CHAPTER 8

STURM-LIOUVILLE THEORY

8.1 INTRODUCTION

Chapter 7 examined methods for solving ordinary differential equations (ODEs), with emphasis on techniques that can generate the solutions. In the present chapter we shift the focus to the general properties that solutions must have to be appropriate for specific physics problems, and to discuss the solutions using the notions of vector spaces and eigenvalue problems that were developed in Chapters 5 and 6.

A typical physics problem controlled by an ODE has two important properties: (1) Its solution must satisfy **boundary conditions**, and (2) It contains a parameter whose value must be set in a way that satisfies the boundary conditions. From a vector-space perspective, the boundary conditions (plus continuity and differentiability requirements) define the Hilbert space of our problem, while the parameter normally occurs in a way that permits the ODE to be written as an eigenvalue equation within that Hilbert space.

These ideas can be made clearer by examining a specific example. The standing waves of a vibrating string clamped at its ends are governed by the ODE

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0, \tag{8.1}$$

where $\psi(x)$ is the amplitude of the transverse displacement at the point x along the string, and k is a parameter. This ODE has solutions for any value of k, but the solutions of relevance to the string problem must have $\psi(x) = 0$ for the values of x at the ends of the string.

The boundary conditions of this problem can be interpreted as defining a Hilbert space whose members are differentiable functions with zeros at the boundary values of x; the ODE itself can be written as the eigenvalue equation

$$\mathcal{L}\psi = k^2\psi, \quad \mathcal{L} = -\frac{d^2}{dx^2}. \tag{8.2}$$

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For practical reasons the eigenvalue is given the name k^2. It is required to find functions $\psi(x)$ that solve Eq. (8.2) subject to the boundary conditions, i.e., to find members $\psi(x)$ of our Hilbert space that solve the eigenvalue equation.

We could now follow the procedures developed in Chapter 5, namely (1) choose a basis for our Hilbert space (a set of functions with zeros at the boundary values of x), (2) define a scalar product for our space, (3) expand $\mathcal{L}$ and ψ in terms of our basis, and (4) solve the resulting matrix equation. However, that procedure makes no use of any specific features of the current ODE, and in particular ignores the fact that it is easily solved.

Instead, we continue with the example defined by Eq. (8.1), using our ability to solve the ODE involved.

Example 8.1.1 STANDING WAVES, VIBRATING STRING

We consider a string clamped at $x = 0$ and $x = l$ and undergoing transverse vibrations. As already indicated, its standing wave amplitudes $\psi(x)$ are solutions of the differential equation

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0, \tag{8.3}$$

where k is not initially known and $\psi(x)$ is subject to the boundary conditions that the ends of the string be fixed in position: $\psi(0) = \psi(l) = 0$. This is the eigenvalue problem defined in Eq. (8.2).

The general solution to this differential equation is $\psi(x) = A\sin kx + B\cos kx$, and in the absence of the boundary conditions solutions would exist for all values of k, A, and B. However, the boundary condition at $x = 0$ requires us to set $B = 0$, leaving $\psi(x) = A\sin kx$. We have yet to satisfy the boundary condition at $x = l$. The fact that A is as yet unspecified is not helpful for this purpose, as $A = 0$ leaves us with only the trivial solution $\psi = 0$. We must, instead, require $\sin kl = 0$, which is accomplished by setting $kl = n\pi$, where n is a nonzero integer, leading to

$$\psi_n(x) = A\sin\left(\frac{n\pi x}{l}\right), \quad k^2 = \frac{n^2\pi^2}{l^2}, \quad n = 1, 2, \ldots. \tag{8.4}$$

Because Eq. (8.3) is homogeneous, it will have solutions of arbitrary scale, so A can have any value. Since our purpose is usually to identify linearly independent solutions, we disregard changes in the sign or magnitude of A. In the vibrating string problem, these quantities control the amplitude and phase of the standing waves. Since changing the sign of n simply changes the sign of ψ, $+n$ and $-n$ in Eq. (8.4) are regarded here as equivalent, so we restricted n to positive values. The first few ψ_n are shown in Fig. 8.1. Note that the number of nodes increases with n: ψ_n has $n + 1$ nodes (including the two nodes at the ends of the string).

The fact that our problem has solutions only for discrete values of k is typical of eigenvalue problems, and in this problem the discreteness in k can be traced directly to the presence of the boundary conditions. Figure 8.2 shows what happens when k is varied in either direction from the acceptable value π/l, with the boundary condition at $x = 0$ maintained for all k. It is obvious that the eigenvalues (here k^2) lie at separated points, and

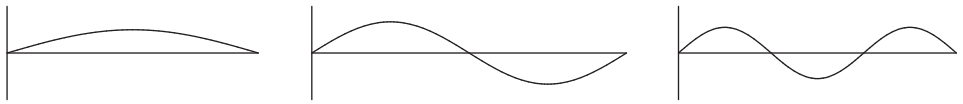

FIGURE 8.1 Standing wave patterns of a vibrating string.

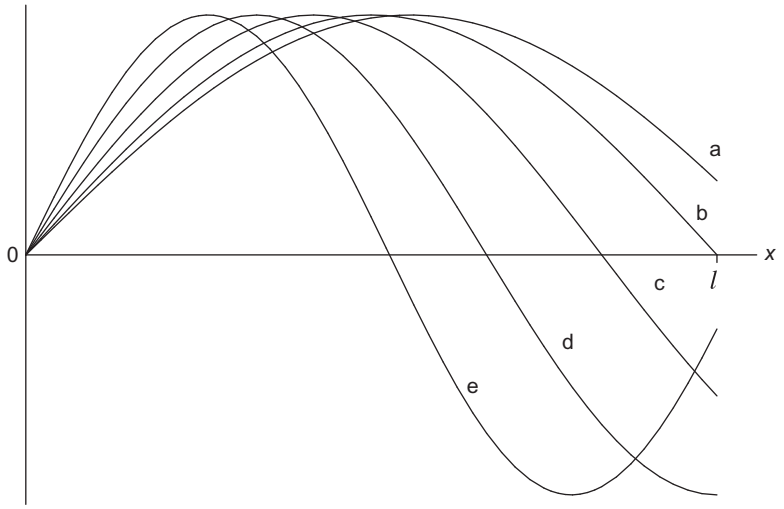

FIGURE 8.2 Solutions to Eq. (8.3) on the range $0 \leq x \leq l$ for: (a) $k = 0.9\pi/l$, (b) $k = \pi/l$, (c) $k = 1.2\pi/l$, (d) $k = 1.5\pi/l$, (e) $k = 1.9\pi/l$.

that the boundary condition at $x = l$ cannot be satisfied for $k < \pi/l$. Moreover, the first acceptable k value larger than π/l is clearly larger than $1.9\pi/l$ (it is actually $2\pi/l$).

As already noted, the solution to this eigenvalue problem is undetermined as to scale because the underlying equation (together with its boundary conditions) is homogeneous. However, if we introduce a scalar product of definition

$$\langle f|g\rangle = \int_0^l f^*(x)g(x)dx, \tag{8.5}$$

we can define solutions that are normalized; requiring $\langle \psi_n|\psi_n\rangle = 1$, we have, with arbitrary sign,

$$\psi_n(x) = \sqrt{\frac{2}{l}}\sin\left(\frac{n\pi x}{l}\right). \tag{8.6}$$

Although we did not solve Eq. (8.2) by an expansion technique, the solutions (the eigenfunctions) will still have properties that depend on whether the operator $\mathcal{L}$ is Hermitian. As we saw in Chapter 5, the Hermitian property depends both on $\mathcal{L}$ and the definition of the scalar product, and a topic for discussion in the present chapter is the identification of conditions making an operator Hermitian. This issue is important because Hermiticity implies real eigenvalues as well as orthogonality and completeness of the eigenfunctions. ■

Summarizing, the matters of interest here, and the subject matter of the current chapter, include:

1. The conditions under which an ODE can be written as an eigenvalue equation with a self-adjoint (Hermitian) operator,
2. Methods for the solution of ODEs subject to boundary conditions, and
3. The properties of the solutions to ODE eigenvalue equations.

8.2 HERMITIAN OPERATORS

Characterization of the general features of eigenproblems arising from second-order differential equations is known as **Sturm-Liouville theory**. It therefore deals with eigenvalue problems of the form

$$\mathcal{L}\psi(x) = \lambda\psi(x), \tag{8.7}$$

where $\mathcal{L}$ is a linear second-order differential operator, of the general form

$$\mathcal{L}(x) = p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x). \tag{8.8}$$

The key matter at issue here is to identify the conditions under which $\mathcal{L}$ is a Hermitian operator.

Self-Adjoint ODEs

$\mathcal{L}$ is known in differential equation theory as **self-adjoint** if

$$p_0'(x) = p_1(x). \tag{8.9}$$

This feature enables $\mathcal{L}(x)$ to be written

$$\mathcal{L}(x) = \frac{d}{dx}\left[p_0(x)\frac{d}{dx}\right] + p_2(x), \tag{8.10}$$

and the operation of $\mathcal{L}$ on a function $u(x)$ then takes the form

$$\mathcal{L}u = (p_0u')' + p_2u. \tag{8.11}$$

Inserting Eq. (8.11) into an integral of the form $\int_a^b v^*(x)\mathcal{L}u(x)dx$, we proceed by applying an integration by parts to the p_0 term (assuming that p_0 is real):

$$\begin{aligned}\int_a^b v^*(x)\mathcal{L}u(x)\,dx &= \int_a^b \left[v^*\left(p_0u'\right)' + v^*p_2u\right]dx \\ &= \left[v^*p_0u'\right]_a^b + \int_a^b \left[-(v^*)'p_0u' + v^*p_2u\right]dx.\end{aligned}$$

Another integration by parts leads to

$$\int_a^b v^*(x)\mathcal{L}u(x)\,dx = \Big[\, v^* p_0 u' - (v^*)' p_0 u \Big]_a^b + \int_a^b \Big[\big[p_0 (v^*)'\big]' u + v^* p_2 u \Big] dx$$

$$= \Big[\, v^* p_0 u' - (v^*)' p_0 u \Big]_a^b + \int_a^b (\mathcal{L}v)^* u\,dx. \tag{8.12}$$

Equation (8.12) shows that, if the boundary terms $\big[\,\cdots\big]_a^b$ vanish and the scalar product is an unweighted integral from a to b, then the operator $\mathcal{L}$ is self-adjoint, as that term was defined for operators. In passing, we observe that the notion of self-adjointness in differential equation theory is weaker than the corresponding concept for operators in our Hilbert spaces, due to the lack of a requirement on the boundary terms. We again stress that the Hilbert-space definition of self-adjoint depends not only on the form of $\mathcal{L}$ but also on the definition of the scalar product and the boundary conditions.

Looking further at the boundary terms, we see that they are surely zero if u and v both vanish at the endpoints $x = a$ and $x = b$ (a case of what are termed **Dirichlet boundary conditions**). The boundary terms are also zero if both u' and v' vanish at a and b (**Neumann boundary conditions**). Even if neither Dirichlet nor Neumann boundary conditions apply, it may happen (particularly in a periodic system, such as a crystal lattice) that the boundary terms vanish because $v^* p_0 u'\big|_a = v^* p_0 u'\big|_b$ for all u and v.

Specializing Eq. (8.12) to the case that u and v are eigenfunctions of $\mathcal{L}$ with respective real eigenvalues λ_u and λ_v, that equation reduces to

$$(\lambda_u - \lambda_v) \int_a^b v^* u\,dx = \Big[\, p_0 (v^* u' - (v^*)' u) \Big]_a^b. \tag{8.13}$$

It is thus apparent that if the boundary terms vanish and $\lambda_u \neq \lambda_v$, then u and v must be orthogonal on the interval (a, b). This is a specific illustration of the orthogonality requirement for eigenfunctions of a Hermitian operator in a Hilbert space.

Making an ODE Self-Adjoint

Some of the differential equations that are important in physics involve operators $\mathcal{L}$ that are self-adjoint in the differential-equation sense, meaning that they satisfy Eq. (8.9); others are not. However, if an operator does not satisfy Eq. (8.9), it is known how to multiply it by a quantity that converts it into self-adjoint form. Letting such a quantity be designated $w(x)$, the Sturm-Liouville eigenvalue problem of Eq. (8.7) becomes

$$w(x)\mathcal{L}(x)\psi(x) = w(x)\lambda\psi(x), \tag{8.14}$$

an equation that has the same eigenvalues λ and eigenfunctions $\psi(x)$ as the original problem in Eq. (8.7). If now $w(x)$ is chosen to be

$$w(x) = p_0^{-1} \exp\left(\int \frac{p_1(x)}{p_0(x)}\,dx \right), \tag{8.15}$$

where p_0 and p_1 are the quantities in $\mathcal{L}$ as given in Eq. (8.8), we can by direct evaluation find that

$$w(x)\mathcal{L}(x) = \overline{p}_0 \frac{d^2}{dx^2} + \overline{p}_1 \frac{d}{dx} + w(x)p_2(x), \tag{8.16}$$

where

$$\overline{p}_0 = \exp\left(\int \frac{p_1(x)}{p_0(x)}\,dx\right), \quad \overline{p}_1 = \frac{p_1}{p_0}\exp\left(\int \frac{p_1(x)}{p_0(x)}\,dx\right). \tag{8.17}$$

It is then straightforward to show that $\overline{p}_0' = \overline{p}_1$, so $w\mathcal{L}$ satisfies the self-adjoint condition.

If we now apply the process represented by Eq. (8.12) to $w\mathcal{L}$, we get

$$\int_a^b v^*(x)w(x)\mathcal{L}u(x)\,dx = \Big[v^*\overline{p}_0 u' - \left(v^*\right)'\overline{p}_0 u\Big]_a^b + \int_a^b w(x)\,(\mathcal{L}v)^*\,u\,dx. \tag{8.18}$$

If the boundary terms vanish, Eq. (8.18) is equivalent to $\langle v|\mathcal{L}|u\rangle = \langle \mathcal{L}v|u\rangle$ when the scalar product is defined to be

$$\langle v|u\rangle = \int_a^b v^*(x)u(x)w(x)\,dx. \tag{8.19}$$

Again considering the case that u and v are eigenfunctions of $\mathcal{L}$, with respective eigenvalues λ_u and λ_v, Eq. (8.18) reduces to

$$(\lambda_u - \lambda_v)\int_a^b v^*u\,w\,dx = \Big[wp_0\left(v^*u' - (v^*)'u\right)\Big]_a^b, \tag{8.20}$$

where p_0 is the coefficient of y'' in the original ODE. We thus see that if the right-hand side of Eq. (8.20) vanishes, then u and v are orthogonal on (a, b) with weight factor w when $\lambda_u \neq \lambda_v$. In other words, our choice of scalar product definition and boundary conditions have made $\mathcal{L}$ a self-adjoint operator in our Hilbert space, thereby producing an eigenfunction orthogonality condition.

Summarizing, we have the useful and important result:

> *If a second-order differential operator $\mathcal{L}$ has coefficients p_0(x) and p_1(x) that satisfy the self-adjoint condition, Eq. (8.9), then it is Hermitian, given (a) a scalar product of uniform weight and (b) boundary conditions that remove the endpoint terms of Eq. (8.12).*
>
> *If Eq. (8.9) is not satisfied, then $\mathcal{L}$ is Hermitian if (a) the scalar product is defined to include the weight factor given in Eq. (8.15), and (b) boundary conditions cause removal of the endpoint terms in Eq. (8.18).*

Note that once the problem has been defined such that $\mathcal{L}$ is Hermitian, then the general properties proved for Hermitian problems apply: the eigenvalues are real; the eigenfunctions are (or if degenerate can be made) orthogonal, **using the relevant scalar product definition**.

Example 8.2.1 LAGUERRE FUNCTIONS

Consider the eigenvalue problem $\mathcal{L}\psi = \lambda\psi$, with

$$\mathcal{L} = x\frac{d^2}{dx^2} + (1-x)\frac{d}{dx}, \tag{8.21}$$

subject to (a) ψ nonsingular on $0 \le x < \infty$, and (b) $\lim_{x\to\infty} \psi(x) = 0$. Condition (a) is simply a requirement that we use the solution of the differential equation that is regular at $x = 0$; and condition (b) is a typical Dirichlet boundary condition.

The operator $\mathcal{L}$ is not self-adjoint, with $p_0 = x$ and $p_1 = 1 - x$. But we can form

$$w(x) = \frac{1}{x}\exp\left(\int \frac{1-x}{x}dx\right) = \frac{1}{x}e^{\ln x - x} = e^{-x}. \tag{8.22}$$

The boundary terms, for arbitrary eigenfunctions u and v, are of the form

$$\Big[xe^{-x}\Big(v^*u' - (v^*)'u\Big)\Big]_0^\infty;$$

their contributions at $x = \infty$ vanish because u and v go to zero; the common factor x causes the $x = 0$ contribution to vanish also. We therefore have a self-adjoint problem, with u and v of different eigenvalues orthogonal under the definition

$$\langle v|u\rangle = \int_0^\infty v^*(x)u(x)e^{-x}dx.$$

The eigenvalue equation of this example is that whose solutions are the Laguerre polynomials; what we have shown here is that they are orthogonal on $(0, \infty)$ with weight e^{-x}. ■

Exercises

8.2.1 Show that Laguerre's ODE, Table 7.1, may be put into self-adjoint form by multiplying by e^{-x} and that $w(x) = e^{-x}$ is the weighting function.

8.2.2 Show that the Hermite ODE, Table 7.1, may be put into self-adjoint form by multiplying by e^{-x^2} and that this gives $w(x) = e^{-x^2}$ as the appropriate weighting function.

8.2.3 Show that the Chebyshev ODE, Table 7.1, may be put into self-adjoint form by multiplying by $(1-x^2)^{-1/2}$ and that this gives $w(x) = (1-x^2)^{-1/2}$ as the appropriate weighting function.

8.2.4 The Legendre, Chebyshev, Hermite, and Laguerre equations, given in Table 7.1, have solutions that are polynomials. Show that ranges of integration that guarantee that the Hermitian operator boundary conditions will be satisfied are

(a) Legendre $[-1, 1]$, (b) Chebyshev $[-1, 1]$,
(c) Hermite $(-\infty, \infty)$, (d) Laguerre $[0, \infty)$.

8.2.5 The functions $u_1(x)$ and $u_2(x)$ are eigenfunctions of the same Hermitian operator but for distinct eigenvalues λ_1 and λ_2. Prove that $u_1(x)$ and $u_2(x)$ are linearly independent.

8.2.6 Given that

$$P_1(x) = x \quad \text{and} \quad Q_0(x) = \frac{1}{2}\ln\left(\frac{1+x}{1-x}\right)$$

are solutions of Legendre's differential equation (Table 7.1) corresponding to different eigenvalues:

(a) Evaluate their orthogonality integral

$$\int_{-1}^{1} \frac{x}{2}\ln\left(\frac{1+x}{1-x}\right) dx.$$

(b) Explain why these two functions are not orthogonal, that is, why the proof of orthogonality does not apply.

8.2.7 $T_0(x) = 1$ and $V_1(x) = (1-x^2)^{1/2}$ are solutions of the Chebyshev differential equation corresponding to different eigenvalues. Explain, in terms of the boundary conditions, why these two functions are not orthogonal on the range $(-1, 1)$ with the weighting function found in Exercise 8.2.3.

8.2.8 A set of functions $u_n(x)$ satisfies the Sturm-Liouville equation

$$\frac{d}{dx}\left[p(x)\frac{d}{dx}u_n(x)\right] + \lambda_n w(x) u_n(x) = 0.$$

The functions $u_m(x)$ and $u_n(x)$ satisfy boundary conditions that lead to orthogonality. The corresponding eigenvalues λ_m and λ_n are distinct. Prove that for appropriate boundary conditions, $u'_m(x)$ and $u'_n(x)$ are orthogonal with $p(x)$ as a weighting function.

8.2.9 Linear operator A has n distinct eigenvalues and n corresponding eigenfunctions: $A\psi_i = \lambda_i \psi_i$. Show that the n eigenfunctions are linearly independent. Do not assume A to be Hermitian.
Hint. Assume linear dependence, i.e., that $\psi_n = \sum_{i=1}^{n-1} a_i \psi_i$. Use this relation and the operator-eigenfunction equation first in one order and then in the reverse order. Show that a contradiction results.

8.2.10 The ultraspherical polynomials $C_n^{(\alpha)}(x)$ are solutions of the differential equation

$$\left\{(1-x^2)\frac{d^2}{dx^2} - (2\alpha+1)x\frac{d}{dx} + n(n+2\alpha)\right\} C_n^{(\alpha)}(x) = 0.$$

(a) Transform this differential equation into self-adjoint form.

(b) Find an interval of integration and weighting factor that make $C_n^{(\alpha)}(x)$ of the same α but different n orthogonal.

Note. Assume that your solutions are polynomials.

8.3 ODE EIGENVALUE PROBLEMS

Now that we have identified the conditions that make a second-order ODE eigenvalue problem Hermitian, let's examine several such problems to gain further understanding of the processes involved and to illustrate techniques for finding solutions.

Example 8.3.1 LEGENDRE EQUATION

The Legendre equation,

$$\mathcal{L}y(x) = -(1-x^2)y''(x) + 2xy'(x) = \lambda y(x), \tag{8.23}$$

defines an eigenvalue problem that arises when ∇^2 is written in spherical polar coordinates, with x identified as $\cos\theta$, where θ is the polar angle of the coordinate system. The range of x in this context is $-1 \le x \le 1$, and in typical circumstances one needs solutions to Eq. (8.23) that are nonsingular on the entire range of x. It turns out that this is a nontrivial requirement, mainly because $x = \pm 1$ are singular points of the Legendre ODE. If we regard nonsingularity of y at $x = \pm 1$ as a set of boundary conditions, we shall find that this requirement is sufficient to define eigenfunctions of the Legendre operator.

This eigenvalue problem, namely Eq. (8.23) plus nonsingularity at $x = \pm 1$, is conveniently handled by the method of Frobenius. We assume solutions of the form

$$y = \sum_{j=0}^{\infty} a_j x^{s+j}, \tag{8.24}$$

with indicial equation $s(s-1) = 0$, whose solutions are $s = 0$ and $s = 1$. For $s = 0$, we obtain the following recurrence relation for the coefficients a_j:

$$a_{j+2} = \frac{j(j+1) - \lambda}{(j+1)(j+2)} a_j. \tag{8.25}$$

We may set $a_1 = 0$, thereby causing all a_j of odd j to vanish, so (for $s = 0$) our series will contain only even powers of x. The boundary condition comes into play because Eq. (8.24) diverges at $x = \pm 1$ for all λ except those that actually cause the series to terminate after a finite number of terms.

To see how the divergence arises, note that for large j and $|x| = 1$ the ratio of successive terms of the series approaches

$$\frac{a_j x^j}{a_{j+2} x^{j+2}} \to \frac{j(j+1)}{(j+1)(j+2)} \to 1,$$

so the ratio test is indeterminate. However, application of the Gauss test shows that this series diverges, as was discussed in more detail in Example 1.1.7.

The series in Eq. (8.24) can be made to terminate after a_l for some even l by choosing $\lambda = l(l+1)$, a value that makes $a_{l+2} = 0$. Then $a_{l+4}, a_{l+6}, \ldots$ will also vanish, and our solution will be a polynomial, which is clearly nonsingular for all $|x| \le 1$. Summarizing, we have, **for even** l, solutions that are polynomials of degree l as eigenfunctions, and the corresponding eigenvalues are $l(l+1)$.

For $s = 1$ we must set $a_1 = 0$ and the recurrence relation is

$$a_{j+2} = \frac{(j+1)(j+2) - \lambda}{(j+2)(j+3)} a_j, \tag{8.26}$$

which also leads to divergence at $|x| = 1$. However, the divergence can now be avoided by setting $\lambda = (l+1)(l+2)$ for some even value of l, thereby causing $a_{l+2}, a_{l+4}, \ldots$ to vanish. The result will be a polynomial of degree $l + s$, i.e., of an odd degree $l + 1$. These solutions can be described equivalently as, for odd l, polynomials of degree l with eigenvalues $\lambda = l(l+1)$, so the overall set of eigenfunctions consists of polynomials of all integer degrees l, with respective eigenvalues $l(l+1)$. When given the conventional scaling, these polynomials are called **Legendre polynomials**. Verification of these properties of solutions to the Legendre equation is left to Exercise 8.3.1.

Before leaving the Legendre equation, note that its ODE is self-adjoint, and that the coefficient of d^2/dx^2 in the Legendre operator is $p_0 = -(1 - x^2)$, which vanishes at $x = \pm 1$. Comparing with Eq. (8.12), we see that this value of p_0 causes the vanishing of the boundary terms when we take the adjoint of $\mathcal{L}$, so the Legendre operator on the range $-1 \le x \le 1$ is Hermitian, and therefore has orthogonal eigenfunctions. In other words, the Legendre polynomials are orthogonal with unit weight on $(-1, 1)$. ■

Let's examine one more ODE that leads to an interesting eigenvalue problem.

Example 8.3.2 HERMITE EQUATION

Consider the Hermite differential equation,

$$\mathcal{L}y = -y'' + 2xy' = \lambda y, \tag{8.27}$$

which we wish to regard as an eigenvalue problem on the range $-\infty < x < \infty$. To make $\mathcal{L}$ Hermitian, we define a scalar product with a weight factor as given by Eq. (8.15),

$$\langle f | g \rangle = \int_{-\infty}^{\infty} f^*(x) g(x) e^{-x^2} \, dx, \tag{8.28}$$

and demand (as a boundary condition) that our eigenfunctions y_n have finite norms using this scalar product, meaning that $\langle y_n | y_n \rangle < \infty$.

Again we obtain a solution by the method of Frobenius, as a series of the form given in Eq. (8.24). Again the indicial equation is $s(s-1) = 0$, and for $s = 0$ we can develop a series of even powers of x with coefficients satisfying the recurrence relation

$$a_{j+2} = \frac{2j - \lambda}{(j+1)(j+2)} a_j. \tag{8.29}$$

This series converges for all x, but (assuming it does not terminate) it behaves asymptotically for large $|x|$ as e^{x^2} and therefore does not describe a function of finite norm, even with the e^{-x^2} weight factor in the scalar product. Thus, even though the series solution always converges, our boundary conditions require that we arrange to terminate the series, thereby producing polynomial solutions. From Eq. (8.29) we see that the condition for obtaining an even polynomial of degree j is that $\lambda = 2j$. Odd polynomial solutions can be obtained

using the indicial equation solution $s = 1$. Details of both the solutions and the asymptotic properties are the subject of Exercise 8.3.3.

Since we have established that this is a Hermitian eigenvalue problem with the scalar product as defined in Eq. (8.28), its solutions (when scaled conventionally they are called **Hermite polynomials**) are orthogonal using that scalar product. ■

Some ODE eigenvalue problems can be attacked by dividing the space in which they reside into regions that are most naturally treated in different ways. The following example illustrates this situation, with a potential that is assumed nonzero only within a finite region.

Example 8.3.3 DEUTERON GROUND STATE

The deuteron is a bound state of a neutron and a proton. Due to the short range of the nuclear force, the deuteron properties do not depend much on the detailed shape of the interaction potential. Thus, this system may be modeled by a spherically symmetric square well potential with the value $V = V_0 < 0$ when the nucleons are within a distance a of each other, but with $V = 0$ when the internucleon distance is greater than a. The Schrödinger equation for the relative motion of the two nucleons assumes the form

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi + V\psi = E\psi,$$

where μ is the reduced mass of the system (approximately half the mass of either particle). This eigenvalue equation must be solved subject to the boundary conditions that ψ be finite at $r = 0$ and approach zero at $r = \infty$ sufficiently rapidly to be a member of an $\mathcal{L}^2$ Hilbert space. The eigenfunctions ψ must also be continuous and differentiable for all r, including $r = a$.

It can be shown that if there is to be a bound state, E will have to have a negative value in the range $V_0 < E < 0$, and the lowest state (the **ground state**) will be described by a wave function ψ that is spherically symmetric (thereby having no angular momentum). Thus, taking $\psi = \psi(r)$ and using a result from Exercise 3.10.34 to write

$$\nabla^2\psi = \frac{1}{r}\frac{d^2u}{dr^2}, \quad \text{with } u(r) = r\psi(r),$$

the Schrödinger equation reduces to an ODE that assumes the form, for $r < a$,

$$\frac{d^2u_1}{dr^2} + k_1^2 u_1 = 0, \quad \text{with} \quad k_1^2 = \frac{2\mu}{\hbar^2}(E - V_0) > 0,$$

while, for $r > a$,

$$\frac{d^2u_2}{dr^2} - k_2^2 u_2 = 0, \quad \text{with} \quad k_2^2 = -\frac{2\mu E}{\hbar^2} > 0.$$

The solutions for these two ranges of r must connect smoothly, meaning that both u and du/dr must be continuous across $r = a$, and therefore must satisfy the **matching conditions** $u_1(a) = u_2(a)$, $u_1'(a) = u_2'(a)$. In addition, the requirement that ψ be finite at $r = 0$ dictates that $u_1(0) = 0$, and the boundary condition at $r = \infty$ requires that $\lim_{r\to\infty} u_2(r) = 0$.

For $r < a$, our Schrödinger equation has the general solution

$$u_1(r) = A \sin k_1 r + C \cos k_1 r,$$

and the boundary condition at $r = 0$ is only met if we set $C = 0$. The Schrödinger equation for $r > a$ has the general solution

$$u_2(r) = C' \exp(k_2 r) + B \exp(-k_2 r), \tag{8.30}$$

and the boundary condition at $r = \infty$ requires us to set $C' = 0$. The matching conditions at $r = a$ then take the form

$$A \sin k_1 a = B \exp(-k_2 a) \quad \text{and} \quad A k_1 \cos k_1 a = -k_2 B \exp(-k_2 a).$$

Using the second of these equations to eliminate $B \exp(-k_2 a)$ from the first, we reach

$$A \sin k_1 a = -A \frac{k_1}{k_2} \cos k_1 a, \tag{8.31}$$

showing that the overall scale of the solution (i.e., A) is arbitrary, which is of course a consequence of the fact that the Schrödinger equation is homogeneous.

Rearranging Eq. (8.31), and inserting values for k_1 and k_2, our matching conditions become

$$\tan k_1 a = -\frac{k_1}{k_2}, \quad \text{or} \quad \tan\left[\frac{2\mu a^2}{\hbar^2}(E - V_0)\right]^{1/2} = -\sqrt{\frac{E - V_0}{-E}}. \tag{8.32}$$

This is an admittedly unpleasant implicit equation for E; if it has solutions with E in the range $V_0 < E < 0$, our model predicts deuteron bound state(s).

One way to search for solutions to Eq. (8.32) is to plot its left- and right-hand sides as a function of E, identifying the E values, if any, for which they are equal. Taking $V_0 = -4.046 \times 10^{-12}$ J, $a = 2.5$ fermi,[1] $\mu = 0.835 \times 10^{-27}$ kg, and $\hbar = 1.05 \times 10^{-34}$ J-s (joule-seconds), the two sides of Eq. (8.32) are plotted in Fig. 8.3 for the range of E in which a bound state is possible. The E values have been plotted in MeV (mega electron volts), the energy unit most frequently used in nuclear physics (1 MeV $\approx 1.6 \times 10^{-13}$ J). The curves cross at only one point, indicating that the model predicts just one bound state. Its energy is at approximately $E = -2.2$ MeV.

It is instructive to see what happens if we take E values that may or may not solve Eq. (8.32), using $u(r) = A \sin k_1 r$ for $r < a$ (thereby satisfying the $r = 0$ boundary condition) but for $r > a$ using the general form of $u(r)$ as given in Eq. (8.30), with the coefficient values B and C' that are required by the matching conditions for the chosen E value. Letting E_- and E_+, respectively, denote values of E less than and greater than the eigenvalue E, we find that by forcing a smooth connection at $r = a$ we lose the required asymptotic behavior except at the eigenvalue. See Fig. 8.4. ■

[1] 1 fermi $= 10^{-15}$ m.

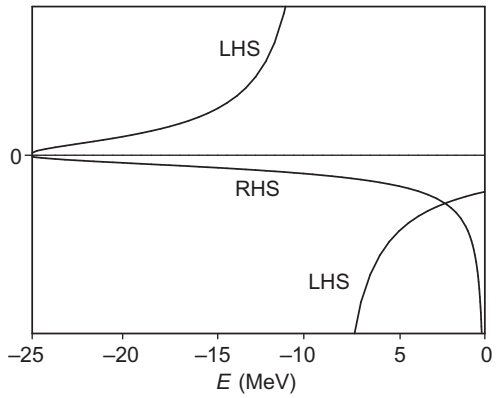

FIGURE 8.3 Left- and right-hand sides of Eq. (8.32) as a function of E for the model parameters given in the text.

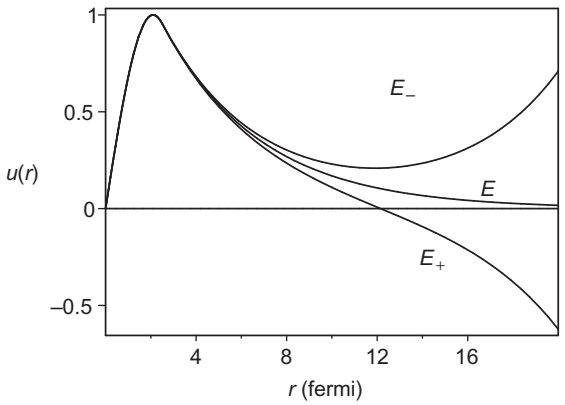

FIGURE 8.4 Wavefunctions for the deuteron problem when the energy is chosen to be less than the eigenvalue E ($E_- < E$) or greater than E ($E_+ > E$).

Exercises

8.3.1 Solve the Legendre equation

$$(1-x^2)y'' - 2xy' + n(n+1)y = 0$$

by direct series substitution.

(a) Verify that the indicial equation is

$$s(s-1) = 0.$$

(b) Using $s = 0$ and setting the coefficient $a_1 = 0$, obtain a series of even powers of x:

$$y_{\text{even}} = a_0\left[1 - \frac{n(n+1)}{2!}x^2 + \frac{(n-2)n(n+1)(n+3)}{4!}x^4 + \cdots\right],$$

where

$$a_{j+2} = \frac{j(j+1) - n(n+1)}{(j+1)(j+2)} a_j.$$

(c) Using $s = 1$ and noting that the coefficient a_1 must be zero, develop a series of odd powers of x:

$$y_{\text{odd}} = a_0 \left[x - \frac{(n-1)(n+2)}{3!} x^3 + \frac{(n-3)(n-1)(n+2)(n+4)}{5!} x^5 + \cdots \right],$$

where

$$a_{j+2} = \frac{(j+1)(j+2) - n(n+1)}{(j+2)(j+3)} a_j.$$

(d) Show that both solutions, y_{even} and y_{odd}, diverge for $x = \pm 1$ **if the series continue to infinity**. (Compare with Exercise 1.2.5.)

(e) Finally, show that by an appropriate choice of n, one series at a time may be converted into a polynomial, thereby avoiding the divergence catastrophe. In quantum mechanics this restriction of n to integral values corresponds to **quantization of angular momentum**.

8.3.2 Show that with the weight factor $\exp(-x^2)$ and the interval $-\infty < x < \infty$ for the scalar product, the Hermite ODE eigenvalue problem is Hermitian.

8.3.3 (a) Develop series solutions for Hermite's differential equation

$$y'' - 2xy' + 2\alpha y = 0.$$

ANS. $s(s-1) = 0$, indicial equation.

For $s = 0$,

$$a_{j+2} = 2a_j \frac{j - \alpha}{(j+1)(j+2)} \quad (j \text{ even}),$$

$$y_{\text{even}} = a_0 \left[1 + \frac{2(-\alpha)x^2}{2!} + \frac{2^2(-\alpha)(2-\alpha)x^4}{4!} + \cdots \right].$$

For $s = 1$,

$$a_{j+2} = 2a_j \frac{j + 1 - \alpha}{(j+2)(j+3)} \quad (j \text{ even}),$$

$$y_{\text{odd}} = a_1 \left[x + \frac{2(1-\alpha)x^3}{3!} + \frac{2^2(1-\alpha)(3-\alpha)x^5}{5!} + \cdots \right].$$

(b) Show that both series solutions are convergent for all x, the ratio of successive coefficients behaving, for a large index, like the corresponding ratio in the expansion of $\exp(x^2)$.

(c) Show that by appropriate choice of α, the series solutions may be cut off and converted to finite polynomials. (These polynomials, properly normalized, become the Hermite polynomials in Section 18.1.)

8.3.4 Laguerre's ODE is

$$xL_n''(x) + (1-x)L_n'(x) + nL_n(x) = 0.$$

Develop a series solution and select the parameter n to make your series a polynomial.

8.3.5 Solve the Chebyshev equation

$$(1-x^2)T_n'' - xT_n' + n^2T_n = 0,$$

by series substitution. What restrictions are imposed on n if you demand that the series solution converge for $x = \pm 1$?

ANS. The infinite series does converge for $x = \pm 1$ and no restriction on n exists (compare with Exercise 1.2.6).

8.3.6 Solve

$$(1-x^2)U_n''(x) - 3xU_n'(x) + n(n+2)U_n(x) = 0,$$

choosing the root of the indicial equation to obtain a series of **odd** powers of x. Since the series will diverge for $x = 1$, choose n to convert it into a polynomial.

8.4 VARIATION METHOD

We saw in Chapter 6 that the expectation value of a Hermitian operator H for the normalized function ψ can be written as

$$\langle H \rangle \equiv \langle \psi | H | \psi \rangle,$$

and that the expansion of this quantity in a basis consisting of the orthonormal eigenfunctions of H had the form given in Eq. (6.30):

$$\langle H \rangle = \sum_\mu |a_\mu|^2 \lambda_\mu,$$

where a_μ is the coefficient of the μth eigenfunction of H and λ_i is the corresponding eigenvalue. As we noted when we obtained this result, one of its consequences is that $\langle H \rangle$ is a weighted average of the eigenvalues of H, and therefore is at least as large as the smallest eigenvalue, and equal to the smallest eigenvalue only if ψ is actually an eigenfunction to which that eigenvalue corresponds.

The observations of the foregoing paragraph hold true even if we do not actually make an expansion of ψ and even if we do not actually know or have available the eigenfunctions or eigenvalues of H. The knowledge that $\langle H \rangle$ is an upper limit to the smallest eigenvalue of H is sufficient to enable us to devise a method for approximating that eigenvalue and the associated eigenfunction. This eigenfunction will be the member of the Hilbert space of our problem that yields the smallest expectation value of H, and a strategy for finding it is to search for the minimum in $\langle H \rangle$ within our Hilbert space. This is the essential idea

behind what is known as the **variation method** for the approximate solution of eigenvalue problems.

Since in many problems (including most that arise in quantum mechanics) it is impractical to compute $\langle H \rangle$ for all members of a Hilbert space, the actual approach is to define a portion of the Hilbert space by introducing an assumed functional form for ψ that contains parameters, and then to minimize $\langle H \rangle$ with respect to the parameters; this is the source of the name "variation method." The success of the method will depend on whether the functional form that is chosen is capable of representing functions that are "close" to the desired eigenfunction (meaning that its coefficient in the expansion is relatively large, with other coefficients much smaller). The great advantage of the variation method is that we do not need to know anything about the exact eigenfunction and we do not actually have to make an expansion; we simply choose a suitable functional form and minimize $\langle H \rangle$.

Since eigenvalue equations for energies and related quantities in quantum mechanics usually have finite smallest eigenvalues (e.g., ground energy levels), the variation method is frequently applicable. We point out that it is not a method having only academic interest; it is at the heart of some of the most powerful methods for solving the Schrödinger eigenvalue equation for complex quantum systems.

Example 8.4.1 VARIATION METHOD

Given a single-electron wave function (in three-dimensional space) of the form

$$\psi = \left(\frac{\zeta^3}{\pi}\right)^{1/2} e^{-\zeta r}, \tag{8.33}$$

where the factor $(\zeta/\pi)^{3/2}$ makes ψ normalized, it can be shown that, in units with the electron mass, its charge, and $\hbar$ (Planck's constant divided by 2π) all set to unity (so-called **Hartree atomic units**), the quantum-mechanical kinetic energy operator has expectation value $\langle \psi | T | \psi \rangle = \zeta^2/2$, and the potential energy of interaction between the electron and a fixed nucleus of charge $+$Z has $\langle \psi | V | \psi \rangle = -Z\zeta$. For a one-electron atom with a nucleus of charge $+Z$ at $r = 0$, the total energy will be less than or equal to the expectation value of the Hamiltonian $H = T + V$, given for the ψ of Eq. (8.33) as

$$\langle H \rangle = \langle T \rangle + \langle V \rangle = \frac{\zeta^2}{2} - Z\zeta. \tag{8.34}$$

As is customary when the meaning is clear, we no longer explicitly show ψ within all the angle brackets. We can now optimize our upper bound to the lowest eigenvalue of H by minimizing the expectation value $\langle H \rangle$ with respect to the parameter ζ in ψ. To do so, we set

$$\frac{d}{d\zeta}\left[\frac{\zeta^2}{2} - Z\zeta\right] = 0,$$

leading to $\zeta - Z = 0$, or $\zeta = Z$. This tells us that the wave function yielding the energy closest to the smallest eigenvalue is that with $\zeta = Z$, and the energy expectation value for this value of ζ is $Z^2/2 - Z^2 = -Z^2/2$.

The result we have just found is exact, because, with malice aforethought and with appropriate knowledge, we chose a functional form that included the exact wave function. But now let us continue to a two-electron atom, taking a wave function of the form $\Psi = \psi(1)\psi(2)$, with both ψ of the same ζ value. For this two-electron atom, the scalar product is defined as integration over the coordinates of both electrons, and the Hamiltonian is now $H = T(1) + T(2) + V(1) + V(2) + U(1,2)$, where $T(i)$ and $V(i)$ denote the kinetic energy and the electron-nuclear potential energy for electron i; $U(1,2)$ is the electron-electron repulsion energy operator, equal in Hartree units to $1/r_{12}$, where r_{12} is the distance between the positions of the two electrons. For the wave function in use here, the electron-electron repulsion has expectation value $\langle U\rangle = 5\zeta/8$ and the expectation value $\langle H\rangle$ (for $Z = 2$, thereby representing the He atom) is

$$\langle H\rangle = \frac{\zeta^2}{2} + \frac{\zeta^2}{2} - Z\zeta - Z\zeta + \frac{5\zeta}{8} = \zeta^2 - \frac{27\zeta}{8}.$$

Minimizing $\langle H\rangle$ with respect to ζ, we obtain the optimum value $\zeta = 27/16$, and for this value of ζ we have $\langle H\rangle = -(27/16)^2 = -2.8477$ hartree. This is the best approximation available using a wave function of the form we chose. It cannot be exact, as the exact solution for this system with two interacting electrons cannot be a product of two one-electron functions. We have therefore not included in our variational search the exact ground-state eigenfunction. A highly precise value of the smallest eigenvalue for this problem can only be obtained numerically, and in fact was produced by using the variation method with a trial function containing thousands of parameters and yielding a result accurate to about 40 decimal places.[2] The value found here by very simple means is higher than the exact value, $-2.9037\cdots$ hartree, by only about 2%, and already conveys much physically relevant information. If the two electrons did not interact, they would each have had an optimum wave function with $\zeta = 2$; the fact that the optimum ζ is somewhat smaller shows that each electron partially screens the nucleus from the other electron.

From the viewpoint of the mathematical method in use here, it is desirable to note that we did not need to assume any relation between the trial wave function and the exact form of the eigenfunction; the variational optimization adjusts the trial function to give an energetically optimum fit. The quality of the final result of course depends on the degree to which the trial function can mimic the actual eigenfunction, and trial functions are ordinarily chosen in a way that balances inherent quality against convenience of use. ■

Exercises

8.4.1 A function that is normalized on the interval $0 \le x < \infty$ with an unweighted scalar product is

$$\psi = 2\alpha^{3/2} x e^{-\alpha x}.$$

(a) Verify the normalization.

(b) Verify that for this ψ, $\langle x^{-1}\rangle = \alpha$.

[2] C. Schwartz, Experiment and theory in computations of the He atom ground state, *Int. J. Mod. Phys. E: Nuclear Physics* **15**: 877 (2006).

(c) Verify that for this ψ, $\langle d^2/dx^2 \rangle = -\alpha^2$.

(d) Use the variation method to find the value of α that minimizes

$$\left\langle \psi \left| -\frac{1}{2}\frac{d^2}{dx^2} - \frac{1}{x} \right| \psi \right\rangle,$$

and find the minimum value of this expectation value.

8.5 SUMMARY, EIGENVALUE PROBLEMS

Because any Hermitian operator on a Hilbert space can be expanded in a basis and is therefore mathematically equivalent to a matrix, all the properties derived for matrix eigenvalue problems automatically apply whether or not a basis-set expansion is actually carried out. It may be helpful to summarize some of those results, along with some that were developed in the present chapter.

1. A second-order differential operator is Hermitian if it is self-adjoint in the differential-equation sense and the functions on which it operates are required to satisfy appropriate boundary conditions. In that event, the scalar product consistent with Hermiticity is an unweighted integral over the range between its boundaries.
2. If a second-order differential operator is not self-adjoint in the differential-equation sense, it will nevertheless be Hermitian if it satisfies appropriate boundary conditions and if the scalar product includes the weight function that makes the original differential equation self-adjoint.
3. A Hermitian operator on a Hilbert space has a complete set of eigenfunctions. Thus, they span the space and can be used as basis for an expansion.
4. The eigenvalues of a Hermitian operator are real.
5. The eigenfunctions of a Hermitian operator corresponding to different eigenvalues are orthogonal, using the appropriate scalar product.
6. Degenerate eigenfunctions of a Hermitian operator can be orthogonalized using the Gram-Schmidt or any other orthogonalization process.
7. Two operators have a common set of eigenfunctions if and only if they commute.
8. An algebraic function of an operator has the same eigenfunctions as the original operator, and its eigenvalues are the corresponding function of the eigenvalues of the original operator.
9. Eigenvalue problems involving a differential operator may be solved either by expressing the problem in any basis and solving the resulting matrix problem or by using relevant properties of the differential equation.
10. The matrix representation of a Hermitian operator can be brought to diagonal form by a unitary transformation. In diagonal form, the diagonal elements are the eigenvalues, and the eigenvectors are the basis functions. The orthonormal eigenvectors are the columns of the unitary matrix U^{-1} when a Hermitian matrix H is transformed to the diagonal matrix UHU^{-1}.

11. Hermitian-operator eigenvalue problems which have a finite smallest eigenvalue may have their solutions approximated by the variation method, which is based on the theorem that for all members of the relevant Hilbert space, the expectation value of the operator will be larger than its smallest eigenvalue (or equal to it only if the Hilbert space member is actually a corresponding eigenfunction).

Additional Readings

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