of the triumphs of kinetic theory is the proof that in such a situation with a physically realizable scattering function, the solution for  $\psi$  is an isotropic-in-angle Maxwellian distribution [8]. This result gives

$$\psi^{(0)}(\vec{r}, \hat{\Omega}, E, t) = \frac{\phi_{\text{th}}^{(0)}(\vec{r}, t)}{4\pi} M(E, T) \quad (10)$$

where

$$\phi_{\text{th}}^{(0)}(\vec{r}, t) = \int_0^{\infty} dE \int_{4\pi} d\Omega \psi^{(0)}(\vec{r}, \hat{\Omega}, E, t),$$

and  $M(E, T)$  is the Maxwellian distribution defined by

$$M(E, T) \equiv \frac{E}{(kT)^2} e^{-\frac{E}{kT}}, \quad (11)$$

with  $k$  being the Boltzmann constant and  $T$  being the material temperature, which varies with  $\vec{r}$  and  $t$ . Because the temperature in the medium could vary in space and time, Eq. (10) says that to leading order

the angular flux has an energy distribution that is Maxwell-Boltzmann at the local temperature at any given time.

The Maxwell-Boltzmann distribution has the following property.

$$\int_0^\infty M(E, T) dE = 1, \quad (12)$$

and  $\phi_{\text{th}}^{(0)}$  is related to the number density of neutrons by

$$\phi_{\text{th}}^{(0)}(\vec{r}, t) = \sqrt{\frac{8kT(\vec{r}, t)}{\pi m_n}} n_{\text{th}}(\vec{r}, t), \quad (13)$$

where  $m_n$  is the mass of the neutron. Note at this point the value of  $n_{\text{th}}$  is not yet determined, and we will need to derive an auxiliary equation to solve for this quantity. All we know at this point in the analysis is that to leading order  $\psi$  is isotropic in angle and has a Maxwell-Boltzmann distribution in energy.

The isotropy of the leading-order solution deserves further discussion. If we divide Eq. (9) by  $\sigma_s(\vec{r}, E, t)$  and then operate with  $\int_{4\pi} d\Omega Y_{lm}^*(\hat{\Omega})(\cdot)$  we obtain, by orthogonality of the spherical-harmonics functions, the following.

$$\phi_l^{m(0)}(\vec{r}, E, t) = \frac{1}{\sigma_s(\vec{r}, E, t)} \int dE' \sigma_s(\vec{r}, E', t) f_l(\vec{r}, E' \rightarrow E, t) \phi_l^{m(0)}(\vec{r}, E', t). \quad (14)$$

If we define the integral operator operator  $\mathcal{S}_l$  as

$$[\mathcal{S}_l]g(E) = \frac{1}{\sigma_s(E)} \int_0^\infty dE' \sigma_s(E') f_l(E' \rightarrow E) g(E'), \quad (15)$$

then we can rewrite our  $(l, m)$ -moment equation as

$$[I - \mathcal{S}_l] \phi_l^{m(0)} = 0. \quad (16)$$

In the appendix we show that  $[I - \mathcal{S}_l]$  is invertible for all  $l > 0$ , at least for physically realizable scattering laws. It follows that  $\phi_l^{m(0)} = 0$  for all  $l > 0$ , which means there are no anisotropic components in the leading-order angular flux. We also affirm in the appendix that  $[I - \mathcal{S}_0]$  is not invertible, which agrees with the known result stated above, namely that an isotropic solution (the Maxwell-Boltzmann distribution) does satisfy the  $l = 0$  equation. Thus, the leading-order angular flux in our setting is isotropic in direction and has a Maxwell-Boltzmann distribution in energy.

### 3.2 The $O(1)$ equations

If we continue our analysis of Eq. (7) and examine the next order in  $\epsilon$  (the order- $\epsilon^0$  or  $O(1)$  terms), we find

$$\begin{aligned} \hat{\Omega} \cdot \vec{\nabla} \psi^{(0)}(\vec{r}, \hat{\Omega}, E, t) + \sigma_s(\vec{r}, E, t) \psi^{(1)}(\vec{r}, \hat{\Omega}, E, t) \\ = \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \int dE' \sigma_s(\vec{r}, E', t) f_l(\vec{r}, E' \rightarrow E, t) \phi_l^{m(1)}(\vec{r}, E', t). \end{aligned} \quad (17)$$

If we operate on Eq. (17) with  $\int_{4\pi} d\Omega(\cdot)$ , recognizing that  $\psi^{(0)}$  is isotropic  $\equiv \phi^{(0)}/4\pi$ , we obtain

$$\sigma_s(\vec{r}, E, t) \phi^{(1)}(\vec{r}, E, t) = \int_0^\infty dE' \sigma_s(\vec{r}, E', t) f_0(E' \rightarrow E, t) \phi^{(1)}(\vec{r}, E', t). \quad (18)$$

Here we have used the definition of  $\phi$ :

$$\phi = \int_{4\pi} d\Omega \psi,$$

and recognized the identity

$$\int_{4\pi} d\Omega \hat{\Omega} = \vec{0}.$$

Equation (18) is a source-free infinite-medium equation without absorption. As before, the solution of this equation is Maxwell-Boltzmann in energy,

$$\phi^{(1)}(\vec{r}, E, t) = \phi_{\text{th}}^{(1)}(\vec{r}, t)M(E, T), \quad (19)$$

with  $T$  the material temperature at position  $\vec{r}$  and time  $t$ , where the amplitude function  $\phi_{\text{th}}^{(1)}$  is yet unknown. That is, the isotropic portion of the  $O(\epsilon)$  component of the angular flux,  $\psi^{(1)}$ , has a Maxwell-Boltzmann distribution in energy, at the local temperature. However, in this case the anisotropic portions are not necessarily zero as they were in the leading-order component of  $\psi$ . We must proceed further to assess this.

When we operate on Eq. (17) with  $\int_{4\pi} d\Omega \hat{\Omega}(\cdot)$  we obtain:

$$\frac{1}{3}\vec{\nabla}\phi^{(0)}(\vec{r}, E, t) + \sigma_s(\vec{r}, E, t)\vec{J}^{(1)}(\vec{r}, E, t) = \int_0^\infty dE' \sigma_s(\vec{r}, E', t)f_1(\vec{r}, E' \rightarrow E, t)\vec{J}^{(1)}(\vec{r}, E', t), \quad (20)$$

where we have used the definitions of  $\phi$  and  $\vec{J}$ :

$$\phi = \int_{4\pi} d\Omega \psi, \quad \text{and} \quad \vec{J} = \int_{4\pi} d\Omega \hat{\Omega}\psi,$$

used the orthogonality of the spherical-harmonics functions, and noted that

$$\left[ \int_{4\pi} d\Omega \hat{\Omega}\hat{\Omega} \right] \cdot \frac{\vec{\nabla}\phi}{4\pi} = \frac{1}{3}\vec{\nabla}\phi.$$

In operator form Eq. (20) can be written as

$$[I - \mathcal{S}_1]\vec{J}^{(1)}(\vec{r}, E, t) = -\frac{1}{3\sigma_s(\vec{r}, E, t)}\vec{\nabla}\phi^{(0)}(\vec{r}, E, t). \quad (21)$$

To proceed beyond Eq. (21) we need to know whether the operator  $[I - \mathcal{S}_1]$  is invertible. It may not be obvious that this operator is invertible, given that the operator  $[I - \mathcal{S}_0]$  is singular, but in the appendix we show that  $[I - \mathcal{S}_l]$  is indeed invertible for  $l > 0$  for any physically realizable neutron scattering function.

With the knowledge that  $[I - \mathcal{S}_1]$  is invertible we can develop a version of Fick's law (i.e., a statement that says the "current" of neutrons is proportional to the negative gradient of the density). We rearrange Eq. (21):

$$\begin{aligned} \vec{J}^{(1)}(\vec{r}, E, t) &= -[I - \mathcal{S}_1]^{-1} \left[ \frac{1}{3\sigma_s(\vec{r}, E, t)}\vec{\nabla}\phi^{(0)}(\vec{r}, E, t) \right] \\ &= -[I - \mathcal{S}_1]^{-1} \left[ \frac{1}{3\sigma_s(\vec{r}, E, t)}\vec{\nabla} \left( \phi_{\text{th}}^{(0)}(\vec{r}, t)M(E, T) \right) \right], \end{aligned} \quad (22)$$

and then integrate over all energy:

$$\vec{J}^{(1)}(\vec{r}, t) = - \int_0^\infty dE [I - \mathcal{S}_1]^{-1} \left[ \frac{1}{3\sigma_s(\vec{r}, E, t)}\vec{\nabla} \left( \phi_{\text{th}}^{(0)}(\vec{r}, t)M(E, T) \right) \right]. \quad (23)$$

Using the product rule for derivatives we can rearrange Eq. (23) to obtain

$$\begin{aligned} \vec{J}^{(1)}(\vec{r}, t) &= -\phi_{\text{th}}^{(0)}(\vec{r}, t)\vec{\nabla}T(\vec{r}, t) \int_0^\infty dE [I - \mathcal{S}_1]^{-1} \left[ \frac{1}{3\sigma_s(\vec{r}, E, t)}\frac{\partial}{\partial T}M(E, T) \right] \\ &\quad - \vec{\nabla}\phi_{\text{th}}^{(0)}(\vec{r}, t) \int_0^\infty dE [I - \mathcal{S}_1]^{-1} \left[ \frac{M(E, T)}{3\sigma_s(\vec{r}, E, t)} \right], \end{aligned} \quad (24)$$

or

$$\vec{J}^{(1)}(\vec{r}, t) = \vec{b}(\vec{r}, t)\phi_{\text{th}}^{(0)}(\vec{r}, t) - D(\vec{r}, t)\vec{\nabla}\phi_{\text{th}}^{(0)}(\vec{r}, t), \quad (25)$$

where

$$\vec{b}(\vec{r}, t) = -\vec{\nabla}T(\vec{r}, t) \int_0^\infty dE [I - \mathcal{S}_1]^{-1} \left[ \frac{1}{3\sigma_s(\vec{r}, E, t)} \frac{\partial}{\partial T} M(E, T) \right] \quad (26)$$

and

$$D(\vec{r}, t) = \int_0^\infty dE [I - \mathcal{S}_1]^{-1} \left[ \frac{M(E, T)}{3\sigma_s(\vec{r}, E, t)} \right]. \quad (27)$$

Equation (25) is Fick's Law plus a drift term (the  $\vec{b}$  term). Note that we could define a transport cross-section [8] from this equation as

$$\bar{\sigma}_{\text{tr}}(\vec{r}, t) = \left( \int_0^\infty \frac{dE}{\sigma_s(\vec{r}, E, t)} [I - \mathcal{S}_1]^{-1} M(E, T) \right)^{-1}.$$

This transport cross section and the corresponding diffusion coefficient are analogous to the Rosseland mean opacity and its corresponding diffusion coefficient, commonly used in diffusion approximations for radiative transfer [9]. In this case, however, we do not have a derivative of the Maxwellian in the definition, as the derivative of the Planckian appears in radiative transfer.

We have operated on the  $O(1)$  equations with  $\int_{4\pi} d\Omega(\cdot)$  and  $\int_{4\pi} d\Omega\hat{\Omega}(\cdot)$ , which is equivalent to operating with  $\int_{4\pi} d\Omega Y_{00}^*(\cdot)$  and  $\int_{4\pi} d\Omega Y_{1,m}^*(\cdot)$  with  $|m| \leq 1$ . We continue by operating with  $\int_{4\pi} d\Omega Y_{lm}^*(\cdot)$  for  $l > 1$ , obtaining:

$$\sigma_s(\vec{r}, E, t)\phi_l^{m(1)}(\vec{r}, E, t) = \int_0^\infty dE' \sigma_s(\vec{r}, E', t) f_l(\vec{r}, E' \rightarrow E, t)\phi_l^{m(1)}(\vec{r}, E', t), \quad l > 1, \quad (28)$$

where we have recognized that the orthogonality of the spherical-harmonics functions implies that

$$\int_{4\pi} d\Omega Y_{lm}(\hat{\Omega})\hat{\Omega} = 0 \quad \text{for } l > 1.$$

We can rewrite this as

$$[I - \mathcal{S}_l]\phi_l^{m(1)}(\vec{r}, E, t) = 0, \quad l > 1. \quad (29)$$

The invertibility of  $[I - \mathcal{S}_l]$  for  $l > 0$  (see appendix) implies that

$$\phi_l^{m(1)} = 0 \quad \text{for } l > 1.$$

That is, the  $O(\epsilon)$  component of the solution,  $\psi^{(1)}$ , is at most *linearly anisotropic* and satisfies:

$$\begin{aligned} \psi^{(1)}(\vec{r}, \hat{\Omega}, E, t) &= \frac{1}{4\pi}\phi_{\text{th}}^{(1)}(\vec{r}, t)M(E, T) + \frac{3}{4\pi}\hat{\Omega} \cdot \vec{J}^{(1)}(\vec{r}, E, t) \\ &= \frac{1}{4\pi}\phi_{\text{th}}^{(1)}(\vec{r}, t)M(E, T) - \frac{3}{4\pi}\hat{\Omega} \cdot [I - \mathcal{S}_1]^{-1} \left[ \frac{1}{3\sigma_s(\vec{r}, E, t)} \vec{\nabla} \left( \phi_{\text{th}}^{(0)}(\vec{r}, t)M(E, T) \right) \right]. \end{aligned} \quad (30)$$

At this point in the analysis, the functions  $\phi_{\text{th}}^{(0)}$  and  $\phi_{\text{th}}^{(1)}$  are yet to be determined.

### 3.3 The $O(\epsilon)$ equations

We can derive a drift-diffusion equation for  $\phi_{\text{th}}^{(0)}$  from the  $O(\epsilon)$  terms in Eq. (7). These terms are

$$\begin{aligned} \frac{1}{v} \frac{\partial \psi^{(0)}}{\partial t} + \hat{\Omega} \cdot \vec{\nabla} \psi^{(1)} + \sigma_s(\vec{r}, E, t)\psi^{(2)}(\vec{r}, \hat{\Omega}, E, t) + \sigma_a(\vec{r}, E, t)\psi^{(0)}(\vec{r}, \hat{\Omega}, E, t) \\ = \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \int dE' \sigma_s(\vec{r}, E', t) f_l(\vec{r}, E' \rightarrow E, t)\phi_l^{m(2)}(\vec{r}, E', t) + q(\vec{r}, \hat{\Omega}, E, t). \end{aligned} \quad (31)$$

Upon operating on this equation by  $\int_0^\infty dE \int_{4\pi} d\Omega(\cdot)$  we obtain

$$\frac{\partial}{\partial t} \left( \frac{\phi_{\text{th}}^{(0)}}{\bar{v}(\vec{r}, t)} \right) + \vec{\nabla} \cdot \vec{\mathcal{J}}^{(1)}(\vec{r}, t) + \bar{\sigma}_a(\vec{r}, t) \phi_{\text{th}}^{(0)}(\vec{r}, t) = \bar{Q}(\vec{r}, t), \quad (32)$$

where we have defined several averaged and integrated quantities:

$$\bar{v}(\vec{r}, t) = \frac{\int_0^\infty dE \phi_{\text{th}}^{(0)}(\vec{r}, t) M(E, T)}{\int_0^\infty dE \frac{1}{v(E)} \phi_{\text{th}}^{(0)}(\vec{r}, t) M(E, T)} = \frac{1}{\int_0^\infty dE \frac{1}{v(E)} M(E, T)}, \quad (33)$$

$$\bar{\sigma}_a(\vec{r}, t) = \frac{\int_0^\infty dE \sigma_a(\vec{r}, E) \phi_{\text{th}}^{(0)}(\vec{r}, t) M(E, T)}{\int_0^\infty dE \phi_{\text{th}}^{(0)}(\vec{r}, t) M(E, T)} = \int_0^\infty dE \sigma_a(\vec{r}, E) M(E, T), \quad (34)$$

$$\bar{Q}(\vec{r}, t) = \int_0^\infty dE \int_{4\pi} d\Omega q(\vec{r}, \hat{\Omega}, E, t). \quad (35)$$

In these expressions the temperature  $T$  is understood to be evaluated at position  $\vec{r}$  and time  $t$ . Using the definition of  $\vec{\mathcal{J}}^{(1)}$  from Eq. (25) we see that Eq. (32) is a drift-diffusion equation for the leading-order thermal-flux amplitude:

$$\frac{\partial}{\partial t} \left( \frac{\phi_{\text{th}}^{(0)}}{\bar{v}} \right) - \vec{\nabla} \cdot D \vec{\nabla} \phi_{\text{th}}^{(0)} + \vec{\nabla} \cdot (\vec{b} \phi_{\text{th}}^{(0)}) + \bar{\sigma}_a \phi_{\text{th}}^{(0)} = \bar{Q}. \quad (36)$$

(Every term depends on  $\vec{r}$  and  $t$ .) This is a closed equation for the leading-order scalar-flux amplitude function in the system, which will be satisfied away from boundary and initial layers given the conditions we stipulated above.

### 3.4 Properties of the model

The drift diffusion model for thermal neutrons given above has several notable consequences. First, the energy spectrum at each point in space and time is, to leading order, a Maxwell-Boltzmann distribution at the local temperature. This indicates that in a medium with continuously varying temperatures, we should expect that the leading-order solution should have an energy spectrum that continuously varies as the local Maxwellian. However, the magnitude of the leading-order solution will depend on many factors:

1. the fixed source term,
2. the local absorption cross section averaged with a Maxwell-Boltzmann weighting function,
3. the magnitude of the nearby solution (through the diffusion term)
4. the local diffusion coefficient (through the diffusion term), and
5. the gradient of the temperature inside the medium (via the drift speed  $\vec{b}$ ).

There is a special case of the model where the scattering is isotropic in angle, that is,  $f_1(E' \rightarrow E) = 0$  and hence  $\mathcal{S}_1 = 0$ . In this case the diffusion coefficient,  $D(\vec{r}, t)$ , only involves the Maxwell-Boltzmann average of  $1/\sigma_s(\vec{r}, E, t)$ .

## 4 Conclusions

We have used an asymptotic analysis to develop a model for thermal neutrons in a medium with small amounts of absorption, large amounts of scattering, and without strong localized sources, away from boundaries and material interfaces. Our model has the leading-order neutron energy distribution as a Maxwell-Boltzmann distribution at the local material temperature, and has a drift-diffusion equation to describe the



amplitude of the distribution. The diffusion term in our model shows what the appropriate energy average of the diffusion coefficient should be in the thermal energy range. The drift velocity is proportional to the gradient of the material temperature and points in the opposite direction.

Our results should be a step toward developing a comprehensive simplified model of thermal neutrons in highly scattering media, such as in “thermal columns” near research reactors. Additional work should be performed to derive initial and boundary conditions, and comparisons with energy-resolved transport calculations (such as continuous-energy Monte Carlo calculations) would be an interesting exploration of the accuracy of the model for realistic problems.

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## A Appendix: Invertibility of $[I - \mathcal{S}_l]$ for $l > 0$

Consider an infinite medium that is purely scattering with  $\sigma_s(E) > 0$ . Assume that the scattering law depends only on the dot product of the incident and scattered directions, which means the medium itself is rotationally invariant. This is sometimes referred to as an isotropic medium. In such an instance the transport equation for the steady angular flux of neutrons is [10]

$$\begin{aligned} \sigma_s(E)\psi(\hat{\Omega}, E) &= \int dE' \int_{4\pi} d\Omega' \sigma_s(E') f(E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) \psi(\hat{\Omega}', E') \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \int dE' \sigma_s(E') f_l(E' \rightarrow E) \phi_l^m(E'), \end{aligned} \quad (37)$$

where

$$f_l(E' \rightarrow E) = \int_{-1}^1 d\mu_0 f(E' \rightarrow E, \mu_0) P_l(E', \mu_0), \quad (38)$$

$$\phi_l^m(E') = \int_{4\pi} d\Omega' Y_{lm}^*(\hat{\Omega}') \psi(\hat{\Omega}', E'). \quad (39)$$

Here  $\mu_0$  is the dot product of the incident and scattered angle and  $P_l$  is the  $l^{\text{th}}$ -order Legendre polynomial. If we multiply the transport equation by  $Y_{lm}^*(\hat{\Omega})$  and integrate over  $\hat{\Omega}$  we obtain, via orthonormality of the spherical harmonics functions,

$$\sigma_s(E) \phi_l^m(E) = \int dE' \sigma_s(E') f_l(E' \rightarrow E) \phi_l^m(E'). \quad (40)$$

We can write this equation in operator form as

$$\sigma_s(E) [I - \mathcal{S}_l] \phi_l^m(E) = 0, \quad (41)$$

where

$$\mathcal{S}_l \varphi(E) = \frac{1}{\sigma_s(E)} \int dE' \sigma_s(E') f_l(E' \rightarrow E) \varphi(E'). \quad (42)$$

In this appendix we show that for physically realizable scattering functions, the operator  $[I - \mathcal{S}_l]$  is invertible for  $l > 0$ . We will begin with remarks about the  $l = 0$  case.

**Remark 1.** *The operator  $[I - \mathcal{S}_0]$  is singular for physically realizable scattering functions.*

*Argument.* There is a non-zero solution of the equation

$$(I - \mathcal{S}_0) \varphi(E) = 0, \quad (43)$$

given by

$$\varphi(E) = \hat{\varphi} M(E, T), \quad (44)$$

where  $M(E, T)$  is the Maxwell-Boltzmann distribution (for the scalar flux, not density) at temperature  $T$ , the temperature of the scattering medium, and  $\hat{\varphi}$  is a constant [8]. According to well-known results from statistical mechanics, the solution is unique except for the multiplicative constant  $\hat{\varphi}$ . That is, the Maxwell-Boltzmann distribution is the only possible solution to the given steady-state problem. This means the operator  $[I - \mathcal{S}_0]$  has exactly one zero eigenvalue, with a corresponding eigenfunction equal to the Maxwell-Boltzmann distribution. This in turn means that the operator  $\mathcal{S}_0$  has one eigenvalue equal to unity, with eigenfunction equal to the Maxwell-Boltzmann distribution.

The next remark is a mathematical consequence of the physical reality that scattering does not create particles, but only changes their directions and energies.

**Remark 2.** *The spectral radius of  $\mathcal{S}_0 = 1$ .*

*Argument.* The spectral radius of  $\mathcal{S}_0$  satisfies

$$\rho(\mathcal{S}_0) = \sup_{\varphi} \frac{\|\mathcal{S}_0 \varphi\|}{\|\varphi\|}, \quad (45)$$

where the supremum is taken over all functions in the function space and  $\|f\|$  is a valid norm of  $f$ . For our purposes we define the norm

$$\|\varphi\| \equiv \int dE \sigma_s(E) |\varphi(E)|, \quad (46)$$

and we choose our function space to include only functions of  $E$  whose norms are bounded. We recognize that the integral of the differential scattering cross section is the scattering cross section:

$$\sigma_s(E') \equiv \int dE \sigma_s(E') f_0(E' \rightarrow E). \quad (47)$$

The norm of  $\mathcal{S}_0 \varphi$  satisfies

$$\begin{aligned} \|\mathcal{S}_0 \varphi\| &= \int dE \sigma_s(E) \left| \frac{1}{\sigma_s(E)} \int dE' \sigma_s(E') f_0(E' \rightarrow E) \varphi(E') \right| \\ &= \int dE \left| \int dE' \sigma_s(E') f_0(E' \rightarrow E) \varphi(E') \right| \\ &\leq \int dE \int dE' \sigma_s(E') f_0(E' \rightarrow E) |\varphi(E')| = \int dE' \sigma_s(E') |\varphi(E')| = \|\varphi\|, \end{aligned} \quad (48)$$

from which it follows that the spectral radius of  $\mathcal{S}_0$  is  $\leq 1$ . Equality holds for any non-negative function  $\varphi(E)$ , so the spectral radius equals 1. We saw previously that exactly one eigenvalue equals 1; now we see that there are no eigenvalues with larger magnitude.

The next remark will also be useful.

**Remark 3.** *If the spectral radius of  $\mathcal{S}_l$  is less than 1, then the operator  $[I - \mathcal{S}_l]$  is invertible.*

*Argument.*  $1 - \lambda$  is an eigenvalue of  $[I - \mathcal{S}_l]$  with eigenfunction  $f$  if and only if  $\lambda$  is an eigenvalue of  $\mathcal{S}_l$  with eigenfunction  $f$ . If all eigenvalues of  $\mathcal{S}_l$  have magnitude less than unity (*i.e.*, if the spectral radius  $\rho(\mathcal{S}_l) < 1$ ), then the eigenvalues of  $[I - \mathcal{S}_l]$  lie within a circle of radius  $\rho(\mathcal{S}_l)$  centered in the complex plane at 1 on the real axis. Zero is outside of this circle and is therefore not an eigenvalue of  $[I - \mathcal{S}_l]$ ; thus,  $[I - \mathcal{S}_l]$  is invertible.

**Remark 4.** The spectral radius of  $\mathcal{S}_l$  is less than 1 for  $l > 0$ .

*Argument.* The spectral radius satisfies

$$\rho(\mathcal{S}_l) = \sup_{\varphi} \frac{\|\mathcal{S}_l \varphi\|}{\|\varphi\|}, \quad (49)$$

where the supremum is taken over all functions in the function space and  $\|f\|$  is a valid norm of  $f$ . We continue to use the norm

$$\|\varphi\| \equiv \int dE \sigma_s(E) |\varphi(E)|. \quad (50)$$

In what follows we shall use the following identities and definitions.

$$f_l(E' \rightarrow E) = \int_{-1}^1 d\mu_0 P_l(\mu_0) f(E' \rightarrow E, \mu_0), \quad (51)$$

$$\int dE \int_{-1}^1 d\mu_0 f(E' \rightarrow E) = 1, \quad (52)$$

$$\begin{aligned} \int dE f_l(E' \rightarrow E) &= \int dE \int_{-1}^1 d\mu_0 P_l(\mu_0) f(E' \rightarrow E, \mu_0) \\ &= \frac{\int dE \int_{-1}^1 d\mu_0 P_l(\mu_0) f(E' \rightarrow E, \mu_0)}{\int dE \int_{-1}^1 d\mu_0 f(E' \rightarrow E, \mu_0)}. \end{aligned} \quad (53)$$

Here  $\mu_0 = \hat{\Omega} \cdot \hat{\Omega}'$ . The form of Eq. (53) makes it clear that  $\int dE f_l(E' \rightarrow E)$  is a proper weighted average of  $P_l(\mu_0)$ , with non-negative weight function  $f(E' \rightarrow E, \mu_0)$ , for particles scattering with initial energy  $E'$ . The average of the *absolute value* of  $P_l(\mu_0)$  is a function of  $E'$  and will be a useful quantity in what follows, so we define it here:

$$\langle |P_l(\mu_0)| \rangle \equiv \int dE \int_{-1}^1 d\mu_0 |P_l(\mu_0)| f(E' \rightarrow E, \mu_0). \quad (54)$$

With these definitions, the norm of  $\mathcal{S}_l \varphi$  satisfies the inequality

$$\begin{aligned} \|\mathcal{S}_l \varphi\| &= \int dE \sigma_s(E) \left| \frac{1}{\sigma_s(E)} \int dE' \sigma_s(E') f_l(E' \rightarrow E) \varphi(E') \right| \\ &\leq \int dE \int dE' |\sigma_s(E') f_l(E' \rightarrow E) \varphi(E')| \\ &\leq \int dE' |\sigma_s(E') \varphi(E')| \int dE |f_l(E' \rightarrow E)| \\ &\leq \int dE' \sigma_s(E') |\varphi(E')| \int dE \left| \int_{-1}^1 d\mu_0 P_l(\mu_0) f(E' \rightarrow E, \mu_0) \right| \\ &\leq \int dE' \sigma_s(E') |\varphi(E')| \int dE \int_{-1}^1 d\mu_0 |P_l(\mu_0)| f(E' \rightarrow E, \mu_0) \\ &\leq \int dE' \sigma_s(E') |\varphi(E')| \langle |P_l(\mu_0)| \rangle \\ &\leq |P_l|_{\max} \int dE' \sigma_s(E') |\varphi(E')| \\ &\leq |P_l|_{\max} \|\varphi\|. \end{aligned} \quad (55)$$

Here  $|P_l|_{\max}$  is the supremum over all  $E'$  of the averaged  $|P_l(\mu_0)|$ .  $P_l(\mu_0)$  is between  $-1$  and  $1$  for all values of  $l$ , and  $\mu_0$ . If  $l = 0$ , then  $P_0(\mu_0) = 1$  for all  $\mu_0$  and of course  $|P_0|_{\max} = 1$ . In this case, the equal sign holds throughout Eq. (55), which is in keeping with our previous result that the spectral radius of  $\mathcal{S}_0$  is

unity. However, for  $l > 0$ ,  $\langle |P_l(\mu_0)| \rangle = 1$  only if  $\mu_0 = \pm 1$  for every particle that scatters with initial energy  $E'$ —that is, only if every particle of energy  $E'$  suffers only scattering events that either do not change the particle's direction or that exactly reverse its direction. This is not a physically realizable scattering function for neutrons. That is, for physically realizable scattering functions, the left-hand side of Eq. (55) is strictly less than the right-hand side for  $l > 0$ . It follows that for physically realizable scattering functions, the spectral radius of  $S_l$  is strictly  $< 1$  for  $l > 0$ . For a scattering law where  $\mu_0 = \pm 1$  for every scattering event (non physically realizable for neutrons), our argument would not hold.

Now we can combine our results to demonstrate invertibility.

**Main Result.** The operator  $[I - S_l]$  is invertible for  $l > 0$ , for physically plausible scattering laws.

*Argument.* Remark 4 shows that the conditions of Remark 3 are satisfied and the operator is invertible.

## References

- [1] Edward W. Larsen and Joseph B. Keller. Asymptotic solution of neutron transport problems for small mean free paths. *Journal of Mathematical Physics*, 15(1), January 1974.
- [2] G. J. Habetler and B.J. Matkowsky. Uniform asymptotic expansions in transport theory with small mean free paths, and the diffusion approximation. *Journal of Mathematical Physics*, 16(4), April 1975.
- [3] Richard Sanchez, Jean Ragusa, and Emiliano Masiello. Asymptotic theory of the linear transport equation in anisotropic media. *Journal of Mathematical Physics*, 49(1), January 2008.
- [4] P.A. Markowich, C.A. Ringhofer, and C. Schmeiser. *Semiconductor equations*. Springer-Verlag, 1990.
- [5] E.W. Larsen, G.C. Pomraning, and V.C. Badham. Asymptotic analysis of radiative transfer problems. *J. Quant. Spec. Rad. Transf.*, 29(4), 1983.
- [6] Ryan G. McClarren. Theoretical aspects of the simplified  $P_n$  equations. *Transport Theory and Statistical Physics*, 39(2):73–109, 2011.
- [7] Edward W. Larsen, J. E. Morel, and Warren F. Miller. Asymptotic solutions of numerical transport problems in optically thick, diffusive regimes. *J. Comput. Phys.*, 69(2), 1987.
- [8] George I. Bell and Samuel Glasstone. *Nuclear Reactor Theory*. Robert E. Kreiger Publishing, Malabar, Florida, 1970.
- [9] Gerald C. Pomraning. *The Equations of Radiation Hydrodynamics*. Dover Publications, Mineola, New York, 2005.
- [10] E.E. Lewis and W.F. Miller. *Computational Methods of Neutron Transport*. John Wiley and Sons, 1984.