

Adjoint Transport Equation

(L&M 1.6)

The adjoint TE has two main applications: use in MC variance reduction and use in perturbation theory for eigenvalue problems (estimate changes in the neutron multiplication caused by small changes in material properties).

We will start with some mathematical concepts we will use.

Inner product

- An inner product is a binary operation (takes 2 arguments) that combines 2 vectors into a scalar quantity.
- in Euclidean space, which comprises all 3D vectors, the inner product is the project of one vector onto another ($\vec{v}_1 \cdot \vec{v}_2 = |\vec{v}_1||\vec{v}_2| \cos(\theta)$).
- A function space comprises all functions that have a given property. e.g. all continuous functions; all functions with Dirichlet BCs; etc.
- for $f \in$ a function space: f satisfies the properties of the space
- one way to define an inner product: $\langle f, g \rangle \equiv \int_{\rho} d\rho f^*(\rho)g(\rho)$, where superscript $*$ indicates complex conjugate.
- Inner products are linear: $\langle f, [ag_1 + bg_2] \rangle = a \langle f, g_1 \rangle + b \langle f, g_2 \rangle$, where a and b are scalars.

The *adjoint operator* obeys the following identity: $\langle A^\dagger f, g \rangle = \langle f, Ag \rangle$ for all f and g in the vector space. Superscript \dagger indicates adjoint quantities.

Note that if M_1^\dagger and M_2^\dagger are both adjoints of M_1 and M_2 , respectively, then $(M_1 + M_2)^\dagger = M_1^\dagger + M_2^\dagger$.

We can relate the forward and adjoint eigenspaces

Forward: $Mf = \lambda f$ with homogeneous BCs;

Adjoint: $M^\dagger f^\dagger = \lambda^\dagger f^\dagger$ with homogeneous BCs.

$$\begin{aligned}\langle M^\dagger f^\dagger, f \rangle - \langle f^\dagger, Mf \rangle &= \langle \lambda^\dagger f^\dagger, f \rangle - \langle f^\dagger, \lambda f \rangle \\ 0 &= \langle \lambda^\dagger - \lambda \rangle \langle f^\dagger, f \rangle \quad \text{orthogonality condition}\end{aligned}$$

If $\lambda^{\dagger,*} \neq \lambda$ then $\langle f^\dagger, f \rangle = 0$.

If $\langle f^\dagger, f \rangle \neq 0$ then $\lambda^{\dagger,*} = \lambda \rightarrow \lambda^\dagger = \lambda$.

If $M = M^\dagger$, the operator is called self-adjoint.

Adjoint Transport Equation for non-multiplying media

Note that we're going to use ζ to indicate this could be applied to any appropriate function (though in practice we'll use ψ).

We will use vacuum boundary conditions: $\zeta(\vec{r}_s, \hat{\Omega}, E) = 0$, $\hat{n} \cdot \hat{\Omega} < 0$, where \vec{r}_s is on the surface and \hat{n} is the outward normal at \vec{r}_s .

Recall that $\zeta(\vec{r}_s, \hat{\Omega}, E)$ must be continuous in the direction of particle travel.

We will call our transport operator H .

Our goal is to find H^\dagger such that $\langle \zeta^\dagger, H\zeta \rangle = \langle \zeta, H^\dagger \zeta^\dagger \rangle$.

To do this, we'll start with the LHS : we will multiply the regular TE by ζ^\dagger , integrate over all phase space, and manipulate the result to get ζ in front of the operator.

$$\int_\rho d\rho \zeta^\dagger(\rho) \left[[\hat{\Omega} \cdot \nabla + \Sigma_t] \zeta(\vec{r}, E, \hat{\Omega}) - \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE' \Sigma_s(E', \hat{\Omega}' \rightarrow E, \hat{\Omega}) \zeta(\vec{r}, E', \hat{\Omega}') \right]$$

Let's go through this one term at a time:

- The total interaction is a self-adjoint operator (why?), so we can simply rearrange the order: $\zeta^\dagger \Sigma_t \zeta \rightarrow \zeta \Sigma_t \zeta^\dagger$. That is

$$\int_V dV \zeta^\dagger(\vec{r}, E, \hat{\Omega}) \Sigma_t(E) \zeta(\vec{r}, E, \hat{\Omega}) = \int_V dV \zeta(\vec{r}, E, \hat{\Omega}) \Sigma_t(\vec{r}, E) \zeta^\dagger(\vec{r}, E, \hat{\Omega})$$

- For the streaming term, use $\hat{\Omega} \cdot \nabla = \nabla \cdot \hat{\Omega}$ and the identity (from the chain rule)

$$\nabla \cdot (\hat{\Omega} \zeta^\dagger \zeta) = \zeta^\dagger \hat{\Omega} \cdot \nabla \zeta + \zeta \hat{\Omega} \cdot \nabla \zeta^\dagger,$$

then

$$\int_V d^3r \zeta^\dagger \hat{\Omega} \cdot \nabla \zeta + \int_V d^3r \zeta \hat{\Omega} \cdot \nabla \zeta^\dagger = \int_S d\Gamma \hat{n} \cdot \hat{\Omega} \zeta^\dagger \zeta$$

from divergence theorem.

Now, we apply the boundary condition that we originally had for ζ , which causes the surface integral to vanish for $\hat{\Omega} \cdot \hat{n} < 0$.

We have a *corresponding boundary condition* for ζ^\dagger that at any point \vec{r}_s on the surface, $\zeta^\dagger(\vec{r}, \hat{\Omega}, E) = 0$, $\vec{r} \in \Gamma$ and $\hat{\Omega} \cdot \hat{n} \geq 0$.

This means that the surface integral has to vanish for all $\hat{\Omega}$ giving

$$\int_V d^3r \zeta^\dagger \hat{\Omega} \cdot \nabla \zeta = - \int_V d^3r \zeta \hat{\Omega} \cdot \nabla \zeta^\dagger$$

- Finally we'll look at the scattering term. As with total interaction, we know $\zeta^\dagger \Sigma_s \zeta = \zeta \Sigma_s \zeta^\dagger$. We will also swap E' and E , $\hat{\Omega}'$ and $\hat{\Omega}$ to get (leaving out volume integration but we'll add it later)

$$\begin{aligned} \int d\hat{\Omega} \int dE \zeta^\dagger(\vec{r}, \hat{\Omega}, E) \int d\hat{\Omega}' \int dE' \Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) \zeta(\vec{r}, \hat{\Omega}', E') = \\ \int d\hat{\Omega} \int dE \zeta(\vec{r}, \hat{\Omega}, E) \int d\hat{\Omega}' \int dE' \Sigma_s(\vec{r}, E \rightarrow E', \hat{\Omega} \cdot \hat{\Omega}') \zeta^\dagger(\vec{r}, \hat{\Omega}', E') \end{aligned}$$

We now combine all three terms to get the adjoint form of the transport equation (!):

$$\begin{aligned} \langle \zeta^\dagger, H\zeta \rangle = \int_V dV \int_{4\pi} d\hat{\Omega} \int_0^\infty dE \zeta(\vec{r}, \hat{\Omega}, E) \times \left[-\hat{\Omega} \cdot \nabla \zeta^\dagger(\vec{r}, E, \hat{\Omega}) + \Sigma_t(\vec{r}, E) \zeta^\dagger(\vec{r}, E, \hat{\Omega}) \right. \\ \left. - \int d\hat{\Omega}' \int dE' \Sigma_s(\vec{r}, E \rightarrow E', \hat{\Omega} \cdot \hat{\Omega}') \zeta^\dagger(\vec{r}, \hat{\Omega}', E') \right] \end{aligned}$$

We can see that $\langle \zeta^\dagger, H\zeta \rangle = \langle \zeta, H^\dagger \zeta^\dagger \rangle$ will be satisfied if we define the adjoint operator as

$$H^\dagger = -\hat{\Omega} \cdot \nabla + \Sigma_t(\vec{r}, E) - \int d\hat{\Omega}' \int dE' \Sigma_s(\vec{r}, E \rightarrow E', \hat{\Omega} \cdot \hat{\Omega}')$$

Where key differences are the negative in front of the streaming term and the reversal of energy direction in the scattering cross section.

We also need the boundary condition of zero *outgoing* adjoint flux.

Interpretation of adjoint flux as *neutron importance*

Let's think about a problem with an external source: $H\psi = q_{ex}$, where ψ meets the boundary conditions.

We'd like to find out the response of a detector with cross section Σ_d and volume V_d to that source:

$$R = V_d \int dE \Sigma_d(E) \int_{4\pi} d\hat{\Omega} \psi(\vec{r}_d, \hat{\Omega}, E).$$

- We'll set up the adjoint problem with the detector response as the source

$$H^\dagger \psi^\dagger = q_{ex}^\dagger \equiv V_d \Sigma_d \delta(\vec{r} - \vec{r}_d)$$

where $\psi^\dagger(\vec{r}_s, \hat{\Omega}, E) = 0$ for \vec{r} on Γ and $\hat{\Omega} \cdot \hat{n} > 0$.

- We can multiply the initial equation (forward) by ψ^\dagger and integrate over phase space. We can do the opposite/same to the adjoint equation. This gives

$$\begin{aligned} \langle \psi^\dagger, H\psi \rangle &= \langle \psi^\dagger, q_{ex} \rangle \quad \text{and} \\ \langle \psi, H^\dagger \psi^\dagger \rangle &= \underbrace{\langle \psi, V_d \Sigma_d \delta(\vec{r} - \vec{r}_d) \rangle}_R \end{aligned}$$

- We can subtract the two and then apply the adjoint equivalence identity to see

$$\begin{aligned} \langle \psi^\dagger, H\psi \rangle - \langle \psi, H^\dagger \psi^\dagger \rangle &= \langle \psi^\dagger, q_{ex} \rangle - R \\ R &= \langle \psi^\dagger, q_{ex} \rangle \end{aligned}$$

So what does that mean?

It means that the detector response is the volume integral of the adjoint-weighted source distribution.

What does that mean?

The weighting of the adjoint flux directly corresponds to how influential a given source particle will be on the answer we're looking for (what we defined as the adjoint source).

This is a pretty powerful concept.

We can look at a delta source to clarify this a bit.

$$\begin{aligned} q_{ex} &= \delta(\vec{r} - \vec{r}_0) \delta(E - E_0) \delta(\hat{\Omega} \cdot \hat{\Omega}_0) \\ R &= \psi^\dagger(\vec{r}_0, \hat{\Omega}_0, E_0) \end{aligned}$$

It is clear here that the importance provides the detector response to particles produced at $(\vec{r}_0, \hat{\Omega}_0, E_0)$.

This also makes sense if we think through the differences in the equations:

- $-\hat{\Omega} \cdot \nabla$: by convention, $\hat{\Omega} \cdot \nabla \psi$ implies the *outflow* of ψ from an infinitesimal volume.
A neutron that exits dV has a better chance to contribute to whatever you are measuring and so has a higher importance.
In the adjoint equation the streaming is therefore a *gain* term (recall it's a loss in the forward case, so the negative makes it production in the adjoint).
- Scattering term: transposed E' and E , $\hat{\Omega}'$ and $\hat{\Omega}$.
A neutron with energy E and direction $\hat{\Omega}$ has importance $\psi^\dagger(\vec{r}, \hat{\Omega}, E)$.
If it scatters into E' and $\hat{\Omega}'$ it produces neutrons whose importance is $\psi^\dagger(\vec{r}, \hat{\Omega}', E')$.
Thus, the contribution to $\psi^\dagger(\vec{r}, \hat{\Omega}, E)$ from scattering is:

$$\int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' \Sigma_s(\vec{r}, E \rightarrow E', \hat{\Omega} \cdot \hat{\Omega}') \psi^\dagger(\vec{r}, \hat{\Omega}', E')$$

- Boundary condition: $\psi^\dagger(\vec{r}, \hat{\Omega}, E) = 0$, $\hat{n} \cdot \hat{\Omega} > 0$.
Neutrons exiting the problem configuration cannot scatter back and so cannot contribute to the detector inside.

Let's dig more into the the idea of adjoint flux *neutron importance* since it's an impactful one.

What we're going to show is that the angular adjoint flux can represent a map of how every part of phase space will influence the answer we say we are looking for. You can think of it as the reverse of the transport equation

- forward: ψ represents how the source particles go forward and affect the rest of the problem space.
- adjoint: ψ^\dagger represents how the particles from a source come into the solution space and affect the answer.

Let's think about a problem with an external source: $H\psi = q_{ex}$, where ψ meets the boundary conditions. We will just look at the point source this time

$$q_{ex} = \delta(\vec{r} - \vec{r}_0) \delta(E - E_0) \delta(\hat{\Omega} - \hat{\Omega}_0)$$

$$R = \int_V dV \int dE \int_{4\pi} d\hat{\Omega} q_{ex} \psi(\vec{r}_d, \hat{\Omega}, E)$$

Here's how we went through this (last time with a detector response as the adjoint source):

- We'll again set up the adjoint problem but with a different source

$$H^\dagger \psi^\dagger = q_{ex}^\dagger \equiv \delta(\vec{r} - \vec{r}_0) \delta(E - E_0) \delta(\hat{\Omega} - \hat{\Omega}_0)$$

where $\psi^\dagger(\vec{r}_s, \hat{\Omega}, E) = 0$ for \vec{r} on Γ and $\hat{\Omega} \cdot \hat{n} > 0$.

- We multiply the initial equation (forward) by ψ^\dagger and integrate over phase space. We can do the opposite/same to the adjoint equation. This gives

$$\begin{aligned} \langle \psi^\dagger, H\psi \rangle &= \langle \psi^\dagger, q_{ex} \rangle \quad \text{and} \\ \langle \psi, H^\dagger \psi^\dagger \rangle &= \underbrace{\langle \psi, \delta(\vec{r} - \vec{r}_0) \delta(E - E_0) \delta(\hat{\Omega} - \hat{\Omega}_0) \rangle}_R \end{aligned}$$

- We can subtract the two and then apply the adjoint equivalence identity to see

$$\begin{aligned} \langle \psi^\dagger, H\psi \rangle - \langle \psi, H^\dagger \psi^\dagger \rangle &= \langle \psi^\dagger, q_{ex} \rangle - R \\ R &= \langle \psi^\dagger, q_{ex} \rangle \end{aligned}$$

So what does that mean?

It means that the response is the phase-space integral of the adjoint-weighted source distribution.

$$R = \int_V dV \int dE \int_{4\pi} d\hat{\Omega} q_{ex} \psi(\vec{r}_d, \hat{\Omega}, E) = \psi^\dagger(\vec{r}_0, \hat{\Omega}_0, E_0)$$

What does that mean?

The weighting of the adjoint flux directly corresponds to how influential a given source particle will be on the answer we're looking for (what we defined as the adjoint source).

The importance provides the detector response to particles produced at $(\vec{r}_0, \hat{\Omega}_0, E_0)$.

We also talked through how looking at the differences in the equations we can see this as well.