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## ChAPTER 10

## STURM-LIOUVILLE THEORY - ORTHOGONAL Functions

In the preceding chapter we developed two linearly independent solutions of the secondorder linear homogeneous differential equation and proved that no third, linearly independent solution existed. In this chapter the emphasis shifts from solving the differential equation to developing and understanding general properties of the solutions. There is a close analogy between the concepts in this chapter and those of linear algebra in Chapter 3. Functions here play the role of vectors there, and linear operators that of matrices in Chapter 3. The diagonalization of a real symmetric matrix in Chapter 3 corresponds here to the solution of an ODE defined by a self-adjoint operator $\mathcal{L}$ in terms of its eigenfunctions, which are the "continuous" analog of the eigenvectors in Chapter 3. Examples for the corresponding analogy between Hermitian matrices and Hermitian operators are Hamiltonians in quantum mechanics and their energy eigenfunctions.

In Section 10.1 the concepts of self-adjoint operator, eigenfunction, eigenvalue, and Hermitian operator are presented. The concept of adjoint operator, given first in terms of differential equations, is then redefined in accordance with usage in quantum mechanics, where eigenfunctions take complex values. The vital properties of reality of eigenvalues and orthogonality of eigenfunctions are derived in Section 10.2. In Section 10.3 we discuss the Gram-Schmidt procedure for systematically constructuring sets of orthogonal functions. Finally, the general property of the completeness of a set of eigenfunctions is explored in Section 10.4, and Green's functions from Chapter 9 are continued in Section 10.5.

### 10.1 SELf-AdJOINT ODEs

In Chapter 9 we studied, classified, and solved linear, second-order ODEs corresponding to linear, second-order differential operators of the general form

$$
\begin{equation*}
\mathcal{L} u(x)=p_{0}(x) \frac{d^{2}}{d x^{2}} u(x)+p_{1}(x) \frac{d}{d x} u(x)+p_{2}(x) u(x) . \tag{10.1}
\end{equation*}
$$

The coefficients $p_{0}(x), p_{1}(x)$, and $p_{2}(x)$ are real functions of $x$, and over the region of interest, $a \leq x \leq b$, the first $2-i$ derivatives of $p_{i}(x)$ are continuous. Reference to Eq. (9.118) shows that $P(x)=p_{1}(x) / p_{0}(x)$ and $Q(x)=p_{2}(x) / p_{0}(x)$. Hence, $p_{0}(x)$ must not vanish for $a<x<b$. Now, the zeros of $p_{0}(x)$ are singular points (Section 9.4), and the preceding statement means that our interval $[a, b]$ must be given so that there are no singular points in the interior of the interval. There may be and often are singular points on the boundaries.

For a linear operator $\mathcal{L}$, the analog of a quadratic form for a matrix in Chapter 3 is the integral

$$
\begin{align*}
\langle u| \mathcal{L}|u\rangle & \equiv\langle u \mid \mathcal{L} u\rangle \equiv \int_{a}^{b} u(x) \mathcal{L} u(x) d x \\
& =\int_{a}^{b} u\left\{p_{0} u^{\prime \prime}+p_{1} u^{\prime}+p_{2} u\right\} d x \tag{10.2}
\end{align*}
$$

where the primes on the real function $u(x)$ denote derivatives, as usual, and, for simplicity, $u(x)$ is taken to be real. If we shift the derivatives to the first factor, $u$, in Eq. (10.2) by integrating by parts once or twice, we are led to the equivalent expression,

$$
\begin{align*}
\langle u| \mathcal{L}|u\rangle= & {\left[u(x)\left(p_{1}-p_{0}^{\prime}\right) u(x)\right]_{x=a}^{b} } \\
& +\int_{a}^{b}\left\{\frac{d^{2}}{d x^{2}}\left[p_{0} u\right]-\frac{d}{d x}\left[p_{1} u\right]+p_{2} u\right\} u d x . \tag{10.3}
\end{align*}
$$

If we require that the integrals in Eqs. (10.2) and (10.3) be identical for all (twice differentiable) functions $u$, then the integrands have to be equal. The comparison then yields

$$
u\left(p_{0}^{\prime \prime}-p_{1}^{\prime}\right) u+2 u\left(p_{0}^{\prime}-p_{1}\right) u^{\prime}=0
$$

or

$$
\begin{equation*}
p_{0}^{\prime}(x)=p_{1}(x) \tag{10.4}
\end{equation*}
$$

and, as a bonus, the terms at the boundaries $x=a$ and $x=b$ in Eq. (10.3) then also vanish.
Because of the analogy with the transposed matrix in Chapter 3, it is convenient to define the linear operator in Eq. (10.3),

$$
\begin{align*}
\overline{\mathcal{L}} u & =\frac{d^{2}}{d x^{2}}\left[p_{0} u\right]-\frac{d}{d x}\left[p_{1} u\right]+p_{2} u \\
& =p_{0} \frac{d^{2} u}{d x^{2}}+\left(2 p_{0}^{\prime}-p_{1}\right) \frac{d u}{d x}+\left(p_{0}^{\prime \prime}-p_{1}^{\prime}+p_{2}\right) u \tag{10.5}
\end{align*}
$$

as the adjoint ${ }^{1}$ operator $\overline{\mathcal{L}}$. We have defined the adjoint operator $\overline{\mathcal{L}}$ and have shown that if Eq. (10.4) is satisfied, $\langle\overline{\mathcal{L}} u \mid u\rangle=\langle u \mid \mathcal{L} u\rangle$. Following the same procedure we can show more generally that $\langle v \mid \mathcal{L} u\rangle=\langle\mathcal{L} v \mid u\rangle$. When this condition is satisfied,

$$
\begin{equation*}
\overline{\mathcal{L}} u=\mathcal{L} u=\frac{d}{d x}\left[p(x) \frac{d u(x)}{d x}\right]+q(x) u(x) \tag{10.6}
\end{equation*}
$$

the operator $\mathcal{L}$ is said to be self-adjoint. Here, for the self-adjoint case, $p_{0}(x)$ is replaced by $p(x)$ and $p_{2}(x)$ by $q(x)$ to avoid unnecessary subscripts. The form of Eq. (10.6) allows carrying out two integrations by parts in Eq. (10.3) (and Eq. (10.22) and following) without integrated terms. ${ }^{2}$ Note that a given operator is not inherently self-adjoint; its selfadjointness depends on the properties of the function space in which it acts and on the boundary conditions.

In a survey of the ODEs introduced in Section 9.3, Legendre's equation and the linear oscillator equation are self-adjoint, but others, such as the Laguerre and Hermite equations, are not. However, the theory of linear, second-order, self-adjoint differential equations is perfectly general because we can always transform the non-self-adjoint operator into the required self-adjoint form. Consider Eq. (10.1) with $p_{0}^{\prime} \neq p_{1}$. If we multiply $\mathcal{L}$ by $^{3}$

$$
\frac{1}{p_{0}(x)} \exp \left[\int^{x} \frac{p_{1}(t)}{p_{0}(t)} d t\right]
$$

we obtain

$$
\begin{align*}
\frac{1}{p_{0}(x)} \exp \left[\int^{x} \frac{p_{1}(t)}{p_{0}(t)} d t\right] \mathcal{L} u(x)= & \frac{d}{d x}\left\{\exp \left[\int^{x} \frac{p_{1}(t)}{p_{0}(t)} d t\right] \frac{d u(x)}{d x}\right\} \\
& +\frac{p_{2}(x)}{p_{0}(x)} \cdot \exp \left[\int^{x} \frac{p_{1}(t)}{p_{0}(t)} d t\right] u \tag{10.7}
\end{align*}
$$

which is clearly self-adjoint (see Eq. (10.6)). Notice the $p_{0}(x)$ in the denominator. This is why we require $p_{0}(x) \neq 0, a<x<b$. In the following development we assume that $\mathcal{L}$ has been put into self-adjoint form.
${ }^{1}$ The adjoint operator bears a somewhat forced relationship to the adjoint matrix. A better justification for the nomenclature is found in a comparison of the self-adjoint operator (plus appropriate boundary conditions) with the self-adjoint matrix. The significant properties are developed in Section 10.2. Because of these properties, we are interested in self-adjoint operators.
${ }^{2}$ The full importance of the self-adjoint form (plus boundary conditions) will become apparent in Section 10.2. In addition, self-adjoint forms will be required for developing Green's functions in Section 10.5 .
${ }^{3}$ If we multiply $\mathcal{L}$ by $f(x) / p_{0}(x)$ and then demand that

$$
f^{\prime}(x)=\frac{f p_{1}}{p_{0}},
$$

so that the new operator will be self-adjoint, we obtain

$$
f(x)=\exp \left[\int^{x} \frac{p_{1}(t)}{p_{0}(t)} d t\right] .
$$

## Eigenfunctions, Eigenvalues

Schrödinger's wave equation

$$
H \psi(x)=E \psi(x)
$$

is the major example of an eigenvalue equation in physics; here the differential operator $\mathcal{L}$ is defined by the Hamiltonian $H$ and may no longer be real, and the eigenvalue becomes the total energy $E$ of the system. The eigenfunction $\psi(x)$ may be complex and is usually called a wave function. A variational formulation of this Schrödinger equation appears in Section 17.7. Based on spherical, cylindrical, or some other symmetry properties, a three- or four-dimensional PDE or eigenvalue equation such as the Schrödinger equation may separate into eigenvalue equations in a single variable each. Examples are Eqs. (9.41), (9.42), (9.50), and (9.53). However, sometimes an eigenvalue equation takes the more general self-adjoint form

$$
\begin{equation*}
\mathcal{L} u(x)+\lambda w(x) u(x)=0, \tag{10.8}
\end{equation*}
$$

where the constant $\lambda$ is the eigenvalue ${ }^{4}$ and $w(x)$ is a known weight or density function; $w(x)>0$ except possibly at isolated points at which $w(x)=0$. (In Section 10.1, $w(x) \equiv 1$.) For a given choice of the parameter $\lambda$, a function $u_{\lambda}(x)$, which satisfies Eq. (10.8) and the imposed boundary conditions, is called an eigenfunction corresponding to $\lambda$. The constant $\lambda$ is then called an eigenvalue by mathematicians. There is no guarantee that an eigenfunction $u_{\lambda}(x)$ will exist for an arbitrary choice of the parameter $\lambda$. Indeed, the requirement that there be an eigenfunction often restricts the acceptable values of $\lambda$ to a discrete set. Examples of this for the Legendre, Hermite, and Chebyshev equations appear in the exercises of Section 9.5. Here we have the mathematical approach to the process of quantization in quantum mechanics.

The inner product of two functions, $\langle v \mid u\rangle=\int_{a}^{b} v^{*}(x) w(x) u(x) d x$, depends on the weight function and generalizes our previous definition, where $w(x) \equiv 1$. The weight function also modifies the definition of orthogonality of two eigenfunctions: They are orthogonal if their inner product $\left\langle u_{\lambda^{\prime}} \mid u_{\lambda}\right\rangle=0$. The extra weight function $w(x)$ appears sometimes as an asymptotic wave function $\psi_{\infty}$ that is a common factor in all solutions of a PDE such as the Schrödinger equation, for example, when the potential $V(x) \rightarrow 0$ as $x \rightarrow \infty$ in $H=T+V$. We can find $\psi_{\infty}$ when we set $V=0$ in the Schrödinger equation. Another source for $w(x)$ may be a nonzero angular momentum barrier $l(l+1) / x^{2}$ in a PDE or separated ODE Eq. (9.65) that has a regular singularity and dominates at $x \rightarrow 0$. In such a case the indicial equation, such as Eq. (9.87) or (9.103), shows that the wave function has $x^{l}$ as an overall factor. Since the wave function enters twice in matrix elements and orthogonality relations, the weight functions in Table 10.1 come from these common factors in both radial wave functions. This is how the $\exp (-x)$ for Laguerre polynomials arises and $x^{k} \exp (-x)$ for associated Laguerre polynomials in Table 10.1.

[^0]Table 10.1

| Equation | $p(x)$ | $q(x)$ | $\lambda$ | $w(x)$ |
| :---: | :---: | :---: | :---: | :---: |
| Legendre ${ }^{\text {a }}$ | $1-x^{2}$ | 0 | $l(l+1)$ | 1 |
| Shifted Legendre ${ }^{a}$ | $x(1-x)$ | 0 | $l(l+1)$ | 1 |
| Associated Legendre ${ }^{a}$ | $1-x^{2}$ | $-m^{2} /\left(1-x^{2}\right)$ | $l(l+1)$ | 1 |
| Chebyshev I | $\left(1-x^{2}\right)^{1 / 2}$ | 0 | $n^{2}$ | $\left(1-x^{2}\right)^{-1 / 2}$ |
| Shifted Chebyshev I | $[x(1-x)]^{1 / 2}$ | 0 | $n^{2}$ | $[x(1-x)]^{-1 / 2}$ |
| Chebyshev II | $\left(1-x^{2}\right)^{3 / 2}$ | 0 | $n(n+2)$ | $\left(1-x^{2}\right)^{1 / 2}$ |
| Ultraspherical (Gegenbauer) | $\left(1-x^{2}\right)^{\alpha+1 / 2}$ | 0 | $n(n+2 \alpha)$ | $\left(1-x^{2}\right)^{\alpha-1 / 2}$ |
| Bessel $^{b}, 0 \leq x \leq a$ | $x$ | $-n^{2} / x$ | $a^{2}$ | $x$ |
| Laguerre, $0 \leq x<\infty$ | $x e^{-x}$ | 0 | $\alpha$ | $e^{-x}$ |
| Associated Laguerre ${ }^{c}$ | $x^{k+1} e^{-x}$ | 0 | $\alpha-k$ | $x^{k} e^{-x}$ |
| Hermite, $0 \leq x<\infty$ | $e^{-x^{2}}$ | 0 | $2 \alpha$ | $e^{-x^{2}}$ |
| Simple harmonic oscillator ${ }^{d}$ | 1 | 0 | $n^{2}$ | 1 |

${ }^{a} l=0,1, \ldots,-l \leq m \leq l$ are integers and $-1 \leq x \leq 1,0 \leq x \leq 1$ for shifted Legendre.
${ }^{b}$ Orthogonality of Bessel functions is rather special. Compare Section 11.2. for details. A second type of orthogonality is developed in Eq. (11.174).
${ }^{c} k$ is a non-negative integer. For more details, see Table 10.2.
${ }^{d}$ This will form the basis for Chapter 14, Fourier series.

## Example 10.1.1

Legendre's Equation

Legendre's equation is given by

$$
\begin{equation*}
\left(1-x^{2}\right) u^{\prime \prime}-2 x u^{\prime}+n(n+1) u=0, \quad-1 \leq x \leq 1 \tag{10.9}
\end{equation*}
$$

From Eqs. (10.1), (10.8), and (10.9),

$$
\begin{aligned}
& p_{0}(x)=1-x^{2}=p, \quad w(x)=1, \\
& p_{1}(x)=-2 x=p^{\prime}, \quad \lambda=n(n+1), \\
& p_{2}(x)=0=q .
\end{aligned}
$$

Recall that our series solutions of Legendre's equation (Exercise 9.5.5) ${ }^{5}$ diverged unless $n$ was restricted to one of the integers. This represents a quantization of the eigenvalue $\lambda$.

When the equations of Chapter 9 are transformed into the self-adjoint form, we find the following values of the coefficients and parameters (Table 10.1). The coefficient $p(x)$ is the coefficient of the second derivative of the eigenfunction. The eigenvalue $\lambda$ is the parameter that is available in a term of the form $\lambda w(x) u(x)$; any $x$ dependence apart from the eigenfunction becomes the weighting function $w(x)$. If there is another term containing the eigenfunction (not the derivatives), the coefficient of the eigenfunction in this additional term is identified as $q(x)$. If no such term is present, $q(x)$ is zero.

[^1]
## Example 10.1.2 Deuteron

Further insight into the concepts of eigenfunction and eigenvalue may be provided by an extremely simple model of the deuteron, a bound state of a neutron and proton. From experiment, the binding energy of about $2 \mathrm{MeV} \ll M c^{2}$, with $M=M_{p}=M_{n}$, the common neutron and proton mass whose small mass difference we neglect. 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, the neutron-proton nuclear interaction may be modeled by a spherically symmetric square well potential: $V=V_{0}<0$ for $0 \leq r<a, V=0$ for $r>a$. The Schrödinger wave equation is

$$
\begin{equation*}
-\frac{\hbar^{2}}{M} \nabla^{2} \psi+V \psi=E \psi \tag{10.10}
\end{equation*}
$$

where the energy eigenvalue $E<0$ for a bound state. For the ground state the orbital angular momentum $l=0$ because for $l \neq 0$ there is the additional positive angular momentum barrier. So, with $\psi=\psi(r)$, we may write $u(r)=r \psi(r)$, and, using Exercise 2.5.18, the wave equation becomes

$$
\begin{equation*}
\frac{d^{2} u}{d r^{2}}+k_{1}^{2} u=0 \tag{10.11}
\end{equation*}
$$

with

$$
\begin{equation*}
k_{1}^{2}=\frac{M}{\hbar^{2}}\left(E-V_{0}\right)>0 \tag{10.12}
\end{equation*}
$$

for the interior range, $0 \leq r<a$. For $a<r<\infty$, we have

$$
\begin{equation*}
\frac{d^{2} u}{d r^{2}}-k_{2}^{2} u=0 \tag{10.13}
\end{equation*}
$$

with

$$
\begin{equation*}
k_{2}^{2}=-\frac{M E}{\hbar^{2}}>0 . \tag{10.14}
\end{equation*}
$$

The boundary condition that $\psi$ remain finite at $r=0$ implies $u(0)=0$ and

$$
\begin{equation*}
u_{1}(r)=\sin k_{1} r, \quad 0 \leq r<a . \tag{10.15}
\end{equation*}
$$

In the range outside the potential well, we have a linear combination of the two exponentials,

$$
\begin{equation*}
u_{2}(r)=A \exp k_{2} r+B \exp \left(-k_{2} r\right), \quad a<r<\infty \tag{10.16}
\end{equation*}
$$

Continuity of particle and current density demand that $u_{1}(a)=u_{2}(a)$ and that $u_{1}^{\prime}(a)=$ $u_{2}^{\prime}(a)$. These joining, or matching, conditions give

$$
\begin{align*}
\sin k_{1} a & =A \exp k_{2} a+B \exp \left(-k_{2} a\right),  \tag{10.17}\\
k_{1} \cos k_{1} a & =k_{2} A \exp k_{2} a-k_{2} B \exp \left(-k_{2} a\right) .
\end{align*}
$$

The condition that we actually have a bound proton-neutron combination is that $\int_{0}^{\infty} u^{2}(r) d r=1$. This constraint can be met if we impose a boundary condition that $\psi(r)$


Figure 10.1 A deuteron eigenfunction.
remain finite as $r \rightarrow \infty$. And this, in turn, means that $A=0$. Dividing the preceding pair of equations (to cancel $B$ ), we obtain

$$
\begin{equation*}
\tan k_{1} a=-\frac{k_{1}}{k_{2}}=-\sqrt{\frac{E-V_{0}}{-E}}, \tag{10.18}
\end{equation*}
$$

a transcendental equation for the energy $E$ with only certain discrete solutions. If $E$ is such that Eq. (10.18) can be satisfied, our solutions $u_{1}(r)$ and $u_{2}(r)$ can satisfy the boundary conditions. If Eq. (10.18) is not satisfied, no acceptable solution exists. The values of $E$ for which Eq. (10.18) is satisfied are the eigenvalues; the corresponding functions $u_{1}$ and $u_{2}$ (or $\psi$ ) are the eigenfunctions. For the deuteron, problem there is one (and only one) negative value of $E$ satisfying Eq. (10.18); that is, the deuteron has one and only one bound state.

Now, what happens if $E$ does not satisfy Eq. (10.18), that is, if $E \neq E_{0}$ is not an eigenvalue? In graphical form, imagine that $E$ and therefore $k_{1}$ are varied slightly. For $E=E_{1}<E_{0}, k_{1}$ is reduced and $\sin k_{1} a$ has not turned down enough to match $\exp \left(-k_{2} a\right)$. The joining conditions, Eq. (10.17), require $A>0$ and the wave function goes to $+\infty$ exponentially. For $E=E_{2}>E_{0}, k_{1}$ is larger, $\sin k_{1} a$ peaks sooner and has descended more rapidly at $r=a$. The joining conditions demand $A<0$, and the wave function goes to $-\infty$ exponentially. Only for $E=E_{0}$, an eigenvalue, will the wave function have the required negative exponential asymptotic behavior (see Fig. 10.1).

## Boundary Conditions

In the foregoing definition of eigenfunction, it was noted that the eigenfunction $u_{\lambda}(x)$ was required to satisfy certain imposed boundary conditions. The term boundary conditions includes as a special case the concept of initial conditions. For instance, specifying the initial position $x_{0}$ and the initial velocity $v_{0}$ in some dynamical problem would correspond to the Cauchy boundary conditions. The only difference in the present usage of boundary
conditions in these one-dimensional problems is that we are going to apply the conditions on both ends of the allowed range of the variable.

Usually the form of the differential equation or the boundary conditions on the solutions will guarantee that at the ends of our interval (that is, at the boundary, as suggested by Eq. (10.3)) the following products will vanish:

$$
\begin{equation*}
\left.p(x) v^{*}(x) \frac{d u(x)}{d x}\right|_{x=a}=0 \quad \text { and }\left.\quad p(x) v^{*}(x) \frac{d u(x)}{d x}\right|_{x=b}=0 . \tag{10.19}
\end{equation*}
$$

Here $u(x)$ and $v(x)$ are solutions of the particular ODE (Eq. (10.8)) being considered. A reason for this particular form of Eq. (10.19) is suggested shortly. If we recall the radial wave function $u$ of the hydrogen atom with $u(0)=0$ and $d u / d r \sim e^{-k r} \rightarrow 0$ as $r \rightarrow \infty$, then both boundary conditions are satisfied. Similarly in the deuteron Example 10.1.2, $\sin k_{1} r \rightarrow 0$ as $r \rightarrow 0$ and $d\left(e^{-k_{2} r}\right) / d r \rightarrow 0$ as $r \rightarrow \infty$, both boundary conditions are obeyed. We can, however, work with a somewhat less restrictive set of boundary conditions,

$$
\begin{equation*}
\left.v^{*} p u^{\prime}\right|_{x=a}=\left.v^{*} p u^{\prime}\right|_{x=b} \tag{10.20}
\end{equation*}
$$

in which $u(x)$ and $v(x)$ are solutions of the differential equation corresponding to the same or to different eigenvalues. Equation (10.20) might well be satisfied if we were dealing with a periodic physical system, such as a crystal lattice.

Equations (10.19) and (10.20) are written in terms of $v^{*}$, complex conjugate. When the solutions are real, $v=v^{*}$ and the asterisk may be ignored. However, in Fourier exponential expansions and in quantum mechanics the functions will be complex and the complex conjugate will be needed.

## Example 10.1.3 integration Interval [a, b]

For $\mathcal{L}=d^{2} / d x^{2}$, a possible eigenvalue equation is

$$
\begin{equation*}
\frac{d^{2}}{d x^{2}} u(x)+n^{2} u(x)=0 \tag{10.21}
\end{equation*}
$$

with eigenfunctions

$$
u_{n}=\cos n x, \quad v_{m}=\sin m x
$$

Equation (10.20) becomes

$$
-\left.n \sin m x \sin n x\right|_{a} ^{b}=0, \quad \text { or }\left.\quad m \cos m x \cos n x\right|_{a} ^{b}=0,
$$

interchanging $u_{n}$ and $v_{m}$. Since $\sin m x$ and $\cos n x$ are periodic with period $2 \pi$ (for $n$ and $m$ integral), Eq. (10.20) is clearly satisfied if $a=x_{0}$ and $b=x_{0}+2 \pi$. If a problem prescribes a different interval, the eigenfunctions and eigenvalues will change along with the boundary conditions. The functions must always be chosen so that the boundary conditions (Eq. (10.20) etc.) are satisfied. For this case (Fourier series) the usual choices are $x_{0}=0$ leading to $(0,2 \pi)$ and $x_{0}=-\pi$ leading to $(-\pi, \pi)$. Here and throughout the following several chapters the orthogonality interval is so that the boundary conditions (Eq. (10.20)) will be satisfied. The interval $[a, b]$ and the weighting factor $w(x)$ for the most commonly encountered second-order differential equations are listed in Table 10.2.

Table 10.2

| Equation | $a$ | $b$ | $w(x)$ |
| :--- | ---: | :---: | :---: |
| Legendre | -1 | 1 | 1 |
| Shifted Legendre | 0 | 1 | 1 |
| Associated Legendre | -1 | 1 | 1 |
| Chebyshev I | -1 | 1 | $\left(1-x^{2}\right)^{-1 / 2}$ |
| Shifted Chebyshev I | 0 | 1 | $[x(1-x)]^{-1 / 2}$ |
| Chebyshev II | -1 | 1 | $\left(1-x^{2}\right)^{1 / 2}$ |
| Laguerre | 0 | $\infty$ | $e^{-x}$ |
| Associated Laguerre | 0 | $\infty$ | $x^{k} e^{-x}$ |
| Hermite | $-\infty$ | $\infty$ | $e^{-x^{2}}$ |
| Simple harmonic oscillator | 0 | $2 \pi$ | 1 |
|  | $-\pi$ | $\pi$ | 1 |

1. The orthogonality interval $[a, b]$ is determined by the boundary conditions of Section 10.1.
2. The weighting function is established by putting the ODE in selfadjoint form.

## Hermitian Operators

We now prove an important property of the self-adjoint, second-order differential operator (Eq. (10.8)), in conjunction with solutions $u(x)$ and $v(x)$ that satisfy boundary conditions given by Eq. (10.20). This is motivated by applications in quantum mechanics.

By integrating $v^{*}$ (complex conjugate) times the second-order self-adjoint differential operator $\mathcal{L}$ (operating on $u$ ) over the range $a \leq x \leq b$, we obtain

$$
\begin{equation*}
\int_{a}^{b} v^{*} \mathcal{L} u d x=\int_{a}^{b} v^{*}\left(p u^{\prime}\right)^{\prime} d x+\int_{a}^{b} v^{*} q u d x \tag{10.22}
\end{equation*}
$$

using Eq. (10.6). Integrating by parts, we have

$$
\begin{equation*}
\int_{a}^{b} v^{*}\left(p u^{\prime}\right)^{\prime} d x=\left.v^{*} p u^{\prime}\right|_{a} ^{b}-\int_{a}^{b} v^{* \prime} p u^{\prime} d x \tag{10.23}
\end{equation*}
$$

The integrated part vanishes on application of the boundary conditions (Eq. (10.20)). Integrating the remaining integral by parts a second time, we have

$$
\begin{equation*}
-\int_{a}^{b} v^{* \prime} p u^{\prime} d x=-\left.v^{*^{\prime}} p u\right|_{a} ^{b}+\int_{a}^{b} u\left(p v^{* \prime}\right)^{\prime} d x \tag{10.24}
\end{equation*}
$$

Again, the integrated part vanishes in an application of Eq. (10.20). A combination of Eqs. (10.22) to (10.24) gives us

$$
\begin{equation*}
\int_{a}^{b} v^{*} \mathcal{L} u d x=\int_{a}^{b} u(\mathcal{L} v)^{*} d x \tag{10.25}
\end{equation*}
$$

This property, given by Eq. (10.25), is expressed by saying that the operator $\mathcal{L}$ is Hermitian with respect to the functions $u(x)$ and $v(x)$, which satisfy the boundary conditions specified by Eq. (10.20). Note that if this Hermitian property follows from self-adjointness in a Hilbert space, then it includes that boundary conditions are imposed on all functions of that space.

## Hermitian Operators in Quantum Mechanics

The proceeding development in this section has focused on the classical second-order differential operators of mathematical physics. Generalizing our Hermitian operator theory as required in quantum mechanics, we have an extension: The operators need be neither second-order differential operators nor real. $p_{x}=-i \hbar(\partial / \partial x)$ will be a Hermitian operator. We simply assume (as is customary in quantum mechanics) that the wave functions satisfy appropriate boundary conditions: vanishing sufficiently strongly at infinity or having periodic behavior (as in a crystal lattice, or unit intensity for scattering problems). The operator $\mathcal{L}$ is called Hermitian if

$$
\begin{equation*}
\int \psi_{1}^{*} \mathcal{L} \psi_{2} d \tau=\int\left(\mathcal{L} \psi_{1}\right)^{*} \psi_{2} d \tau \tag{10.26}
\end{equation*}
$$

Apart from the simple extension to complex quantities, this definition is identical with Eq. (10.25).

The adjoint $A^{\dagger}$ of an operator $A$ is defined by

$$
\begin{equation*}
\int \psi_{1}^{*} A^{\dagger} \psi_{2} d \tau \equiv \int\left(A \psi_{1}\right)^{*} \psi_{2} d \tau \tag{10.27}
\end{equation*}
$$

This generalizes our classical, second-derivative-operator-oriented definition, Eq. (10.5). Here the adjoint is defined in terms of the resultant integral, with the $A^{\dagger}$ as part of the integrand. Clearly, if $A=A^{\dagger}$ (self-adjoint) and satisfies the aforementioned boundary conditions, then $A$ is Hermitian.

The expectation value of an operator $\mathcal{L}$ is defined as

$$
\begin{equation*}
\langle\mathcal{L}\rangle=\int \psi^{*} \mathcal{L} \psi d \tau \tag{10.28a}
\end{equation*}
$$

In the framework of quantum mechanics $\langle\mathcal{L}\rangle$ corresponds to the result of a measurement of the physical quantity represented by $\mathcal{L}$ when the physical system is in a state described by the wave function $\psi$. If we require $\mathcal{L}$ to be Hermitian, it is easy to show that $\langle\mathcal{L}\rangle$ is real (as would be expected from a measurement in a physical theory). Taking the complex conjugate of Eq. (10.28a), we obtain

$$
\langle\mathcal{L}\rangle^{*}=\left[\int \psi^{*} \mathcal{L} \psi d \tau\right]^{*}=\int \psi \mathcal{L}^{*} \psi^{*} d \tau
$$

Rearranging the factors in the integrand, we have

$$
\langle\mathcal{L}\rangle^{*}=\int(\mathcal{L} \psi)^{*} \psi d \tau
$$

Then, applying our definition of Hermitian operator, Eq. (10.26), we get

$$
\begin{equation*}
\langle\mathcal{L}\rangle^{*}=\int \psi^{*} \mathcal{L} \psi d \tau=\langle\mathcal{L}\rangle \tag{10.28b}
\end{equation*}
$$

or $\langle\mathcal{L}\rangle$ is real. It is worth noting that $\psi$ is not necessarily an eigenfunction of $\mathcal{L}$.

## Exercises

10.1.1 Show that Laguerre's ODE, Eq. (13.52), may be put into self-adjoint form by multiplying by $e^{-x}$ and that $w(x)=e^{-x}$ is the weighting function.
10.1.2 Show that the Hermite ODE, Eq. (13.10), 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 density function.
10.1.3 Show that the Chebyshev (type I) ODE, Eq. (13.100), may be put into self-adjoint form by multiplying by $\left(1-x^{2}\right)^{-1 / 2}$ and that this gives $w(x)=\left(1-x^{2}\right)^{-1 / 2}$ as the appropriate density function.
10.1.4 Show the following when the linear second-order differential equation is expressed in self-adjoint form:
(a) The Wronskian is equal to a constant divided by the initial coefficient $p$ :

$$
W(x)=\frac{C}{p(x)} .
$$

(b) A second solution is given by

$$
y_{2}(x)=C y_{1}(x) \int^{x} \frac{d t}{p(t)\left[y_{1}(t)\right]^{2}} .
$$

10.1.5 $U_{n}(x)$, the Chebyshev polynomial (type II), satisfies the ODE, Eq. (13.101),

$$
\left(1-x^{2}\right) U_{n}^{\prime \prime}(x)-3 x U_{n}^{\prime}(x)+n(n+2) U_{n}(x)=0
$$

(a) Locate the singular points that appear in the finite plane, and show whether they are regular or irregular.
(b) Put this equation in self-adjoint form.
(c) Identify the complete eigenvalue.
(d) Identify the weighting function.
10.1.6 For the very special case $\lambda=0$ and $q(x)=0$ the self-adjoint eigenvalue equation becomes

$$
\frac{d}{d x}\left[p(x) \frac{d u(x)}{d x}\right]=0
$$

satisfied by

$$
\frac{d u}{d x}=\frac{1}{p(x)}
$$

Use this to obtain a "second" solution of the following:
(a) Legendre's equation,
(b) Laguerre's equation,
(c) Hermite's equation.


These second solutions illustrate the divergent behavior usually found in a second solution.
Note. In all three cases $u_{1}(x)=1$.
10.1.7 Given that $\mathcal{L} u=0$ and $g \mathcal{L} u$ is self-adjoint, show that for the adjoint operator $\overline{\mathcal{L}}, \overline{\mathcal{L}}(g u)=0$.
10.1.8 For a second-order differential operator $\mathcal{L}$ that is self-adjoint show that

$$
\int_{a}^{b}\left[y_{2} \mathcal{L} y_{1}-y_{1} \mathcal{L} y_{2}\right] d x=\left.p\left(y_{1}^{\prime} y_{2}-y_{1} y_{2}^{\prime}\right)\right|_{a} ^{b}
$$

10.1.9 Show that if a function $\psi$ is required to satisfy Laplace's equation in a finite region of space and to satisfy Dirichlet boundary conditions over the entire closed bounding surface, then $\psi$ is unique.
Hint. One of the forms of Green's theorem, Section 1.11, will be helpful.
10.1.10 Consider the solutions of the Legendre, Chebyshev, Hermite, and Laguerre equations to be polynomials. Show that the 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 $[0, \infty)$.
10.1.11 Within the framework of quantum mechanics (Eqs. (10.26) and following), show that the following are Hermitian operators:
(a) momentum $\mathbf{p}=-i \hbar \nabla \equiv-i \frac{h}{2 \pi} \nabla$
(b) angular momentum $\mathbf{L}=-i \hbar \mathbf{r} \times \nabla \equiv-i \frac{h}{2 \pi} \mathbf{r} \times \nabla$.

Hint. In Cartesian form $\mathbf{L}$ is a linear combination of noncommuting Hermitian operators.
10.1.12 (a) $A$ is a non-Hermitian operator. In the sense of Eqs. (10.26) and (10.27), show that

$$
A+A^{\dagger} \quad \text { and } \quad i\left(A-A^{\dagger}\right)
$$

are Hermitian operators.
(b) Using the preceding result, show that every non-Hermitian operator may be written as a linear combination of two Hermitian operators.
10.1.13 $U$ and $V$ are two arbitrary operators, not necessarily Hermitian. In the sense of Eq. (10.27), show that

$$
(U V)^{\dagger}=V^{\dagger} U^{\dagger}
$$

Note the resemblance to Hermitian adjoint matrices.
Hint. Apply the definition of adjoint operator, Eq. (10.27).
10.1.14 Prove that the product of two Hermitian operators is Hermitian (Eq. (10.26)) if and only if the two operators commute.
10.1.15 $A$ and $B$ are noncommuting quantum mechanical operators:

$$
A B-B A=i C .
$$

Show that $C$ is Hermitian. Assume that appropriate boundary conditions are satisfied.
10.1.16 The operator $\mathcal{L}$ is Hermitian. Show that $\left\langle\mathcal{L}^{2}\right\rangle \geq 0$.
10.1.17 A quantum mechanical expectation value is defined by

$$
\langle A\rangle=\int \psi^{*}(x) A \psi(x) d x
$$

where $A$ is a linear operator. Show that demanding that $\langle A\rangle$ be real means that $A$ must be Hermitian - with respect to $\psi(x)$.
10.1.18 From the definition of adjoint, Eq. (10.27), show that $A^{\dagger \dagger}=A$ in the sense that $\int \psi_{1}^{*} A^{\dagger \dagger} \psi_{2} d \tau=\int \psi_{1}^{*} A \psi_{2} d \tau$. The adjoint of the adjoint is the original operator.
Hint. The functions $\psi_{1}$ and $\psi_{2}$ of Eq. (10.27) represent a class of functions. The subscripts 1 and 2 may be interchanged or replaced by other subscripts.
10.1.19 The Schrödinger wave equation for the deuteron (with a Woods-Saxon potential) is

$$
-\frac{\hbar^{2}}{2 M} \nabla^{2} \psi+\frac{V_{0}}{1+\exp \left[\left(r-r_{0}\right) / a\right]} \psi=E \psi .
$$

Here $E=-2.224 \mathrm{MeV}, a$ is a "thickness parameter," $0.4 \times 10^{-13} \mathrm{~cm}$. Expressing lengths in fermis ( $10^{-13} \mathrm{~cm}$ ) and energies in million electron volts ( MeV ), we may rewrite the wave equation as

$$
\frac{d^{2}}{d r^{2}}(r \psi)+\frac{1}{41.47}\left[E-\frac{V_{0}}{1+\exp \left(\left(r-r_{0}\right) / a\right)}\right](r \psi)=0
$$

$E$ is assumed known from experiment. The goal is to find $V_{0}$ for a specified value of $r_{0}$ (say, $r_{0}=2.1$ ). If we let $y(r)=r \psi(r)$, then $y(0)=0$ and we take $y^{\prime}(0)=1$. Find $V_{0}$ such that $y(20.0)=0$. (This should be $y(\infty)$, but $r=20$ is far enough beyond the range of nuclear forces to approximate infinity.)

$$
\text { ANS. For } a=0.4 \text { and } r_{0}=2.1 \mathrm{fm}, V_{0}=-34.159 \mathrm{MeV} \text {. }
$$

10.1.20 Determine the nuclear potential well parameter $V_{0}$ of Exercise 10.1 .19 as a function of $r_{0}$ for $r=2.00(0.05) 2.25$ fermis. Express your results as a power law

$$
\left|V_{0}\right| r_{0}^{v}=k
$$

Determine the exponent $v$ and the constant $k$. This power-law formulation is useful for accurate interpolation.
10.1.21 In Exercise 10.1 .19 it was assumed that 20 fermis was a good approximation to infinity. Check on this by calculating $V_{0}$ for $r \psi(r)=0$ at (a) $r=15$, (b) $r=20$, (c) $r=25$, and (d) $r=30$. Sketch your results. Take $r_{0}=2.10$ and $a=0.4$ (fermis).
10.1.22 For a quantum particle moving in a potential well, $V(x)=\frac{1}{2} m \omega^{2} x^{2}$, the Schrödinger wave equation is

$$
-\frac{\hbar^{2}}{2 m} \frac{d^{2} \psi(x)}{d x^{2}}+\frac{1}{2} m \omega^{2} x^{2} \psi(x)=E \psi(x),
$$

or

$$
\frac{d^{2} \psi(z)}{d z^{2}}-z^{2} \psi(z)=-\frac{2 E}{\hbar \omega} \psi(z)
$$

where $z=(m \omega / \hbar)^{1 / 2} x$. Since this operator is even, we expect solutions of definite parity. For the initial conditions that follow, integrate out from the origin and determine the minimum constant $2 E / \hbar \omega$ that will lead to $\psi(\infty)=0$ in each case. (You may take $z=6$ as an approximation of infinity.)
(a) For an even eigenfunction,

$$
\psi(0)=1, \quad \psi^{\prime}(0)=0 .
$$

(b) For an odd eigenfunction,

$$
\psi(0)=0, \quad \psi^{\prime}(0)=1 .
$$

Note. Analytical solutions appear in Section 13.1.

### 10.2 Hermitian Operators

Hermitian, or self-adjoint, operators with appropriate boundary conditions have three properties that are of extreme importance in physics, both classical and quantum.

1. The eigenvalues of a Hermitian operator are real.
2. A Hermitian operator possesses an orthogonal set of eigenfunctions.
3. The eigenfunctions of a Hermitian operator form a complete set. ${ }^{6}$

## Real Eigenvalues

We proceed to prove the first two of these three properties. Let

$$
\begin{equation*}
\mathcal{L} u_{i}+\lambda_{i} w u_{i}=0 . \tag{10.29}
\end{equation*}
$$

[^2]Assuming the existence of a second eigenvalue and eigenfunction,

$$
\begin{equation*}
\mathcal{L} u_{j}+\lambda_{j} w u_{j}=0 . \tag{10.30}
\end{equation*}
$$

Then, taking the complex conjugate, we obtain

$$
\begin{equation*}
\mathcal{L}^{*} u_{j}^{*}+\lambda_{j}^{*} w u_{j}^{*}=0 . \tag{10.31}
\end{equation*}
$$

Here $w(x) \geq 0$ is a real function. But we permit $\lambda_{k}$, the eigenvalues, and $u_{k}$, the eigenfunctions, to be complex. Multiplying Eq. (10.29) by $u_{j}^{*}$ and Eq. (10.31) by $u_{i}$ and then subtracting, we have

$$
\begin{equation*}
u_{j}^{*} \mathcal{L} u_{i}-u_{i} \mathcal{L}^{*} u_{j}^{*}=\left(\lambda_{j}^{*}-\lambda_{i}\right) w u_{i} u_{j}^{*} . \tag{10.32}
\end{equation*}
$$

We integrate over the range $a \leq x \leq b$ :

$$
\begin{equation*}
\int_{a}^{b} u_{j}^{*} \mathcal{L} u_{i} d x-\int_{a}^{b} u_{i} \mathcal{L}^{*} u_{j}^{*} d x=\left(\lambda_{j}^{*}-\lambda_{i}\right) \int_{a}^{b} u_{i} u_{j}^{*} w d x \tag{10.33}
\end{equation*}
$$

Since $\mathcal{L}$ is Hermitian, the left-hand side vanishes by Eq. (10.26) and

$$
\begin{equation*}
\left(\lambda_{j}^{*}-\lambda_{i}\right) \int_{a}^{b} u_{i} u_{j}^{*} w d x=0 \tag{10.34}
\end{equation*}
$$

If $i=j$, the integral cannot vanish $[w(x)>0$, apart from isolated points], except in the trivial case $u_{i}=0$. Hence the coefficient ( $\lambda_{i}^{*}-\lambda_{i}$ ) must be zero,

$$
\begin{equation*}
\lambda_{i}^{*}=\lambda_{i}, \tag{10.35}
\end{equation*}
$$

which says that the eigenvalue is real. Since $\lambda_{i}$ can represent any one of the eigenvalues, this proves the first property. This is an exact analog of the nature of the eigenvalues of real symmetric (and of Hermitian) matrices (compare Section 3.5).

The analog of the spectral decomposition of a real symmetric matrix in Section 3.5 for a Hermitian operator $\mathcal{L}$ with a discrete set of eigenvalues $\lambda_{i}$ takes the form

$$
\mathcal{L}=\sum_{i} \lambda_{i}\left|u_{i}\right\rangle\left\langle u_{i}\right|, \quad f(\mathcal{L})=\sum_{i} f\left(\lambda_{i}\right)\left|u_{i}\right\rangle\left\langle u_{i}\right|
$$

with eigenvectors $\left|u_{i}\right\rangle$ and any infinitely differentiable function $f$.
Real eigenvalues of Hermitian operators have a fundamental significance in quantum mechanics. In quantum mechanics the eigenvalues correspond to precisely measurable quantities, such as energy and angular momentum. With the theory formulated in terms of Hermitian operators, this proof of real eigenvalues guarantees that the theory will predict real numbers for these measurable physical quantities. In Section 17.8 it will be seen that the set of real eigenvalues has a lower bound (for nonrelativistic problems).

## Orthogonal Eigenfunctions

If we now take $i \neq j$ and if $\lambda_{i} \neq \lambda_{j}$ in Eq. (10.34), the integral of the product of the two different eigenfunctions must vanish:

$$
\begin{equation*}
\int_{a}^{b} u_{i} u_{j}^{*} w d x=0 \tag{10.36}
\end{equation*}
$$

This condition, called orthogonality, is the continuum analog of the vanishing of a scalar product of two vectors. ${ }^{7}$ We say that the eigenfunctions $u_{i}(x)$ and $u_{j}(x)$ are orthogonal with respect to the weighting function $w(x)$ over the interval $[a, b]$. Equation (10.36) constitutes a partial proof of the second property of our Hermitian operators. Again, the precise analogy with matrix analysis should be noted. Indeed, we can establish a one-to-one correspondence between this Sturm-Liouville theory of differential equations and the treatment of Hermitian matrices. Historically, this correspondence has been significant in establishing the mathematical equivalence of matrix mechanics developed by Heisenberg and wave mechanics developed by Schrödinger. Today, the two diverse approaches are merged into the theory of quantum mechanics, and the mathematical formulation that is more convenient for a particular problem is used for that problem. Actually the mathematical alternatives do not end here. Integral equations, Chapter 16, form a third equivalent and sometimes more convenient or more powerful approach.

This proof of orthogonality is not quite complete. There is a loophole, because we may have $u_{i} \neq u_{j}$ but still have $\lambda_{i}=\lambda_{j}$. Such a case is labeled degenerate. Illustrations of degeneracy are given at the end of this section. If $\lambda_{i}=\lambda_{j}$, the integral in Eq. (10.34) need not vanish. This means that linearly independent eigenfunctions corresponding to the same eigenvalue are not automatically orthogonal and that some other method must be sought to obtain an orthogonal set. Although the eigenfunctions in this degenerate case may not be orthogonal, they can always be made orthogonal. One method is developed in the next section. See also Eq. (4.21) for degeneracy due to symmetry.

We shall see in succeeding chapters that it is just as desirable to have a given set of functions orthogonal as it is to have an orthogonal coordinate system. We can work with nonorthogonal functions, but they are likely to prove as messy as an oblique coordinate system.

## Example 10.2.1 Fourier Series - Orthogonalty

To continue Example 10.1.3, the eigenvalue equation, Eq. (10.21),

$$
\frac{d^{2}}{d x^{2}} y(x)+n^{2} y(x)=0
$$

$\overline{{ }^{7} \text { From the definition of Riemann integral, }}$

$$
\int_{a}^{b} f(x) g(x) d x=\lim _{N \rightarrow \infty}\left(\sum_{i=1}^{N} f\left(x_{i}\right) g\left(x_{i}\right) \Delta x\right)
$$

where $x_{0}=a, x_{N}=b$, and $x_{i}-x_{i-1}=\Delta x$. If we interpret $f\left(x_{i}\right)$ and $g\left(x_{i}\right)$ as the $i$ th components of an $N$-component vector, then this sum (and therefore this integral) corresponds directly to a scalar product of vectors, Eq. (1.24). The vanishing of the scalar product is the condition for orthogonality of the vectors - or functions.
may describe a quantum mechanical particle in a box, or perhaps a vibrating violin string, a classical harmonic oscillator with degenerate eigenfunctions - $\cos n x, \sin n x-$ and eigenvalues $n^{2}, n$ an integer.

With $n$ real (here taken to be integral), the orthogonality integrals become
(a) $\int_{x_{0}}^{x_{0}+2 \pi} \sin m x \sin n x d x=C_{n} \delta_{n m}$,
(b) $\int_{x_{0}}^{x_{0}+2 \pi} \cos m x \cos n x d x=D_{n} \delta_{n m}$,
(c) $\int_{x_{0}}^{x_{0}+2 \pi} \sin m x \cos n x d x=0$.

For an interval of $2 \pi$ the preceding analysis guarantees the Kronecker delta in (a) and (b) but not the zero in (c) because (c) may involve degenerate eigenfunctions. However, inspection shows that (c) always vanishes for all integral $m$ and $n$.

Our Sturm-Liouville theory says nothing about the values of $C_{n}$ and $D_{n}$ because homogeneous ODEs have solutions whose scaling is arbitrary. Actual calculation yields

$$
C_{n}=\left\{\begin{array}{ll}
\pi, & n \neq 0, \\
0, & n=0,
\end{array} \quad D_{n}= \begin{cases}\pi, & n \neq 0 \\
2 \pi, & n=0\end{cases}\right.
$$

These orthogonality integrals form the basis of the Fourier series developed in Chapter 14.

## Example 10.2.2 Expansion in Orthogonal Eigenfunctions-Square Wave

The property of completeness (see Eq. (1.190) and Section 10.4) means that certain classes of functions (for example, sectionally or piecewise continuous) may be represented by a series of orthogonal eigenfunctions. Consider the square-wave shape

$$
f(x)= \begin{cases}\frac{h}{2}, & 0<x<\pi  \tag{10.37}\\ -\frac{h}{2}, & -\pi<x<0\end{cases}
$$

This function may be expanded in any of a variety of eigenfunctions - Legendre, Hermite, Chebyshev, and so on. The choice of eigenfunction is made on the basis of convenience or an application. To illustrate the expansion technique, let us choose the eigenfunctions of Example 10.2.1, $\cos n x$ and $\sin n x$.

The eigenfunction series is conveniently (and conventionally) written as

$$
f(x)=\frac{a_{0}}{2}+\sum_{m=1}^{\infty}\left(a_{m} \cos m x+b_{m} \sin m x\right)
$$

Upon multiplying $f(t)$ by $\cos n t$ or $\sin n t$ and integrating, only the $n$th term survives, by the orthogonality integrals of Example 10.2.1, thus yielding the coefficients

$$
a_{n}=\frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \cos n t d t, \quad b_{n}=\frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \sin n t d t, \quad n=0,1,2 \ldots
$$

Direct substitution of $\pm h / 2$ for $f(t)$ yields

$$
a_{n}=0,
$$

which is expected here because of the antisymmetry, $f(-x)=-f(x)$, and

$$
b_{n}=\frac{h}{n \pi}(1-\cos n \pi)= \begin{cases}0, & n \text { even } \\ \frac{2 h}{n \pi}, & n \text { odd }\end{cases}
$$

Hence the eigenfunction (Fourier) expansion of the square wave is

$$
\begin{equation*}
f(x)=\frac{2 h}{\pi} \sum_{n=0}^{\infty} \frac{\sin (2 n+1) x}{2 n+1} \tag{10.38}
\end{equation*}
$$

Additional examples, using other eigenfunctions, appear in Chapters 11 and 12.

## Degeneracy

The concept of degeneracy was introduced earlier. If $N$ linearly independent eigenfunctions correspond to the same eigenvalue, the eigenvalue is said to be $N$-fold degenerate. A particularly simple illustration is provided by the eigenvalues and eigenfunctions of the classical harmonic oscillator equation, Example 10.2.1. For each eigenvalue $n^{2}$, there are two possible solutions: $\sin n x$ and $\cos n x$ (and any linear combination, $n$ an integer). We say the eigenfunctions are degenerate or the eigenvalue is degenerate.

A more involved example is furnished by the physical system of an electron in an atom (nonrelativistic treatment, spin neglected). From the Schrödinger equation, Eq. (13.84) for hydrogen, the total energy of the electron is our eigenvalue. We may label it $E_{n L M}$ by using the quantum numbers $n, L$, and $M$ as subscripts. For each distinct set of quantum numbers ( $n, L, M$ ) there is a distinct, linearly independent eigenfunction $\psi_{n L M}(r, \theta, \varphi)$. For hydrogen, the energy $E_{n L M}$ is independent of $L$ and $M$, reflecting the spherical (and $\mathrm{SO}(4)$ ) symmetry of the Coulomb potential. With $0 \leq L \leq n-1$ and $-L \leq M \leq L$, the eigenvalue is $n^{2}$-fold degenerate (including the electron spin would raise this to $2 n^{2}$ ). In atoms with more than one electron, the electrostatic potential is no longer a simple $r^{-1}$ potential. The energy depends on $L$ as well as on $n$, although not on $M ; E_{n L M}$ is still $(2 L+1)$-fold degenerate. This degeneracy - due to rotational invariance of the potential - may be removed by applying an external magnetic field, breaking spherical symmetry and giving rise to the Zeeman effect. As a rule, the eigenfunctions form a Hilbert space, that is, a complete vector space of functions with a metric defined by the inner product (see Section 10.4 for more details and examples).

Often an underlying symmetry, such as rotational invariance, is causing the degeneracies. States belonging to the same energy eigenvalue then will form a multiplet or representation of the symmetry group. The powerful group-theoretical methods are treated in Chapter 4 in some detail.

## Exercises

10.2.1 The functions $u_{1}(x)$ and $u_{2}(x)$ are eigenfunctions of the same Hermitian operator but for distinct eigenvalues $\lambda_{1}$ and $\lambda_{2}$. Prove that $u_{1}(x)$ and $u_{2}(x)$ are linearly independent.
10.2.2 (a) The vectors $\mathbf{e}_{n}$ are orthogonal to each other: $\mathbf{e}_{n} \cdot \mathbf{e}_{m}=0$ for $n \neq m$. Show that they are linearly independent.
(b) The functions $\psi_{n}(x)$ are orthogonal to each other over the interval $[a, b]$ and with respect to the weighting function $w(x)$. Show that the $\psi_{n}(x)$ are linearly independent.
10.2.3 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 corresponding to different eigenvalues:
(a) Evaluate their orthogonality integral

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

(b) Explain why these two functions are not orthogonal, that is, why the proof of orthogonality does not apply.
10.2.4 $T_{0}(x)=1$ and $V_{1}(x)=\left(1-x^{2}\right)^{1 / 2}$ 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.
10.2.5 (a) Show that the first derivatives of the Legendre polynomials satisfy a self-adjoint differential equation with eigenvalue $\lambda=n(n+1)-2$.
(b) Show that these Legendre polynomial derivatives satisfy an orthogonality relation

$$
\int_{-1}^{1} P_{m}^{\prime}(x) P_{n}^{\prime}(x)\left(1-x^{2}\right) d x=0, \quad m \neq n
$$

Note. In Section 12.5, $\left(1-x^{2}\right)^{1 / 2} P_{n}^{\prime}(x)$ will be labeled an associated Legendre polynomial, $P_{n}^{1}(x)$.
10.2.6 A set of functions $u_{n}(x)$ satisfies the Sturm-Liouville equation

$$
\frac{d}{d x}\left[p(x) \frac{d}{d x} u_{n}(x)\right]+\lambda_{n} w(x) u_{n}(x)=0 .
$$

The functions $u_{m}(x)$ and $u_{n}(x)$ satisfy boundary conditions that lead to orthogonality. The corresponding eigenvalues $\lambda_{m}$ and $\lambda_{n}$ are distinct. Prove that for appropriate boundary conditions, $u_{m}^{\prime}(x)$ and $u_{n}^{\prime}(x)$ are orthogonal with $p(x)$ as a weighting function.
10.2.7 A 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. $A$ is not necessarily Hermitian.
Hint. Assume linear dependence - 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.
10.2.8 (a) Show that the Liouville substitution

$$
u(x)=v(\xi)[p(x) w(x)]^{-1 / 4}, \quad \xi=\int_{a}^{x}\left[\frac{w(t)}{p(t)}\right]^{1 / 2} d t
$$

transforms

$$
\frac{d}{d x}\left[p(x) \frac{d}{d x} u\right]+[\lambda w(x)-q(x)] u(x)=0
$$

into

$$
\frac{d^{2} v}{d \xi^{2}}+[\lambda-Q(\xi)] v(\xi)=0
$$

where

$$
Q(\xi)=\frac{q(x(\xi))}{w(x(\xi))}+[p(x(\xi)) w(x(\xi))]^{-1 / 4} \frac{d^{2}}{d \xi^{2}}(p w)^{1 / 4}
$$

(b) If $v_{1}(\xi)$ and $v_{2}(\xi)$ are obtained from $u_{1}(x)$ and $u_{2}(x)$, respectively, by a Liouville substitution, show that $\int_{a}^{b} w(x) u_{1} u_{2} d x$ is transformed into $\int_{0}^{c} v_{1}(\xi) v_{2}(\xi) d \xi$ with $c=\int_{a}^{b}\left[\frac{w}{p}\right]^{1 / 2} d x$.
10.2.9 The ultraspherical polynomials $C_{n}^{(\alpha)}(x)$ are solutions of the differential equation

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

(a) Transform this differential equation into self-adjoint form.
(b) Show that the $C_{n}^{(\alpha)}(x)$ are orthogonal for different $n$. Specify the interval of integration and the weighting factor.

Note. Assume that your solutions are polynomials.
10.2.10 With $\mathcal{L}$ not self-adjoint,

$$
\mathcal{L} u_{i}+\lambda_{i} w u_{i}=0
$$

and

$$
\overline{\mathcal{L}} v_{j}+\lambda_{j} w v_{j}=0 .
$$


[^0]:    ${ }^{4}$ Note that this mathematical definition of the eigenvalue differs by a sign from the usage in physics.

[^1]:    $\overline{{ }^{5}}$ Compare also Exercise 5.2.15 and 12.10.

[^2]:    ${ }^{6}$ This third property is not universal. It does hold for our linear, second-order differential operators in Sturm-Liouville (selfadjoint) form. Completeness is defined and discussed in Section 10.4. A proof that the eigenfunctions of our linear, second-order, self-adjoint, differential equations form a complete set may be developed from the calculus of variations of Section 17.8.

