The Asymptotic Drift-Diffusion Limit of Thermal Neutrons

Ryan G. McClarren, Marvin L. Adams, Clay Strack

Department of Nuclear Engineering
Texas A&M University

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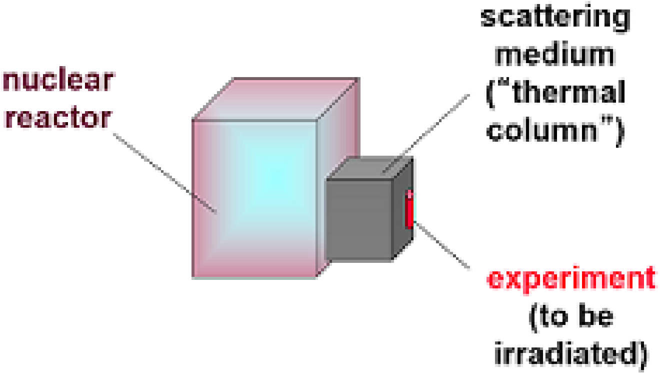
Asymptotic Limits of the Transport Equation

- There are several well known asymptotic limits of the transport equation.
  - In the limit of limit of large scattering cross-sections and small absorption cross-sections,
  - The linear transport equation becomes a diffusion equation.
- In this work we look at, what we feel, is a new limit for the transport equation for thermal neutrons.
- Particularly, we will look at situations of low absorption, small sources and include full energy dependence.
- The material will have a temperature dependence that will help drive the neutron distribution away from a Maxwellian in a particular way.

Possible application: Heavy Water Column



Equilibrium Diffusion Limit for Radiative Transfer

- It is useful to connect this work to previous results for the equilibrium diffusion limit for radiative transfer.
- For a gray transport equation coupled to a material energy equation

$$\frac{\epsilon}{c}\frac{\partial \psi}{\partial t} + \mu \frac{\partial \psi}{\partial x} + \frac{\sigma}{\epsilon}\psi = \frac{\sigma ac}{2\epsilon} T^4$$

$$\epsilon \frac{\partial e_{\mathrm{m}}}{\partial t} = \frac{\sigma}{\epsilon}\left(\int_{-1}^{1} d\mu\, \psi - acT^4\right)$$

- The asymptotic limit gives a non-linear transport equation in the material temperature/energy:

$$\frac{\partial}{\partial t}(e + aT^4) = \frac{\partial}{\partial x} D \frac{\partial}{\partial x} aT^4.$$

Neutron Thermalization

- The radiative transfer problem shares some characteristics with the thermal neutron problem:
  - There is a local temperature equation (in the neutron case it is a specified temperature)
  - The neutron's behavior is influenced by the local temperature
    - In the neutronics case the scattering is affected by the temperature.
    - The source is affected in the radiative transfer case.
- Before proceeding it will be useful to remind the audience that in a source-free, absorption-free, infinite medium, the angular flux becomes

$$\psi(x, \mu, E) = \frac{\Phi_0}{2} M(E, T)$$

where

$$M(E, T) = \frac{E}{(kT)^2} e^{-\frac{E}{kT}}.$$

and T is the material's temperature.

Problem Set Up

- We begin with the slab geometry transport equation,

$$\mu \frac{\partial \psi}{\partial x} + (\sigma_{\mathrm{s}}(E) + \sigma_{\mathrm{a}}(E))\,\psi(x,\mu,E)$$
$$= \int dE' \int d\mu' \sum_{\ell=0}^{\infty} P_\ell(\mu_0) \frac{2\ell+1}{2} \psi(\mu',E') f_\ell(E' \to E)\sigma_{\mathrm{s}}(E') + \frac{Q}{2}$$

- We are going to seek to solve this equation by making the following changes:
  - The scattering cross-section is large: $\sigma_{\mathrm{s}}(E) \to \sigma_{\mathrm{s}}(E)/\epsilon$.
  - The absorption cross-section is small: $\sigma_{\mathrm{a}}(E) \to \epsilon\sigma_{\mathrm{a}}(E)$.
  - The source is small: $Q \to \epsilon Q$.

Problem Set Up

- After making these substitutions, we get

$$\epsilon\mu\frac{\partial\psi}{\partial x} + \left(\sigma_{\rm s}(E) + \epsilon^2\sigma_{\rm a}(E)\right)\psi(x,\mu,E)$$
$$= \int dE' \int d\mu' \sum_{\ell=0}^{\infty} P_\ell(\mu_0)\frac{2\ell+1}{2}\psi(\mu',E')f_\ell(E'\to E)\sigma_{\rm s}(E') + \epsilon^2\frac{Q}{2}$$

- We then look for solutions in the form of a power series in ϵ:

$$\psi(x,\mu,E) = \sum_{j=0}^{\infty}\epsilon^j\psi^{(j)},$$

where the $\psi^{(j)}(x,\mu,E)$ are as yet undetermined functions.

The leading-order equations

- The leading-order equation is an infinite medium equation without source or scattering:

$$\sigma_\mathrm{s}(E)\psi^{(0)} = \int dE' \int d\mu' \sum_{\ell=0}^{\infty} P_\ell(\mu_0)\frac{2\ell+1}{2}\psi^{(0)}(\mu', E')f_\ell(E' \to E)\sigma_\mathrm{s}(E')$$

- The solution to this equation is a Maxwellian at the local temperature with a local normalization:

$$\psi^{(0)}(x,\mu,E) = \frac{\Phi(x)}{2}M(E,T(x)).$$

- $\Phi(x)$ is still undetermined.

The first-order equations

- Moving on to the next order in ϵ we get

$$\mu \frac{\partial \psi^{(0)}}{\partial x} + \sigma(E)\psi^{(1)} = \int dE' \int d\mu' \sum_{\ell=0}^{\infty} P_\ell(\mu_0) \frac{2\ell+1}{2} \psi^{(1)}(\mu', E') f_\ell(E' \to E)\sigma_{\mathrm{s}}(E') \quad (1)$$

- Operating on this equation by $\int_{-1}^{1} d\mu\,(\cdot)$ we get

$$[1 - \mathcal{S}_1]J^{(1)} = -\frac{1}{3}\frac{\partial \phi_0}{\partial x}$$

where the operator $\mathcal{S}_l$ is defined as

$$[\mathcal{S}_l]g(E) \equiv \frac{1}{\sigma_s(E)} \int \mathrm{d}E'\, \sigma_{sl}(E' \to E) g(E').$$

The first-order equations

- We'd like to invert the $[1 - \mathcal{S}_1]$ operator and get a version of Fick's law, but we first need to show that this operator is invertible.
- It's not obvious that it would be, for instance we know that $[1 - \mathcal{S}_0]$ is singular.
- The solution to
$$[1 - \mathcal{S}_0]g(E) = 0,$$
is the Maxwellian.
- It can be shown that this operator is invertible.

The operator $[1 - \mathcal{S}_1]$ is invertible

- To show this we first need to establish the following 4 items:
  1. The operator $[1 - \mathcal{S}_0]$ is singular $\square$
  2.
  3.
  4.

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The spectral radius of $\mathcal{S}_0$ is 1

- From remark 1, we can directly infer that 1 is an eigenvalue of the operator.
- The eigenvalues of the operator are found by seeking non-trivial solutions $\varphi(E)$ and λ's that satisfy $\mathcal{S}_0\varphi(E) = \lambda\varphi(E)$, which can be rewritten as

$$dE \int dE' \, \sigma_{s0}(E' \to E)\varphi(E') = \lambda\sigma_{\mathrm{s}}(E)\varphi(E)dE. \tag{2}$$

In physical terms, this equation says

$$(\text{The scattering rate density into } dE \text{ about } E \text{ from all energies}) = \lambda \times (\text{The scattering rate density from } dE \text{ about } E)$$

Physically, for a solution to exist it must be the case that $\lambda \leq 1$. Otherwise, we could not have a steady solution and φ would have to be time dependent.

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  1. The operator $[1 - \mathcal{S}_0]$ is singular $\square$
  2. The spectral radius of $\mathcal{S}_0$ is 1 $\square$
  3. If the spectral radius of $\mathcal{S}_l$ is less than 1, then the series

     $$(1 - \mathcal{S}_l)^{-1} = 1 + \mathcal{S}_l + \mathcal{S}_l^2 + \dots$$

     converges and the operator $(1 - \mathcal{S}_l)$ is invertible $\square$
  4.

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  converges and the operator $(1 - \mathcal{S}_l)$ is invertible $\square$
  4. The spectral radius of $\mathcal{S}_l$ is less than 1 for $l > 0$.

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- The magnitude of an eigenvalue of the operator can be written as

$$|\lambda| = \left| \frac{\int dE' \, \sigma_{sl}(E' \to E)\varphi(E')}{\sigma_{\mathrm{s}}(E)\varphi(E)} \right| . \tag{3}$$

- We also know that for physically realizable cross-sections $\sigma_{sl}(E) < \sigma_{s0}$ for $l > 0$.
- This leads to

$$|\lambda| < \left| \frac{\int dE' \, \sigma_{s0}(E' \to E)\varphi(E')}{\sigma_{\mathrm{s}}(E)\varphi(E)} \right| = 1, \tag{4}$$

- Therefore, all of the eigenvalues of $\mathcal{S}_l$ are less than 1.

The operator $[1 - \mathcal{S}_1]$ is invertible

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     $$(1 - \mathcal{S}_l)^{-1} = 1 + \mathcal{S}_l + \mathcal{S}_l^2 + \dots$$

     converges and the operator $(1 - \mathcal{S}_l)$ is invertible $\square$
  4. The spectral radius of $\mathcal{S}_l$ is less than 1 for $l > 0$ $\square$
- These combine to say that $[1 - \mathcal{S}_1]$ is invertible.

Fick's Law

- Now we can rearrange our first-order equations to get a version of Fick's Law:

$$J^{(1)}(x,E) = -\frac{1}{3}\left[1-\mathcal{S}_1\right]^{-1}\frac{\partial \phi^{(0)}}{\partial x}.$$

- Integrating this over all energy we get

$$\begin{aligned}\bar{J}^{(1)}(x) &= -\frac{1}{3}\int_0^\infty dE\left[1-\mathcal{S}_1\right]^{-1}\frac{\partial \phi^{(0)}}{\partial x} \\ &= -\frac{1}{3}\int_0^\infty dE\left[1-\mathcal{S}_1\right]^{-1}\frac{\partial}{\partial x}\Phi(x)M(E,T(x)).\end{aligned}$$

Fick's Law

- Using the product rule we can re-write $\bar{J}$ as

$$\bar{J}^{(1)}(x) = -D(x)\left[\frac{d}{dx}\Phi(x)\right] + b(x)\Phi(x)$$

where

$$D(x) = -\frac{1}{3}\left[\int_0^\infty \mathrm{d}E\,[1-\mathcal{S}_1]^{-1}M(E,T)\right] \tag{5}$$

and

$$b(x) = -\frac{1}{3}\frac{dT}{dx}\left[\int_0^\infty \mathrm{d}E\,[1-\mathcal{S}_1]^{-1}\frac{\partial M}{\partial T}\right] \tag{6}$$

The Drift-Diffusion Equation

- Using our equation for $\bar{J}^{(1)}$ we then can get a drift-diffusion equation given by:

$$-\frac{d}{dx}D(x)\left[\frac{d}{dx}\Phi(x)\right]+\frac{d}{dx}b(x)\Phi(x)+\bar{\sigma_{\mathrm{a}}}\Phi(x)=Q.$$

- This equation tells us how the magnitude of the scalar flux changes as a function of the variation in the material temperature.
- We can also show that the energy-dependent scalar flux is a Maxwellian through first order in ϵ.

Comparison of the Model

- We would like to compare the drift-diffusion model derived above to energy-dependent transport results in a material with a temperature gradient.
- We have not done these yet, but have derived how to represent the quantities $D(x)$ and $b(x)$ based on multi-group data.
- First we will need.

$$[I - \hat{\mathcal{S}}_1] = \begin{bmatrix} 1 - \frac{1}{\sigma_s^1}\sigma_{s1}^{1\to 1} & -\frac{1}{\sigma_s^1}\sigma_{s1}^{2\to 1} & \cdots & -\frac{1}{\sigma_s^1}\sigma_{s1}^{G\to 1} \\ -\frac{1}{\sigma_s^2}\sigma_{s1}^{1\to 2} & \ddots & \cdots & -\frac{1}{\sigma_s^2}\sigma_{s1}^{G\to 2} \\ \vdots & \cdots & \ddots & \vdots \\ -\frac{1}{\sigma_s^G}\sigma_{sG}^{1\to G} & \cdots & -\frac{1}{\sigma_s^G}\sigma_{sG}^{G-1\to G} & 1 - \frac{1}{\sigma_s^G}\sigma_{s1}^{G\to G} \end{bmatrix}$$

Multi-group Form

- Using this we can define

$$D(x) = -\frac{1}{3}\left[\int_0^\infty \mathrm{d}E\,[1-\mathcal{S}_1]^{-1} M(E,T)\right] \equiv -\frac{1}{3}\sum_{g=1}^{G}[I-\hat{\mathcal{S}}_l]^{-1}\vec{M}$$

$$b(x) = -\frac{1}{3}\left[\int_0^\infty \mathrm{d}E\,[1-\mathcal{S}_1]^{-1}\frac{\partial M}{\partial T}\right]\frac{dT}{dx} \equiv -\frac{1}{3}\frac{dT}{dx}\sum_{g=1}^{G}[I-\hat{\mathcal{S}}_l]^{-1}\frac{\partial \vec{M}}{\partial T}$$

where

$$M^g = \int_{E_g}^{E_g-1}\mathrm{d}E\,M(E,T) \qquad \frac{\partial M^g}{\partial T} = \int_{E_g}^{E_g-1}\mathrm{d}E\,\frac{\partial M}{\partial T}(E,T)$$

Comparison of the Model

- It's important to note that these quantities will also be functions of temperature.
- It will be a slog to generate $D(x, T)$ and $b(x, T)$ but it is doable.
- For the drift-speed, $b(x, T)$, the temperature derivative can be separated out and the rest could be tabulated.
- We haven't done it yet, but it is a work in progress.

Summary and Future Work

- Under conditions similar to the standard mono-energetic diffusion limit, we derived a drift-diffusion limit for the total scalar-flux.
- The energy dependent scalar flux is a Maxwellian through first-order in ϵ.
- We did not perform a boundary layer analysis, and this should be part of future work.
- I really want to compare the model to full-blown multi-group or continuous energy calculations.