NE 250, F17

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Duderstadt and Hamilton Chp. 5.

** In these notes, ψ is a generic function, the the angular flux **

The last thing we were working on was how to solve the **one-speed** diffusion equation:

$$\frac{1}{v_1}\frac{\partial \phi_1(\vec{r},t)}{\partial t} = S_1(\vec{r},t) - \Sigma_{a,1}(\vec{r})\phi_1(\vec{r},t) + \nabla \cdot [D_1(\vec{r})\nabla\phi_1(\vec{r},t)]$$

We had then looked at steady state and homogeneous to get

$$\nabla^2\phi(\vec{r}) - \frac{1}{L^2}\phi(\vec{r}) = -\frac{S(\vec{r})}{D},$$

The one-group formulation is actually quite useful when thinking through initial design concepts. You can layer together geometry components and see if ideas have any validity at all, and this is something you can do by hand to check computational results.

There are three main ways to solve this. Last time we focused on variation of constants/parameters, which is likely what you learned first in differential equations class. You can get more information in any Diff. Eq. text book, or start at Wikipedia and go from there (`https://en.wikipedia.org/wiki/Variation_of_parameters`).

This class we'll look at **Green's Functions** and the **Eigenfunction Expansion** method. Having multiple tools available can allow you to solve different problems with whichever one is the easiest for that problem. Further, these methods can be used in more sophisticated contexts later on, so it's worth understanding each of them.

Green's Functions

A Green's function is the impulse response of an inhomogeneous linear differential equation defined on a domain, with specified initial conditions or boundary conditions.

Through the superposition principle for linear operator problems, the convolution of a Green's function with an arbitrary function $f(x)$ on that domain is the solution to the inhomogeneous differential equation for $f(x)$. `https://en.wikipedia.org/wiki/Green%27s_function`

To see how this works, we start with two equations. We'll consider a unit source located at $\vec{r'}$. The first equation is the way we're used to seeing it:

$$\begin{aligned} \nabla \cdot D\nabla\phi(\vec{r}) + \Sigma_a\phi(\vec{r}) = -S(\vec{r})\ , \qquad \forall\vec{r} \in V \\ \phi(\vec{r}) = 0\ , \qquad \forall\vec{r} \in \mathcal{S} \equiv \partial V\ . \end{aligned} \tag{1}$$

We will also state that $G(\vec{r}, \vec{r'})$ is the flux at $\vec{r}$ due to a unit source at $\vec{r'}$. Since this is a solution to our problem, we can write:

$$\begin{aligned} \nabla \cdot D\nabla G(\vec{r}, \vec{r'}) + \Sigma_a G(\vec{r}, \vec{r'}) = -\delta(\vec{r} - \vec{r'})\ , \qquad \forall\vec{r} \in V \\ G(\vec{r}, \vec{r'}) = 0\ , \qquad \forall\vec{r} \in \mathcal{S} \equiv \partial V\ . \end{aligned} \tag{2}$$

Now, we'll take the approach of multiplying the LHS of each equation by the opposite solution function, subtracting, and integrating over phase space. This is a common math trick that we'll use again later.

$$\begin{aligned} \int_V dV\ \big[(\nabla \cdot D\nabla\phi(\vec{r}))G(\vec{r}, \vec{r'}) + (\Sigma_a\phi(\vec{r}))G(\vec{r}, \vec{r'}) \\ -(\nabla \cdot D\nabla G(\vec{r}, \vec{r'}))\phi(\vec{r}) - (\Sigma_a G(\vec{r}, \vec{r'}))\phi(\vec{r})\big] = 0 \end{aligned}$$

We can see this by using divergence theorem and the boundary conditions to note:

$$\int_{\mathcal{S}} d\mathcal{S}\ \hat{e}_s \cdot D[\nabla\phi(\vec{r}))G(\vec{r}, \vec{r'}) - \nabla G(\vec{r}, \vec{r'}))\phi(\vec{r})] = 0$$

From there, we can subtract the right hand sides to see:

$$\begin{aligned} \int_V dV\ S(\vec{r})G(\vec{r}, \vec{r'}) - \delta(\vec{r} - \vec{r'})\phi(\vec{r}) = 0 \\ \phi(\vec{r'}) = \int_V dV\ S(\vec{r})G(\vec{r}, \vec{r'}) \\ \text{or}\ \ \phi(\vec{r}) = \int_V dV\ S(\vec{r'})G(\vec{r'}, \vec{r}) \end{aligned}$$

Thus, we have shown that the Green's function is the general solution to the diffusion equation. This is also known as a kernel.

The challenge is: how do we find $G(\vec{r}, \vec{r'})$? We'll use some of the strategies we've already developed. Consider a plane source in an infinite medium:

$$\frac{d^2\phi}{dx^2} - \frac{1}{L^2}\phi(x) = -S(x)\delta(x)$$
$$\lim_{x\to\pm\infty} \phi(x) = 0$$
$$\frac{d^2G(x,x')}{dx^2} - \frac{1}{L^2}G(x,x') = -S(x)\delta(x)$$
$$\lim_{x\to\pm\infty} G(x,x') = 0$$

Now we use variation of constants like we were doing before to get

$$G(x,x') = \frac{L}{2D}H(x-x')\exp[\frac{-|x-x'|}{L}] + \frac{L}{2D}(1-H(x-x'))\exp[\frac{|x-x'|}{L}]$$

Then we substitute this in to get

$$\phi = \int_{-\infty}^{\infty} dx'\, G(x,x')\delta(x')S$$
$$\phi = \frac{SL}{2D}\exp(\frac{-|x|}{L})$$

Eigenfunction Expansion Method

A powerful method for solving boundary value problems is to obtain the solution as an expansion in the set of eigenfunctions.

Eigenvalue Review

Eigenvalues are a special set of scalars associated with a linear system of equations (a matrix equation) that are sometimes also known as characteristic roots.

Each eigenvalue is paired with a corresponding so-called eigenvector.

The decomposition of a square matrix $\mathbf{A}$ into eigenvalues and eigenvectors is known as eigen decomposition, and the fact that **this decomposition is always possible as long as the matrix consisting of the eigenvectors of A is square** is known as the eigen decomposition theorem.

Let $\mathbf{A} \in \mathbb{R}^{n \times n}$. If there is a vector $\vec{x} \in \mathbb{R}^n$ such that

$$\mathbf{A}\vec{x} = \lambda\vec{x}$$

for some scalar λ, then λ is an eigenvalue of $\mathbf{A}$ with a corresponding (right) eigenvector $\vec{x}$. Note that the eigenvalue represents the "stretching factor" in the direction of its associated eigenvector.

(`http://math.stackexchange.com/questions/54176/is-there-a-geometric-meaning-of-the-frobenius-norm`)

We find eigenvalues by re-writing the stated relationship as $(\mathbf{A} - \lambda\mathbf{I})\vec{x} = 0$ and solving for the λs that make this true. The λs are then the eigenvalues and the $\vec{x}$s that go with them are the corresponding eigenvectors.

A linear system of equations has nontrivial solutions iff the determinant vanishes (Cramer's rule; related to the theorem for finding out if a solution exits that we talked about above), so the solutions of this equation are given by

$$\det(\mathbf{A} - \lambda\mathbf{I}) = 0 \ .$$

This equation is known as the characteristic equation of $\mathbf{A}$, and the left-hand side is known as the characteristic polynomial.

Since an n$^{\text{th}}$ degree polynomial has n roots, $\mathbf{A}_{n \times n}$ is guaranteed to have n real and/or complex eigenvalues, some of which may be repeated: $\lambda_1, \lambda_2, \ldots, \lambda_n$.

This gives $\mathbf{A}\vec{u}_1 = \lambda_1\vec{u}_1$, etc.

The spectrum of eigenvalues of a matrix $\mathbf{A}$ are defined formally as

$$\sigma(\mathbf{A}) = [\lambda \in \mathbb{C} : \det(\mathbf{A} - \lambda\mathbf{I}) = 0]$$

and an eigenvalue is

$$\lambda \in \sigma(\mathbf{A}) \ ,$$

We'll start with an example to see how the method works for our problems. We'll look at a similar problem as before:

$$\begin{aligned}
\nabla^2\phi(\vec{r}) - \Sigma_a\phi(\vec{r}) = -\frac{S(\vec{r})}{D}\,, \quad \forall\vec{r}\in V \\
\phi(\vec{r}) \qquad\qquad\qquad\qquad\qquad\qquad\qquad = 0\,, \quad \forall\vec{r}\in\mathcal{S}
\end{aligned}$$

Now, we introduce the eigenfuction expansion, where the subscript n indicates the nth mode:

$$\begin{aligned}
\nabla^2\psi_n(\vec{r}) + B_n^2\psi_n(\vec{r}) = 0\,, \quad \forall\vec{r}\in V \\
\nabla^2\psi_n(\vec{r}) = -B_n^2\psi_n(\vec{r}) \qquad \text{Note: } \mathbf{A} = \nabla^2 \text{ and } \lambda = -B_n^2 \\
\psi_n(\vec{r}) = 0\,, \quad \forall\vec{r}\in\mathcal{S}
\end{aligned}$$

We will use the property that eigenfunctions form a complete set. That is, any function, including our solution, can be expressed as a linear combination of eigenfunctions:

$$\phi(\vec{r}) = \sum_{n=1}^{N} c_n\psi_n\,, \quad \text{where } c_n \text{ are coefficients.}$$

We substitute this, and then our eigenvalue relationship, into the diffusion equation while also expanding the source term:

$$\begin{aligned}
\nabla^2\sum_{n=1}^{N} c_n\psi_n - \Sigma_a\sum_{n=1}^{N} c_n\psi_n = -\frac{-}{D}\sum_{n=1}^{N} S_n\psi_n \\
\sum_{n=1}^{N} c_n(B_n^2+\Sigma_a)\psi_n = -\frac{1}{D}\sum_{n=1}^{N} S_n\psi_n
\end{aligned} \tag{3}$$

Next, we're going to use the orthonormality property of eigenvectors:

$$\int_V dV\ \psi_n\psi_m = \begin{cases} 1 & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases}$$

We will use this to find our c_n by multiplying Equation 3 by ψ_m and integrating over volume:

$$\begin{aligned}\int_V dV \ \sum_{n=1}^{N} c_n(B_n^2+\Sigma_a)\psi_n\psi_m &= -\int_V dV \ \frac{1}{D}\sum_{n=1}^{N} S_n\psi_n\psi_m \\ c_n(B_n^2+\Sigma_a) &= \frac{1}{D}S_n \\ c_n &= \frac{S_n/\Sigma_a}{1+B_n^2L^2}\end{aligned}$$

Noting

$$S_n = \int_V dV \ S(\vec{r})\psi_n$$

We get

$$\phi(\vec{r}) = \int_V dV \ \sum_{n=1}^{N} \frac{S(\vec{r})/\Sigma_a}{1+B_n^2L^2}\psi_n\psi_n$$

—————————————-

Our question now is that are the ψ_n and B_n? We'll look at a real example to figure that out.

$$\begin{aligned}\frac{d^2\phi}{dx^2} - \frac{1}{L^2}\phi(x) &= \frac{-S(x)}{D}\,, \quad -a/2 \le x \le a/2 \\ \phi(\pm\frac{\tilde{a}}{2}) &= 0\end{aligned}$$

We're taking the source to be arbitrary, so we cannot assume symmetry. To solve, we'll take a somewhat roundabout approach to connect our problem to an eigenvalue solution. We'll look at how to solve the similar problem

$$\begin{aligned}\frac{d^2\psi}{dx^2} - B^2\psi(x) &= 0\,, \quad -a/2 \le x \le a/2 \\ \psi(\pm\frac{\tilde{a}}{2}) &= 0\,,\end{aligned}$$

where B^2 is an arbitrary parameter.

We can get the homogeneous solution as a combination of trig functions:

$$\begin{aligned}\psi(x) &= A_1\cos(Bx) + A_2\sin(Bx) \\ \psi(\pm\frac{\tilde{a}}{2}) &= A_1\cos(\frac{B\tilde{a}}{2}) \pm A_2\sin(\frac{B\tilde{a}}{2})\,.\end{aligned}$$

To get a non-trivial solution, we need

$$
\begin{aligned}
c_2 = 0\,, \quad & \cos(\frac{B\tilde{a}}{2}) = 0 \rightarrow \cos(\frac{B\tilde{a}}{2}) = \frac{n\pi}{\tilde{a}} \text{ when } n \text{ is odd} \\
c_1 = 0\,, \quad & \sin(\frac{B\tilde{a}}{2}) = 0 \rightarrow \cos(\frac{B\tilde{a}}{2}) = \frac{n\pi}{\tilde{a}} \text{ when } n \text{ is event} \\
\psi_n(x) = & \begin{cases} A_n \cos(\frac{n\pi x}{\tilde{a}}) & \text{if } n = \text{ odd} \\ A_n \sin(\frac{n\pi x}{\tilde{a}}) & \text{if } n = \text{ even} \end{cases}
\end{aligned}
$$

What we are seeing here is that the eigenvalues are $B_n = \frac{n\pi}{\tilde{a}}$, and the eigenvectors are the ψ_n.

Note that in a symmetric problem, the sin term would drop out b/c it's not symmetric. Further, another term for the eigenvectors or eigenfucntions is *normal modes* or *harmonic modes*.

Also note that the A_n remain undetermined. These are arbitrary, and in a real system would determine the amplitude of the flux shape. What do you think would set A_n in a real system?

What now? Well, we can see clearly that our functions hold the orthogonality property. We can also see that they form a complete set. Thus, we will use our eigenfuctions to create solutions like we did above:

$$
\begin{aligned}
\phi(\vec{r}) &= \sum_{n=1}^{N} c_n \psi_n \\
S(\vec{r}) &= \sum_{n=1}^{N} \phi_n S_n
\end{aligned}
$$

This time our problem has defined boundaries and thus

$$S_n = \frac{2}{\tilde{a}} \int_{-\frac{\tilde{a}}{2}}^{\frac{\tilde{a}}{2}} dx\; S(x)\psi_n$$

To find the c_n we substitute our expansion into our original equation:

$$
\begin{aligned}
\frac{d^2}{dx^2} \sum_{n=1}^{N} c_n \psi_n - \frac{1}{L^2} \sum_{n=1}^{N} c_n \psi_n &= \frac{-1}{D} \sum_{n=1}^{N} \phi_n S_n\,, \\
\sum_{n=1}^{N} c_n \big(B_n + \frac{1}{L^2}\big)\psi_n &= \frac{1}{D} \sum_{n=1}^{N} \phi_n S_n
\end{aligned}
$$

We do our multiply, integrate, orthogonality trick, and we again see

$$c_n = \frac{S_n/\Sigma_a}{1 + B_n^2 L^2}$$

$$\phi(x) = \frac{1}{\Sigma_a} \sum_{n=1}^{N} \frac{s_n}{1 + B_n^2 L^2} \psi_n$$

Only now we know ψ_n and B_n!

Connection to Green's Functions

And finally, we can see this is the same things as Green's Functions. We start by again substitute the source expansion coefficients into the flux:

$$\phi(x) = \int_{-\frac{\tilde{a}}{2}}^{\frac{\tilde{a}}{2}} dx \left[\frac{2}{\tilde{a}\Sigma_a} \sum_{n=1}^{N} \frac{\psi_n(x)\psi_n(x')}{1 + B_n^2 L^2} \right] S(x')$$

If we compare this to how we expect a Green's Function to look

$$\phi_x = \int_{-\frac{\tilde{a}}{2}}^{\frac{\tilde{a}}{2}} dx \, G(x, x') S(x') \, ,$$

we can see that

$$G(x, x') = \frac{2}{\tilde{a}\Sigma_a} \sum_{n=1}^{N} \frac{\psi_n(x)\psi_n(x')}{1 + B_n^2 L^2} \, .$$

This relationship between eigenfunctions and Green's Functions is a general result. The coefficients out front will differ based on the dimensionality of the problem, but the concept always holds.