SELF-ADJOINT DIFFERENTIAL EQUATIONS

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Many ordinary differential equations (ODEs) in physics, especially those in quantum mechanics, have sets of solutions consisting of mutually orthogonal functions. The Hermite polynomials, associated Legendre functions and associated Laguerre polynomials that turn up in systems such as the harmonic oscillator and the hydrogen atom fall into this category.

Here we'll have a look at some of the mathematics behind such ODEs.

We'll begin by considering an ODE of the general form

$$p_0(x)u'' + p_1(x)u' + p_2(x)u + \lambda w(x)u(x) = 0 \tag{1}$$

Here, the p_i functions are known functions of the single variable x, λ is a constant called the *eigenvalue* and $w(x)$ is another function of x known as the *weighting function*, for reasons that we will encounter later. The problem is to find $u(x)$ (and usually along the way, acceptable values for λ) given the other functions.

We will define the linear operator L so that its operation on $u(x)$ is to generate the first three terms in the above equation. That is

$$Lu(x) = p_0(x)u'' + p_1(x)u' + p_2(x)u \tag{2}$$

so we can write the top equation as

$$Lu(x) + \lambda w(x)u(x) = 0 \tag{3}$$

For now we'll concentrate on the $Lu(x)$ term. Suppose we consider two solutions of this equation, which we'll call u and v, and suppose we examine the integral (we suppress explicit dependence on x to simplify the notation):

$$\langle v|Lu \rangle = \int_a^b vLu\,dx \tag{4}$$

$$= \int_a^b v(p_0 u'' + p_1 u' + p_2 u)\,dx \tag{5}$$

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The limits a and b are not specified here, but we will see that they typically have fixed values for certain types of ODE. Now we apply integration by parts on the first two terms of this integral. Considering the first term:

$$\int_a^b v p_0 u'' \, dx = v p_0 u' \Big|_a^b - \int_a^b u'(v p_0)' \, dx \tag{6}$$

$$= v p_0 u' \Big|_a^b - u(v p_0)' \Big|_a^b + \int_a^b u(v p_0)'' \, dx \tag{7}$$

$$= \left[v p_0 u' - u p_0 v' - u p_0' v \right] \Big|_a^b + \int_a^b u(v p_0)'' \, dx \tag{8}$$

Now the second term is

$$\int_a^b v p_1 u' \, dx = v p_1 u \Big|_a^b - \int_a^b u(p_1 v)' \, dx \tag{9}$$

Combining everything we get

$$\langle v | L u \rangle = \left[v p_0 u' - u p_0 v' - u p_0' v + v p_1 u \right] \Big|_a^b + \int_a^b u \left((v p_0)'' - (p_1 v)' + p_2 v \right) dx \tag{10}$$

Now we do something that seems at first to be rather odd: we *require* the initial integral to be equal to the integral term in 10. That is, we are essentially requiring the integrated terms at the start of 10 to be zero. We can get away with this since it turns out in many applications in quantum mechanics these terms *are* zero if we choose the limits of integration correctly. But more on that later. For now, we'll just make this assumption and see where it leads.

Since the two integrals are equal for all functions u and v, their integrands must be equal at every point (this is a theorem which we will accept here). That is

$$v(p_0 u'' + p_1 u' + p_2 u) = u \left((v p_0)'' - (p_1 v)' + p_2 v \right) \tag{11}$$

Expanding the derivatives on the right using the product rule, we get

$$v(p_0 u'' + p_1 u' + p_2 u) = u(v p_0'' + 2v' p_0' + p_0 v'' - v p_1' - v' p_1 + p_2 v) \tag{12}$$

$$= u \left(p_0 v'' + (2p_0' - p_1)v' + (p_0'' - p_1' + p_2)v \right) \tag{13}$$

Now if we further require

$$p_0' = p_1 \tag{14}$$

(which in turn requires $p_0'' = p_1'$), the RHS simplifies and we get

$$v(p_0 u'' + p_1 u' + p_2 u) = u(p_0 v'' + p_1 v' + p_2 v) \tag{15}$$

$$vLu = uLv \tag{16}$$

Operators that satisfy all the conditions here are known as *self-adjoint* operators. Note that the condition 14 also disposes of a couple of the boundary terms in 10, so we now require only that

$$vp_0 u' - up_0 v' \Big|_a^b = 0 \tag{17}$$

Note in particular that in the special case where $u = v$, all the boundary terms are zero without any further assumptions.

A self-adjoint operator can be written in the condensed form

$$Lu = (p_0 u')' + p_2 u \tag{18}$$

Not every ODE is written in terms of a self-adjoint operator, but we can always transform the equation in self-adjoint form, assuming that $p_0 \neq 0$. If we multiply Lu by

$$\frac{1}{p_0} \exp \left[\int^x \frac{p_1(t)}{p_0(t)} dt \right] \tag{19}$$

where the notation in the integral means 'find the indefinite integral and then replace t by x'. Then we get

$$\frac{1}{p_0} \exp \left[\int \frac{p_1(x)}{p_0(x)} dx \right] Lu = \frac{d}{dx} \left\{ \exp \left[\int^x \frac{p_1(t)}{p_0(t)} dt \right] u' \right\} + \frac{p_2}{p_0} u \exp \left[\int^x \frac{p_1(t)}{p_0(t)} dt \right] \tag{20}$$

This works because if we expand the derivative in the curly braces, we get

$$\frac{d}{dx} \left\{ \exp \left[\int^x \frac{p_1(t)}{p_0(t)} dt \right] u' \right\} = \frac{p_1}{p_0} \exp \left[\int^x \frac{p_1(t)}{p_0(t)} dt \right] u' + \exp \left[\int^x \frac{p_1(t)}{p_0(t)} dt \right] u'' \tag{21}$$

The exponential factor then cancels out of all terms, and if we multiply through by p_0, we regain the original expression 2. Since the form of 20 is the same as that of 18, the operator is in self-adjoint form.

As an example, Laguerre's ODE, which arises in the solution of the radial equation for the hydrogen atom, is

$$xu'' + (1 - x)u' + nu = 0 \tag{22}$$

Comparing with 2, we see that

$$p_0 = x \tag{23}$$

$$p_1 = 1 - x \tag{24}$$

This is not in self-adjoint form, since $p_0' \neq p_1$. Using the above method to convert it to self adjoint form means finding

$$\exp\left[\int^x \frac{p_1(t)}{p_0(t)}dt\right] = \exp\left[\int^x \frac{1-t}{t}dt\right] \tag{25}$$

$$= \exp\left[\int^x \left(\frac{1}{t} - 1\right)dt\right] \tag{26}$$

$$= \exp(\ln x - x) \tag{27}$$

$$= xe^{-x} \tag{28}$$

The conversion factor then becomes

$$\frac{1}{p_0}\exp\left[\int^x \frac{p_1(t)}{p_0(t)}dt\right] = \frac{1}{x}(xe^{-x}) \tag{29}$$

$$= e^{-x} \tag{30}$$

and the self-adjoint form is

$$Lu = xe^{-x}u'' + (1-x)e^{-x}u' + ne^{-x}u = 0 \tag{31}$$

and it can be seen that $p_0' = p_1$ since $(xe^{-x})' = (1-x)e^{-x}$.

PINGBACKS

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