The Weight Function

Introduction

The goal of this brief set of Lecture Notes is to discuss the space- and energy-dependent "Weight Function" that is used in a lot of Reactor Physics applications in a bit more detail. For example, this weight function, typically written as $w(\vec{r}, E)$ or $\theta(\vec{r}, E)$, is used extensively in Ref. 1 to develop formal expressions for the "effective" kinetics parameters that are used within the point kinetics equations. It is also often used to write the reactivity worth associated with a cross section change or material change within the reactor -- such as the worth of a partially inserted control rod, for example (e.g. see Ref. 2). In most applications, one multiplies the steady-state or time-varying neutron balance equation (depending on the application of interest) by the weight function and integrates the resultant expression over space and energy, giving a formal weighted integral balance relationship. It is important to note that, in general, this integral relationship is exact for any choice of the weight function, since every term in the "unperturbed" balance equation is multiplied by the same function. However, as shown below, it is often advantageous to select this weight function in a particular way to improve the accuracy associated with the prediction of perturbed conditions within the system, especially when one uses an approximate expression for the flux distribution in the perturbed system. For example, in practical application of the point kinetics equations,[1] one almost always makes the assumption that "the spatial flux distribution does not vary significantly during the transient" or, in mathematical terms, we say that

$$\phi_g(\vec{r}, t) = \psi_g(\vec{r}, t)T(t) \approx \psi_{og}(\vec{r})T(t) \tag{1}$$

where the group-wise spatial distribution with the 'o' subscript represents the initial steady state values and $T(t)$ represents the time-dependent amplitude of the neutron flux. Clearly, replacing the time dependent flux shape with its distribution at $t = 0$ is, in all cases, an approximation -- and it makes sense, if possible, to choose a weight function that minimizes the impact of this approximation within practical applications.

Therefore, the purpose of the development to follow is to show that if we let the weight function be the so-called "adjoint flux" (typically denoted as ϕ^*), we can indeed achieve first-order accuracy in the integral expressions -- even when statements such as those implied by eqn. (1) are made. And this is the real value of letting the weight function be the adjoint flux -- that is, to retain as much accuracy as possible even when we know that the approximations that are being made may indeed be quite large. As part of this development, we will also define a bunch of new terminology, such as what is an "adjoint operator", and what does it mean to be "self-adjoint", and also include some typical examples of how one determines the adjoint operator that corresponds to a particular "forward" operator, etc. etc.. In fact, the goal here is to give the reader a pretty good overview of the terminology, theory, and practical application of "Perturbation Theory Methods", without going into too much detail into this field of specialization. Thus, our objective is not to make the reader an expert in this field but, instead, to give you enough insight so that you can talk intelligently about the subject and, most importantly, understand why we let $\theta(\vec{r}, E) = \phi^*(\vec{r}, E)$ in most practical applications. In keeping this development manageable, we will take the liberty of "cutting a few corners", where appropriate, so that the key ideas are not lost in the notation. Thus, this development is

admittedly rather cursory and rather imprecise, but the goal of having a "pretty good understanding of the key ideas" is achieved -- or, least, this is what I hope to accomplish here. Finally, it should be noted that Perturbation Theory is indeed a very fascinating specialization within the field of Nuclear Reactor Theory that can be utilized in a wide range of interesting applications, and the reader is certainly encouraged to explore further, as desired. In fact, Chapter 13 in the text by Stacey (see Ref. 3) is a good place to start if you do indeed want further information on this subject...

First-Order Perturbation Theory, Adjoint Operators, etc. etc.

We will start our development with the operator form of the steady state diffusion equation for a critical reactor using the notation from Ref. 4,

$$(L - \lambda F)\phi = 0 \tag{2}$$

Now, if we multiply this by an arbitrary space and energy dependent weight function, θ, and integrate over all space and energy, we have the usual expression for the eigenvalue $\lambda = 1/k$, or

$$\langle \theta(L - \lambda F)\phi \rangle = 0 \qquad \text{or} \qquad \lambda = \frac{\langle \theta L\phi \rangle}{\langle \theta F\phi \rangle} \tag{3}$$

Note that in previous work (see Ref. 4) we have written λ as $\lambda = \langle L\phi \rangle / \langle F\phi \rangle$ -- this just assumes that the weight function, θ, is unity. Thus, the above expression in eqn. (3) is just a slight generalization of our previous representation.

Now, if a perturbation is made in the absorption cross section, for example, in some region in the core, then both the L operator and the flux distribution will change, and the first-order variation in λ associated with the perturbation can be written as

$$\Delta\lambda = \left\langle \frac{\partial \lambda}{\partial \Sigma_a} \Delta\Sigma_a \right\rangle + \left\langle \frac{\partial \lambda}{\partial \phi} \Delta\phi \right\rangle + \text{ higher-order terms } \approx \left\langle \frac{\partial \lambda}{\partial \Sigma_a} \Delta\Sigma_a \right\rangle + \left\langle \frac{\partial \lambda}{\partial \phi} \Delta\phi \right\rangle \tag{4}$$

where we have replaced the change in the L operator by the explicit change in the absorption cross section (since none of the other components of L will change if we only perturb the absorption cross section). Note that the far right expression given here is referred to as the **First-Order Perturbation Theory** estimate, since we have dropped all the higher order terms in $\Delta\Sigma_a$ and $\Delta\phi$ within the infinite Taylor series expansion for $\Delta\lambda$.

Before continuing, we first note that $\Delta\lambda$ and our usual definition of reactivity, ρ, are directly related -- one is simply the negative of the other. To see this, we write $\lambda = 1/k$ and $\rho = (k-1)/k$ for two different states (i.e. a reference and perturbed configuration), to give

$$\Delta\lambda = \lambda' - \lambda = \frac{1}{k'} - \frac{1}{k} = \frac{k - k'}{k'k} \tag{5a}$$

and

$$\Delta\rho = \rho' - \rho = \frac{k'-1}{k'} - \frac{k-1}{k} = \frac{k'-k}{k'k} \tag{5b}$$

Thus, we see that $\Delta\rho = -\Delta\lambda$ or simply $\rho' = -\Delta\lambda$ if the reference state is exactly critical (i.e. $\rho = 0$ for a critical system).

Now, if we expand the derivative terms within the 1ˢᵗ-order approximation for $\Delta\lambda$ in eqn. (4) using the definition of λ from eqn. (3), we have

$$\Delta\lambda \approx \frac{\langle\theta\,\Delta\Sigma_a\phi\rangle}{\langle\theta\,F\phi\rangle} + \frac{\langle\theta\,L\Delta\phi\rangle}{\langle\theta\,F\phi\rangle} - \frac{\langle\theta\,L\phi\rangle\langle\theta\,F\Delta\phi\rangle}{\langle\theta\,F\phi\rangle^2} = \frac{\langle\theta\,\Delta\Sigma_a\phi\rangle}{\langle\theta\,F\phi\rangle} + \frac{\langle\theta(L-\lambda F)\Delta\phi\rangle}{\langle\theta\,F\phi\rangle} \tag{6}$$

where we have retained the integration over space and energy with the $<\dots>$ notation. Here we note that the integral containing $\Delta\Sigma_a$ involves only a *local integration* and the integral containing the $\Delta\phi$ distribution is a *global integral* -- since $\Delta\Sigma_a$ is non-zero only in the location of the perturbation, yet this variation generally causes a flux perturbation everywhere in the system. These two terms are also often referred to as the *direct effect* and *indirect effect*, respectively, since $\Delta\Sigma_a$ is associated with the actual change or local perturbation made within the system, but the change in flux throughout the system, $\Delta\phi$, is a secondary or indirect result of the initial physical perturbation.

To actually evaluate eqn. (6) for a given $\Delta\Sigma_a$, we need to know the perturbed flux, $\Delta\phi = \phi' - \phi$, and doing this for each change that we desire to investigate can become quite impractical. This is one of the key points in this whole development -- that is, in practice, we would like to evaluate $\Delta\lambda$ without re-solving the neutron balance equation for each variation in the system parameters. However, we can't just throw away the second term in eqn. (6) without justification -- at least not for an arbitrary choice of the weight function, θ. Thus, the goal here is to make a judicious choice for $\theta(\vec{r},E)$ such that the second term in the latter part of eqn. (6) vanishes completely. If we can do this, then only the reference unperturbed flux distribution and this (yet to be determined) specialized weight function are needed to evaluate $\Delta\lambda$ to first-order accuracy (i.e. the error terms are all proportional to the square of a deviation variable, $\Delta\Sigma_a^2$, $\Delta\phi^2$, or $\Delta\Sigma_a\Delta\phi$). The importance of this capability cannot be overstated, since it says we can get a good estimate of $\Delta\lambda$ (i.e. the change in reactivity) without knowledge of $\Delta\phi$ -- and this is the real power of First-Order Perturbation Theory methods!!!

Now, to perform some "magic" and make the term containing $\Delta\phi$ disappear, we introduce the definition of an **adjoint operator**. In particular, let's define H* as the *adjoint* of operator H, where H* is defined precisely by the equality

$$\langle vHu\rangle = \langle uH*v\rangle + \text{boundary terms} \tag{7}$$

where u and v are general functions defined over the same phase space, they satisfy the same type of operator equation, and they have the same kind of boundary conditions. For our current application involving the neutron diffusion equation, Hu is replaced by $(L - \lambda F)\phi$ and we will write the v function as $\phi*$, where this function is usually referred to as the **regular adjoint flux** or just simply the **adjoint flux**.

Note: Within the Perturbation Theory field, there is also a quantity known as the **generalized adjoint flux**, and the terms "regular" and "generalized" are used to distinguish between the two quantities. However, since our focus here is only introductory in nature, we will not address the generalized problem -- so in all the discussion that follows, the term "adjoint" refers to the regular adjoint problem as described here.

We now rewrite eqn. (7) using the specific notation of interest to reactor theory applications, or

$$\langle \phi*(L-\lambda F)\phi \rangle = \langle \phi(L-\lambda F)*\phi* \rangle + BT \qquad (8)$$

where BT refers to the "boundary terms" noted in eqn. (7) and, in most cases of practical interest, the boundary terms will vanish with appropriate definition of the boundary conditions for the operator equations -- thus, BT = 0 for our current discussions (see Appendix A for further justification of this statement). Also, with the functions ϕ and $\phi*$ satisfying the same type of operator equation and same kind of boundary conditions, we propose that the adjoint flux, $\phi*$, satisfy the equation

$$(L-\lambda F)*\phi* = 0 \qquad (9)$$

which is clearly similar to the operator equation given in eqn. (2) for the forward flux, ϕ. In addition, this also satisfies eqn. (8) with an equality that says $0 = 0$ (with BT = 0). The solution of eqn. (9), with appropriate boundary conditions, represents the formal definition of $\phi*(\vec{r},E)$, the so-called regular adjoint flux.

Now, we can also apply the basic definition of an adjoint operator to the numerator of the last expression in eqn. (6). In particular, letting $\theta = \phi*$, we have

$$\langle \phi*(L-\lambda F)\Delta\phi \rangle = \langle \Delta\phi(L-\lambda F)*\phi* \rangle + 0 = 0 \qquad (10)$$

where the first equality is true because of eqn. (8) with BT = 0, and both these terms are zero because of the definition of the adjoint flux given by eqn. (9). Thus, the last term in eqn. (6) simply goes to zero if the weight function is chosen to be the adjoint flux defined via eqn. (9). Clearly, from this development, if $\theta = \phi*$, the whole term containing $\Delta\phi$ vanishes identically, and the expression for the reactivity change from critical due to a change in material composition or an absorption cross section reduces to an equation of the form

$$\rho = -\Delta\lambda = -\frac{\langle \phi*\Delta\Sigma_a\phi \rangle}{\langle \phi*F\phi \rangle} \qquad (11)$$

Thus, if the chosen weight function is the adjoint flux (or the ***importance function*** as it is often called), then the expression for a reactivity change in the system simplifies greatly, and it becomes relatively insensitive to flux changes from reference -- since the term containing $\Delta\phi$ completely vanishes, leaving only errors that are proportional to the second order deviation variables (i.e. terms containing variables such as $\Delta\Sigma_a^2$, $\Delta\phi^2$, and $\Delta\Sigma_a\Delta\phi$).

The goal of this brief introduction to Perturbation Theory Methods was to define what is meant by the adjoint flux and to justify that $\phi*(\vec{r},E)$ is the best choice for the weight function that occurs in the weighted integral form of the neutron balance equation -- especially when integral expressions for reactivity are involved -- and we have just completed this task. However, we purposely left out a lot of detail so that our primary goal was not clouded with too much notation and too much tedious mathematics. However, to get a feel for what some of the abstract integral operator notation (such as $<\phi*H\phi>$) really means, a few explicit detailed examples are given in Appendix A. In addition, using the adjoint operators defined in Appendix A, the full multigroup adjoint diffusion equation is given in Appendix B along with a comparison to the usual forward balance equation. Furthermore, explicit forward and adjoint equations using 2-group theory for a

critical system are also summarized in Appendix B. Finally, Appendix B also contains a brief overview of the basic solution strategy for solving both the forward and adjoint forms of the multigroup diffusion equations. These appendices simply add some specificity to the operator notation used here -- and these details can be quite useful if you are ever involved with actually solving the rather unconventional adjoint form of the multigroup balance equation.

Summary

As stated previously, the goal of this set of Lecture Notes is to give the reader a pretty good overview of the terminology, theory, and practical application of "Perturbation Theory Methods", without going into too much detail into this field of specialization. Thus, the objective here was not to make the reader an expert in this field but, instead, to give you enough insight so that you can talk intelligently about the subject and, most importantly, **understand why we let $\theta(\vec{r},E) = \phi*(\vec{r},E)$ in most practical applications**. As part of this development, we also defined a bunch of new terminology, such as what is an adjoint operator, the importance function, etc. Finally, in the appendices, we also included some typical examples of how one determines the adjoint operator that corresponds to a particular forward operator, and also showed how the adjoint multigroup diffusion equation differs from it forward counterpart. There is a bit of detail in all this development -- all really good stuff in fact -- but the real goal was to show clearly that the weight function used for performing weighted integral neutron balances should be the adjoint flux, $\phi*(\vec{r},E)$, since, when using this weight function, the weighted integral results becomes less sensitive to variations or perturbations in the reference flux distribution. This understanding should be the real take-away from this set of Lecture Notes...

References

1. J. R. White, "Formal Derivation of the Point Kinetics Equations Using Multigroup Diffusion Theory," part of a series of Lecture Notes for the Nuclear Engineering Program at UMass-Lowell.

2. J. R. White, "The Time Dependent Reactor," part of a series of Lecture Notes for the Nuclear Engineering Program at UMass-Lowell.

3. W. M. Stacey, **Nuclear Reactor Physics**, Wiley-VCH Verlag GmbH & Co KGaA, Weinheim, Federal Republic of Germany (2007).

4. J. R. White, "The Multigroup Neutron Balance Equation," part of a series of Lecture Notes for the Nuclear Engineering Program at UMass-Lowell.

Appendix A   Some Common Forward and Adjoint Operators

In general, for any forward operator H, we can define the adjoint operator H* by applying the formal definition given in eqn. (7) in the main body of this set of Lecture Notes. The purpose of this appendix is to give some explicit examples of several common operators of interest in typical reactor physics analyses (in fact these operators are usually of general interest for many applications). These examples should give some specificity to the general notation used in the main notes.

Example 1: 1st Derivative Operator   H = $\partial/\partial x$

Applying the basic definition of an adjoint operator, one has

$$\langle \phi * H\phi \rangle = \langle \phi H * \phi * \rangle + BT$$

and, if written in detail for H = $\partial/\partial x$, the left hand side (LHS) becomes

$$\langle \phi * H\phi \rangle = \int_a^b \phi *(x) \frac{\partial}{\partial x} \phi(x)dx \qquad (A.1)$$

Now, if we integrate this expression by parts, where $\int_a^b u\,dv = uv\big|_a^b - \int_a^b v\,du$, and we let

$$u = \phi * \quad \text{and} \quad dv = \frac{\partial \phi}{\partial x}dx \qquad \text{with} \qquad du = \frac{\partial \phi *}{\partial x}dx \quad \text{and} \quad v = \phi$$

then we have

$$\langle \phi * H\phi \rangle = \phi * \phi\big|_a^b - \int_a^b \phi \frac{\partial \phi *}{\partial x}dx = BT + \langle \phi H * \phi * \rangle \qquad (A.2)$$

Therefore, from eqns. (A.1) and (A.2), we see that for H = $\partial/\partial x$, the adjoint operator becomes H* = $-\partial/\partial x$. Also note that, in general, the multidimensional forward and adjoint gradient operators can be written in vector form as

$$H = \vec{\nabla}, \quad H* = -\vec{\nabla} \qquad (A.3)$$

Example 2: Laplacian Operator   H = $\partial^2/\partial x^2$

From the basic definition of our bracket notation for H = $\partial^2/\partial x^2$, we have

$$\langle \phi * H\phi \rangle = \int_a^b \phi *(x) \frac{\partial^2}{\partial x^2} \phi(x)dx \qquad (A.4)$$

Integrating by parts as above, we have

$$u = \phi * \quad \text{and} \quad dv = \frac{\partial}{\partial x}\left(\frac{\partial \phi}{\partial x}\right)dx \qquad \text{with} \qquad du = \frac{\partial \phi *}{\partial x}dx \quad \text{and} \quad v = \frac{\partial \phi}{\partial x}$$

and, upon substitution, this gives

$$\langle \phi * H\phi \rangle = \phi * \frac{\partial \phi}{\partial x}\bigg|_a^b - \int_a^b \frac{\partial \phi}{\partial x} \frac{\partial \phi *}{\partial x}dx$$

Since we desire a form of the integral where the operator is operating completely on ϕ^*, let's try integration by parts once again. This time we have

$$u = \frac{\partial \phi^*}{\partial x} \quad \text{and} \quad dv = \frac{\partial \phi}{\partial x} dx \qquad \text{with} \qquad du = \frac{\partial}{\partial x}\left(\frac{\partial \phi^*}{\partial x}\right) dx \quad \text{and} \quad v = \phi$$

and, after substitution, we have

$$\langle \phi^* H\phi \rangle = \phi^* \frac{\partial \phi}{\partial x}\bigg|_a^b - \phi \frac{\partial \phi^*}{dx}\bigg|_a^b + \int_a^b \phi \frac{\partial^2 \phi^*}{\partial x^2} dx = BT + \langle \phi H^* \phi^* \rangle \tag{A.5}$$

Thus, by comparing eqns. (A.4) and (A.5), we see that for $H = \partial^2/\partial x^2$, the adjoint operator becomes $H^* = H = \partial^2/\partial x^2$. When this occurs (i.e. when $H^* = H$), the operator is said to be ***self-adjoint***. Also note that, in general, we can write this relationship in terms of the multidimensional Laplacian,

$$H = \vec{\nabla} \cdot \vec{\nabla} = \nabla^2, \qquad H^* = H = \vec{\nabla} \cdot \vec{\nabla} = \nabla^2 \tag{A.6}$$

and also, for the special case of the leakage term within the neutron diffusion equation, we have

$$H = -\vec{\nabla} \cdot D\vec{\nabla}, \qquad H^* = H = -\vec{\nabla} \cdot D\vec{\nabla} \tag{A.7}$$

Before giving another example, we should also mention the Boundary Terms (BT) again. Recall that the general defining equation for an adjoint operator contains this term. However, we argued that, with the typical boundary conditions that are applied to physical systems, these terms usually vanish. To illustrate this behavior, notice that the boundary terms from the above example are

$$BT = \phi^* \frac{\partial \phi}{\partial x}\bigg|_a^b - \phi \frac{\partial \phi^*}{\partial x}\bigg|_a^b = \phi^*(b)\frac{d\phi}{dx}\bigg|_b - \phi^*(a)\frac{d\phi}{dx}\bigg|_a - \phi(b)\frac{d\phi^*}{dx}\bigg|_b + \phi(a)\frac{d\phi^*}{dx}\bigg|_a$$

Now, for a 1-D Cartesian geometry reactor model, for example, a typical set of boundary conditions for the forward flux solution is

1. symmetry at $x = a$ (zero current at the center of the system at $x = a = 0$)

    at $x = a$ $\qquad \dfrac{d\phi}{dx}\bigg|_{x=a} = 0$

2. flux goes to zero at the extrapolation distance (zero flux at $x = b$)

    at $x = b$ $\qquad \phi(x)\big|_{x=b} = 0$

Now let's choose an identical set of boundary conditions for the adjoint flux, ϕ^*, that is

1. symmetry at $x = a$

    at $x = a$ $\qquad \dfrac{\partial \phi^*}{\partial x}\bigg|_{x=a} = 0$

2. adjoint flux (or importance) goes to zero at the extrapolated boundary (i.e. the importance of a neutron is zero here)

at $x = b$ $\qquad \phi*(x)\big|_{x=b} = 0$

Thus, with these boundary conditions, we see that every term in the BT expansion does indeed vanish. This specific example can also be generalized. In particular, for general reactor physics applications using the steady-state diffusion equation, the boundary conditions for the adjoint flux equation are usually identical to those for the forward flux equation -- and with these boundary conditions, the BT component within the definition of the adjoint operator expression will always vanish.

Example 3: Matrix Operator $\mathbf{H} \rightarrow \underline{\underline{H}} = [H_{ij}]$

Another important operator that occurs frequently in applications is the matrix operator. Recall that the multigroup neutron balance equation can be written in matrix form[4] as

$\qquad$ Forward Form: $\qquad (\underline{\underline{L}} - \lambda\underline{\underline{F}})\underline{\varphi} = 0$ $\qquad\qquad\qquad\qquad\qquad$ (A.8)

$\qquad$ Adjoint Form: $\qquad (\underline{\underline{L}} - \lambda\underline{\underline{F}})*\underline{\varphi}* = 0$ $\qquad\qquad\qquad\qquad\qquad$ (A.9)

and, for the case of a matrix operator, the definition of the adjoint operator becomes

$$\left\langle \underline{\phi}*^{\,T}\underline{\underline{H}}\,\underline{\phi}\right\rangle = \left\langle \underline{\phi}^{T}\underline{\underline{H}}*\underline{\phi}*\right\rangle + BT \qquad\qquad\qquad\qquad (A.10)$$

In the context of the diffusion equation, the matrix operation, $\underline{\phi}*^{\,T}\underline{\underline{H}}\,\underline{\phi}$, represents integration over the discrete energy variable, and the brackets in eqn. (A.10) indicate an integration over the spatial variable.

If we concentrate for the moment on just the matrix operations (so that the brackets can be dropped temporarily from the following expressions), we know that these matrix manipulations can also be expressed with discrete summation notation, that is

$$\underline{\underline{H}}\,\underline{\phi} = \sum_{j} H_{ij}\phi_{j}$$

and

$$\underline{\phi}*^{\,T}\underline{\underline{H}}\,\underline{\phi} = \sum_{i}\phi_{i}^{*}\sum_{j}H_{ij}\phi_{j} = \sum_{ij}\phi_{i}^{*}H_{ij}\phi_{j} \qquad\qquad\qquad\qquad (A.11)$$

where the H_{ij}'s are the elements of the $\underline{\underline{H}}$ matrix. Notice also that $\underline{\phi}^{T}\underline{\underline{H}}*\underline{\phi}*$ can be written as

$$\underline{\phi}^{T}\underline{\underline{H}}*\underline{\phi}* = \sum_{ij}\phi_{i}H_{ij}^{*}\phi_{j}^{*} \qquad\qquad\qquad\qquad (A.12))$$

where the H_{ij}^{*} values are the elements of the $\underline{\underline{H}}*$ matrix.

It is important to notice in these discrete representations that the summation indices are dummy variables. For example, eqn. (A.12) can also be written as

$$\underline{\phi}^{T}\underline{\underline{H}}*\underline{\phi}* = \sum_{ij}\phi_{j}H_{ji}^{*}\phi_{i}^{*} \qquad\qquad\qquad\qquad (A.13)$$

where the i and j indices have been interchanged. Note, however, that these indices have been interchanged in a fully consistent manner.

Now for the simple case of the elements of $\underline{\underline{H}}$ being constants (not operators), it should be obvious from comparison of eqns. (A.11) and (A.13) that $H_{ji}^* = H_{ij}$, since by definition of the adjoint operator, $\underline{\phi}^{*T} \underline{\underline{H}} \underline{\phi} = \underline{\phi}^T \underline{\underline{H}}^* \underline{\phi}^*$ (there are no boundary terms here since we have not done any integrals yet). Thus, for constant matrices the adjoint matrix is simply the transpose of the original matrix operator

$$\underline{\underline{H}}^* = \underline{\underline{H}}^T \qquad \text{and} \qquad H_{ij}^* = H_{ji} \qquad \text{(when the elements are constants)} \qquad \text{(A.14)}$$

If the matrix operator contains differential or integral operators as elements, then we need to be careful to carry along the integral notation that was dropped above. In this case, the notation becomes a little messy, but the concept is quite straightforward. Here we have

$$\left\langle \underline{\phi}^{*T} \underline{\underline{H}} \underline{\phi} \right\rangle = \sum_{ij} \left\langle \phi_i^* H_{ij} \phi_j \right\rangle = \sum_{ij} \left\langle \phi_j (H_{ij})^* \phi_i^* \right\rangle + \text{BT} = \sum_{ij} \left\langle \phi_i (H_{ji})^* \phi_j^* \right\rangle \qquad \text{(A.15)}$$

where, in the first step, we have moved H_{ij} from operating on φ_j to having $(H_{ij})^*$ operating on φ_i^* by definition of the adjoint to element H_{ij}. In the second step, we simply interchanged the indices (as before) and assumed that BT = 0 (as before).

Now also writing $\left\langle \underline{\phi}^T \underline{\underline{H}}^* \underline{\phi}^* \right\rangle$ explicitly, we have

$$\left\langle \underline{\phi}^T \underline{\underline{H}}^* \underline{\phi}^* \right\rangle = \sum_{ij} \left\langle \phi_i (H^*)_{ij} \phi_j^* \right\rangle \qquad \text{(A.16)}$$

and, via careful comparison with the last entry of eqn. (A.15), we see that $(H^*)_{ij} = (H_{ji})^*$, or

$$\underline{\underline{H}} = [H_{ij}], \qquad \underline{\underline{H}}^* = [H_{ij}^*] = [H_{ji}]^* \qquad \text{(A.17)}$$

In words, this says that the ij^{th} element of the adjoint operator $\underline{\underline{H}}^*$ is equal to the adjoint of the ji^{th} element of the original matrix $\underline{\underline{H}}$. Or more simply, to find $\underline{\underline{H}}^*$, first transpose $\underline{\underline{H}}$ and then adjoint each element of the transposed matrix. Note that, in practice, this procedure is more straightforward than all this ugly notation implies (see footnote 1) -- where, in general, we have

$$\underline{\underline{H}} = \begin{bmatrix} H_{11} & H_{12} & H_{13}\cdots \\ H_{21} & H_{22} & H_{23} \\ & \vdots & & \ddots \end{bmatrix} \qquad \underline{\underline{H}}^* = \begin{bmatrix} (H_{11})^* & (H_{21})^* & (H_{31})^*\cdots \\ (H_{12})^* & (H_{22})^* & (H_{32})^* \\ & \vdots & & \ddots \end{bmatrix} \qquad \text{(A.18)}$$

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[1] The notation here is a little tricky. The precise definitions are as follows:

H_{ij}^* represents the ij element of the adjoint matrix $\underline{\underline{H}}^*$

$[H_{ij}]^*$ or $(H_{ij})^*$ represents the adjoint of the ij element of the forward matrix $\underline{\underline{H}}$

Appendix B   The Forward and Adjoint Multigroup Balance Equations

The detailed mathematics in Appendix A were necessary to precisely define what is meant by the term adjoint operator where, in particular, we gave explicit examples for all of the operators that are of interest for the multigroup diffusion equation. Thus, with the mathematical preliminaries from Appendix A, we can now define precisely the so-called multigroup adjoint diffusion equation.

In matrix form the forward diffusion equation (see Ref. 4) can be written as $(\underline{\underline{L}} - \lambda \underline{\underline{F}})\underline{\phi} = 0$ or

$$-\vec{\nabla} \cdot \underline{\underline{D}} \vec{\nabla} \underline{\phi} + \underline{\underline{\Sigma}}_R \, \underline{\phi} - \underline{\underline{\Sigma}}_S^I \underline{\phi} - \lambda \underline{\underline{F}} \underline{\phi} = 0 \tag{B.1}$$

Noting that $\underline{\underline{D}}$ and $\underline{\underline{\Sigma}}_R$ are diagonal matrices, that the Laplacian operator is self-adjoint, that the adjoint of a matrix not containing integral or differential operators is simply the transpose of the original matrix, and that $\lambda^* = \lambda$ (which can be easily shown -- see Ref. 3 for example), we can write the regular adjoint diffusion equation, $(\underline{\underline{L}} - \lambda \underline{\underline{F}})^* \underline{\phi}^* = 0$, as

$$-\vec{\nabla} \cdot \underline{\underline{D}} \vec{\nabla} \underline{\phi}^* + \underline{\underline{\Sigma}}_R \, \underline{\phi}^* - \left(\underline{\underline{\Sigma}}_S^I \right)^T \underline{\phi}^* - \lambda \left(\underline{\underline{F}} \right)^T \underline{\phi}^* = 0 \tag{B.2}$$

where explicit definitions for the forward and adjoint inscatter and fission source matrices are given by:

forward inscatter source

$$\underline{\underline{\Sigma}}_S^I \underline{\phi} = \begin{bmatrix} 0 & \Sigma_{2\to1} & \Sigma_{3\to1} & \cdots & \Sigma_{G\to1} \\ \Sigma_{1\to2} & 0 & \Sigma_{3\to2} & \cdots & \\ \Sigma_{1\to3} & \Sigma_{2\to3} & 0 & & \\ & & \vdots & & \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_G \end{bmatrix}$$

adjoint inscatter source

$$\left(\underline{\underline{\Sigma}}_S^I \right)^* \underline{\phi}^* = \left(\underline{\underline{\Sigma}}_S^I \right)^T \underline{\phi}^* = \begin{bmatrix} 0 & \Sigma_{1\to2} & \Sigma_{1\to3} & \cdots & \Sigma_{1\to G} \\ \Sigma_{2\to1} & 0 & \Sigma_{2\to3} & \cdots & \\ \Sigma_{3\to1} & \Sigma_{3\to2} & 0 & & \\ & & \vdots & & \end{bmatrix} \begin{bmatrix} \phi_1^* \\ \phi_2^* \\ \vdots \\ \phi_G^* \end{bmatrix}$$

forward fission source

$$\underline{\underline{F}} \underline{\phi} = \begin{bmatrix} \chi_1 \nu\Sigma_{f1} & \chi_1 \nu\Sigma_{f2} & \chi_1 \nu\Sigma_{f3} & \cdots \\ \chi_2 \nu\Sigma_{f1} & \chi_2 \nu\Sigma_{f2} & \chi_2 \nu\Sigma_{f3} & \cdots \\ & \vdots & & \\ \chi_G \nu\Sigma_{f1} & \chi_G \nu\Sigma_{f2} & \chi_G \nu\Sigma_{f3} & \cdots \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_G \end{bmatrix}$$

adjoint fission source

$$\underline{\underline{F}}^* \underline{\phi}^* = \underline{\underline{F}}^T \underline{\phi}^* = \begin{bmatrix} \chi_1 \nu\Sigma_{f1} & \chi_2 \nu\Sigma_{f1} & \chi_3 \nu\Sigma_{f1} & \cdots \\ \chi_1 \nu\Sigma_{f2} & \chi_2 \nu\Sigma_{f2} & \chi_3 \nu\Sigma_{f2} & \cdots \\ & \vdots & & \\ \chi_1 \nu\Sigma_{fG} & \chi_2 \nu\Sigma_{fG} & \chi_3 \nu\Sigma_{fG} & \cdots \end{bmatrix} \begin{bmatrix} \phi_1^* \\ \phi_2^* \\ \vdots \\ \phi_G^* \end{bmatrix}$$

If written for a discrete energy group g (an arbitrary component of the vector), one has for the multigroup forward equation

$$-\vec{\nabla} \cdot D_g \vec{\nabla} \phi_g + \Sigma_{Rg} \phi_g - \sum_{g' \neq g} \Sigma_{g' \to g} \phi_{g'} - \lambda \chi_g \sum_{g'} \nu \Sigma_{fg'} \phi_{g'} = 0 \tag{B.3}$$

and for the adjoint equation, we have

$$-\vec{\nabla} \cdot D_g \vec{\nabla} \phi_g^* + \Sigma_{Rg} \phi_g^* - \sum_{g \neq g'} \Sigma_{g \to g'} \phi_{g'}^* - \lambda \nu \Sigma_{fg} \sum_{g'} \chi_{g'} \phi_{g'}^* = 0 \tag{B.4}$$

These expressions are the basis for all work associated with the multigroup forward and adjoint diffusion equations. Here one should clearly note the subtle, but extremely important differences between the adjoint inscatter and fission sources and their forward counterparts -- since these differences also suggest that a different approach should be taken when solving these equations (see further discussion below).

Specializing the general equations to the case of the usual 2-group thermal reactor problem (i.e. with no upscatter and $\chi_1 = 1.0$ and $\chi_2 = 0.0$), the expressions for the **forward equations** become

$$-\vec{\nabla} \cdot D_1 \vec{\nabla} \phi_1 + (\Sigma_{a1} + \Sigma_{1 \to 2}) \phi_1 - \lambda (\nu \Sigma_{f1} \phi_1 + \nu \Sigma_{f2} \phi_2) = 0$$
$$-\vec{\nabla} \cdot D_2 \vec{\nabla} \phi_2 + \Sigma_{a2} \phi_2 - \Sigma_{1 \to 2} \phi_1 = 0 \tag{B.5}$$

and the appropriate **two-group adjoint equations** are

$$-\vec{\nabla} \cdot D_1 \vec{\nabla} \phi_1^* + (\Sigma_{a1} + \Sigma_{1 \to 2}) \phi_1^* - \Sigma_{1 \to 2} \phi_2^* - \lambda \nu \Sigma_{f1} \phi_1^* = 0$$
$$-\vec{\nabla} \cdot D_2 \vec{\nabla} \phi_2^* + \Sigma_{a2} \phi_2^* - \lambda \nu \Sigma_{f2} \phi_1^* = 0 \tag{B.6}$$

As mentioned above, one should take special note of the key differences in these equations, primarily in the inscatter and the fission source terms. In fact, the adjoint equation is fundamentally different in the sense that the "inscatter source" for group 1 requires knowledge of the group 2 fluxes. In essence, "neutron importance" scatters (or transfers) from group 2 to group 1, whereas physical neutrons scatter from group 1 to group 2. Also note that the adjoint equations contain a fission source term in each group (both of which are functions of ϕ_1^*).

In practice, since scattering in the adjoint case is from group 2 to group 1, the energy equations are usually solved in reverse order. During the inner iteration of a finite difference calculation for the adjoint equation, for example, the energy loop goes from low to high energy (instead of the standard high to low scheme for the forward solution). Other than this change, and the fact that the scattering and fission source components are "transposed", the numerical solution scheme for the adjoint equation is identical to that for the forward equation. Thus, many deterministic reactor physics code systems solve both forms of the balance equation with little interaction on the part of the user. In fact, in most systems, the choice of a forward/adjoint option switch is all that is required.

If we specialize even further to the 1-group approximation, one has the following result,

Forward Problem: $\quad -\vec{\nabla} \cdot D \vec{\nabla} \varphi + \Sigma_a \varphi - \lambda \nu \Sigma_f \varphi = 0$ (B.7)

Adjoint Problem: $\quad -\vec{\nabla} \cdot D \vec{\nabla} \varphi^* + \Sigma_a \varphi^* - \lambda \nu \Sigma_f \varphi^* = 0$ (B.8)

Close inspection of these expressions shows that they are identical -- that is, the solution to eqn. (B.7) is identical to that of eqn. (B.8). Again, upon reflection, this is to be expected since, for the 1-group approximation, each operator is self-adjoint (i.e. $H^* = H$) and the boundary conditions for the forward and adjoint problems are identical. Thus, for all 1-group problems, independent of the spatial complexity of the geometry, the adjoint flux is identical to the forward flux (i.e. $\varphi^*(\vec{r}) = \varphi(\vec{r})$ for 1-group problems). Unfortunately, this does not hold for multigroup problems since, in this case, the inscatter and fission source components are not self-adjoint.

Note: If you have been following the full set of these Lecture Notes, you may recall that the self-adjoint property was used to advantage in Ref. 2 to develop a simple formula for the worth of a partially inserted control rod in a bare homogeneous system...