9.7 NONHOMOGENEOUS EQUATION—GREEN'S FUNCTION

In this section we turn to a different method of solution— Green's function method, as applied to the solution of a nonhomogeneous PDE

For the second-order, linear, but nonhomogeneous differential

equation ,

$$\mathcal{L}y(\mathbf{r}_1) = -f(\mathbf{r}_1)$$

Then the particular solution ***y(r1) becomes***

$$y(\mathbf{r}_1) = \int G(\mathbf{r}_1, \mathbf{r}_2) f(\mathbf{r}_2)\, d\tau_2$$

The Green's function

$$G(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{4\pi |\mathbf{r}_1 - \mathbf{r}_2|}$$

is taken to be a solution of

$$\mathcal{L}G(\mathbf{r}_1, \mathbf{r}_2) = -\delta(\mathbf{r}_1 - \mathbf{r}_2).$$

Symmetry of Green's Function

An important property of Green's function is the symmetry of its two variables;

$$G(r1, r2) = G(r2, r1)$$

Provided that $G(r, r1)$ ***satisfy self adjoint differential equations with general form***

$$\nabla \cdot \left[p(\mathbf{r}) \nabla G(\mathbf{r}, \mathbf{r}_1) \right] + \lambda q(\mathbf{r}) G(\mathbf{r}, \mathbf{r}_1) = -\delta(\mathbf{r} - \mathbf{r}_1)$$

Form of Green's Functions

assume that *L is a self-adjoint differential operator of the general form*

$$\mathcal{L}_1 = \nabla_1 \cdot \left[p(\mathbf{r}_1)\nabla_1\right] + q(\mathbf{r}_1)$$

Table 9.5 Green's Functions[a] , $\rho = (x^2 + y^2)^{1/2}$

	Laplace ∇^2	Helmholtz $\nabla^2 + k^2$	Modified Helmholtz $\nabla^2 - k^2$
One-dimensional space	No solution for $(-\infty, \infty)$	$\frac{i}{2k}\exp(ik\lvert x_1 - x_2\rvert)$	$\frac{1}{2k}\exp(-k\lvert x_1 - x_2\rvert)$
Two-dimensional space	$-\frac{1}{2\pi}\ln\lvert\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2\rvert$	$\frac{i}{4}H_0^{(1)}(k\lvert\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2\rvert)$	$\frac{1}{2\pi}K_0(k\lvert\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2\rvert)$
Three-dimensional space	$\frac{1}{4\pi}\cdot\frac{1}{\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert}$	$\frac{\exp(ik\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert)}{4\pi\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert}$	$\frac{\exp(-k\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert)}{4\pi\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert}$

[a] These are the Green's functions satisfying the boundary condition $G(\mathbf{r}_1, \mathbf{r}_2) = 0$ as $\mathbf{r}_1 \to \infty$ for the Laplace and modified Helmholtz operators. For the Helmholtz operator, $G(\mathbf{r}_1, \mathbf{r}_2)$ corresponds to an outgoing wave. $H_0^{(1)}$ is the Hankel function of Section 11.4. K_0 is he modified Bessel function of Section 11.5.

Spherical Polar Coordinate Expansion

As an alternate determination of the Green's function of the Laplace operator

$$G(\mathbf{r}_1, \mathbf{r}_2) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{1}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_l^m(\theta_1, \varphi_1) Y_l^{m*}(\theta_2, \varphi_2).$$

or

$$\frac{1}{4\pi} \cdot \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{1}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_l^m(\theta_1, \varphi_1) Y_l^{m*}(\theta_2, \varphi_2).$$

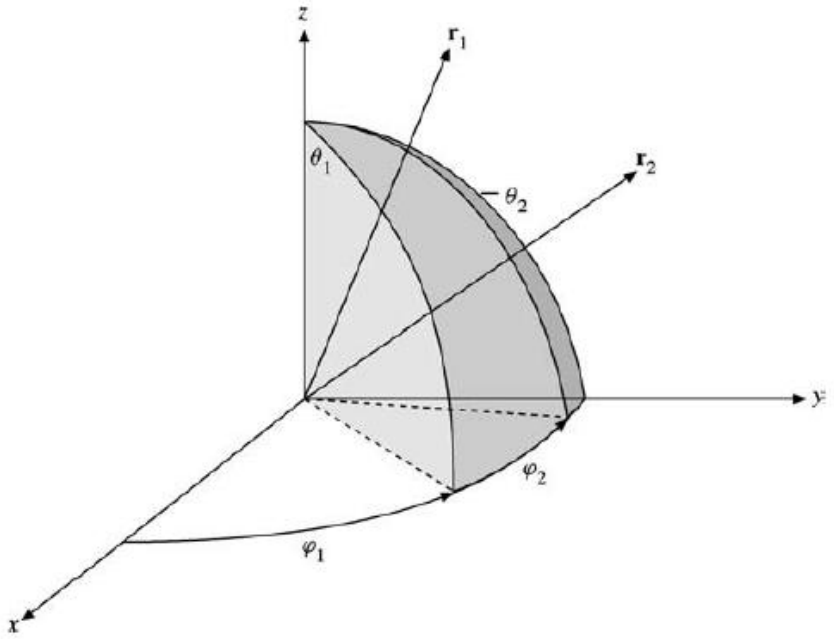
From the generating expression for Legendre polynomials

From the generating expression for Legendre polynomials

$$\frac{1}{4\pi}\cdot\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}=\frac{1}{4\pi}\sum_{l=0}^{\infty}\frac{r_<^l}{r_>^{l+1}}P_l(\cos\gamma),$$

where *γ is the angle included between vectors* ***r1 and r2,***

$$P_l(\cos\gamma)=\frac{4\pi}{2l+1}\sum_{m=-l}^{l}Y_l^m(\theta_1,\varphi_1)Y_l^{m*}(\theta_2,\varphi_2).$$



Spherical polar coordinates.

Example 9.7.1 QUANTUM MECHANICAL SCATTERING — NEUMANN SERIES SOLUTION

The quantum theory of scattering provides a nice illustration of integral equation techniques and an application of a Green's function. Our physical picture of scattering is as follows. A beam of particles moves along the negative z-axis toward the origin. A small fraction of the particles is scattered by the potential $V(\mathbf{r})$ and goes off as an outgoing spherical wave. Our wave function $\psi(\mathbf{r})$ must satisfy the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{9.198a}$$

or

$$\nabla^2\psi(\mathbf{r}) + k^2\psi(\mathbf{r}) = -\left[-\frac{2m}{\hbar^2}V(\mathbf{r})\psi(\mathbf{r})\right], \qquad k^2 = \frac{2mE}{\hbar^2}. \tag{9.198b}$$

From the physical picture just presented we look for a solution having an **asymptotic** form

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k}_0\cdot\mathbf{r}} + f_k(\theta,\varphi)\frac{e^{ikr}}{r}. \tag{9.199}$$

Here $e^{i\mathbf{k}_0\cdot\mathbf{r}}$ is the incident plane wave[28] with $\mathbf{k}_0$ the propagation vector carrying the subscript 0 to indicate that it is in the $\theta = 0$ (z-axis) direction. The magnitudes k_0 and k are equal (ignoring recoil), and e^{ikr}/r is the outgoing spherical wave with an angular (and energy) dependent amplitude factor $f_k(\theta,\varphi)$.[29] Vector $\mathbf{k}$ has the direction of the outgoing scattered wave. In quantum mechanics texts it is shown that the differential probability of scattering, $d\sigma/d\Omega$, the scattering cross section per unit solid angle, is given by $|f_k(\theta,\varphi|^2$.

Identifying $[-(2m/\hbar^2)V(\mathbf{r})\psi(\mathbf{r})]$ with $f(\mathbf{r})$ of Eq. (9.158), we have

$$\psi(\mathbf{r}_1) = -\int \frac{2m}{\hbar^2}V(\mathbf{r}_2)\psi(\mathbf{r}_2)G(\mathbf{r}_1,\mathbf{r}_2)\,d^3r_2 \tag{9.200}$$

by Eq. (9.170). This does not have the desired asymptotic form of Eq. (9.199), but we may add to Eq. (9.200) $e^{i\mathbf{k}_0\cdot\mathbf{r}_1}$, a solution of the homogeneous equation, and put $\psi(\mathbf{r})$ into the desired form:

$$\psi(\mathbf{r}_1) = e^{i\mathbf{k}_0\cdot\mathbf{r}_1} - \int \frac{2m}{\hbar^2} V(\mathbf{r}_2)\psi(\mathbf{r}_2)G(\mathbf{r}_1,\mathbf{r}_2)\,d^3r_2. \tag{9.201}$$

Our Green's function is the Green's function of the operator $\mathcal{L} = \nabla^2 + k^2$ (Eq. (9.198)), satisfying the boundary condition that it describe an outgoing wave. Then, from Table 9.5, $G(\mathbf{r}_1,\mathbf{r}_2) = \exp(ik|\mathbf{r}_1-\mathbf{r}_2|)/(4\pi|\mathbf{r}_1-\mathbf{r}_2|)$ and

$$\psi(\mathbf{r}_1) = e^{i\mathbf{k}_0\cdot\mathbf{r}_1} - \int \frac{2m}{\hbar^2} V(\mathbf{r}_2)\psi(\mathbf{r}_2)\frac{e^{ik|\mathbf{r}_1-\mathbf{r}_2|}}{4\pi|\mathbf{r}_1-\mathbf{r}_2|}d^3r_2. \tag{9.202}$$

This integral equation analog of the original Schrödinger wave equation is **exact**. Employing the Neumann series technique of Section 16.3 (remember, the scattering probability is very small), we have

$$\psi_0(\mathbf{r}_1) = e^{i\mathbf{k}_0\cdot\mathbf{r}_1}, \tag{9.203a}$$

which has the physical interpretation of no scattering.

Substituting $\psi_0(\mathbf{r}_2) = e^{i\mathbf{k}_0\cdot\mathbf{r}_2}$ into the integral, we obtain the first correction term,

$$\psi_1(\mathbf{r}_1) = e^{i\mathbf{k}_0\cdot\mathbf{r}_1} - \int \frac{2m}{\hbar^2} V(\mathbf{r}_2)\frac{e^{ik|\mathbf{r}_1-\mathbf{r}_2|}}{4\pi|\mathbf{r}_1-\mathbf{r}_2|}e^{i\mathbf{k}_0\cdot\mathbf{r}_2}\,d^3r_2. \tag{9.203b}$$

This is the famous **Born approximation**. It is expected to be most accurate for weak potentials and high incident energy. If a more accurate approximation is desired, the Neumann series may be continued.[30] ■

CHAPTER 10
STURM–LIOUVILLE THEORY—ORTHOGONAL FUNCTIONS

•In the preceding chapter we developed two linearly independent solutions of the second order linear homogeneous differential equation

•In this chapter the emphasis shifts 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. Functions here play the role of vectors , and linear operators that of matrices in linear algebra .

10.1 SELF-ADJOINT ODES

If we define a linear, second-order differential operators of the general form

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

$P(x) = p_1(x)/p_0(x)$ and $Q(x) = p_2(x)/p_0(x)$. Hence, $p_0(x)$ must not vanish for *$a < x < b$.* Also if we define the linear operator as the **adjoint operator**

$$\bar{\mathcal{L}}u = \frac{d^2}{dx^2}[p_0 u] - \frac{d}{dx}[p_1 u] + p_2 u$$

When this condition is satisfied, (*$p'_0(x) = p_1(x)$,)*the operator *L is said to be* ***self-adjoint.***

$$\bar{\mathcal{L}}u = \mathcal{L}u = \frac{d}{dx}\left[p(x)\frac{du(x)}{dx}\right] + q(x)u(x),$$

In general we can **always transform the non-self-adjoint operator into the** required self-adjoint form. If we multiply *L by*

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

Eigenfunctions, Eigenvalues

Schrödinger's wave equation

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

is the major example of an eigenvalue equation in physics

- eigenvalue equation takes the more general self-adjoint form

$$\mathcal{L}u(x) + \lambda w(x)u(x) = 0,$$

- *λ is the eigenvalue and w(x) is density function; w(x) > 0.*
- A function *uλ(x), which satisfies* **the imposed boundary conditions, is called an eigenfunction corresponding** to *λ.*
- Indeed, the requirement that there be an eigenfunction often restricts the acceptable values of *λ to a discrete set*

Table 10.1

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

[a] $l = 0, 1, \ldots, -l \le m \le l$ are integers and $-1 \le x \le 1$, $0 \le x \le 1$ 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

$$\left(1-x^2\right)u''-2xu'+n(n+1)u=0, \qquad -1\le x\le 1. \tag{10.9}$$

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

$$p_0(x)=1-x^2=p, \qquad w(x)=1,$$
$$p_1(x)=-2x=p', \qquad \lambda=n(n+1),$$
$$p_2(x)=0=q.$$

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 λ. ■

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 MeV$\ll Mc^2$, 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 $0 \le r < a$, $V = 0$ for $r > a$. The Schrödinger wave equation is

$$-\frac{\hbar^2}{M}\nabla^2\psi + V\psi = E\psi, \tag{10.10}$$

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

$$\frac{d^2u}{dr^2} + k_1^2 u = 0, \tag{10.11}$$

with

$$k_1^2 = \frac{M}{\hbar^2}(E - V_0) > 0 \tag{10.12}$$

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

$$\frac{d^2u}{dr^2} - k_2^2 u = 0, \tag{10.13}$$

with

$$k_2^2 = -\frac{ME}{\hbar^2} > 0. \tag{10.14}$$

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

$$u_1(r) = \sin k_1 r, \qquad 0 \leq r < a. \tag{10.15}$$

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

$$u_2(r) = A \exp k_2 r + B \exp(-k_2 r), \qquad a < r < \infty. \tag{10.16}$$

Continuity of particle and current density demand that $u_1(a) = u_2(a)$ and that $u_1'(a) = u_2'(a)$. These **joining**, or **matching, conditions** give

$$\begin{aligned} \sin k_1 a &= A \exp k_2 a + B \exp(-k_2 a), \\ k_1 \cos k_1 a &= k_2 A \exp k_2 a - k_2 B \exp(-k_2 a). \end{aligned} \tag{10.17}$$

The condition that we actually have a bound proton–neutron combination is that $\int_0^\infty u^2(r)\, dr = 1$. This constraint can be met if we impose a boundary condition that $\psi(r)$

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

$$\tan k_1 a = -\frac{k_1}{k_2} = -\sqrt{\frac{E - V_0}{-E}}, \tag{10.18}$$

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 ψ) 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.

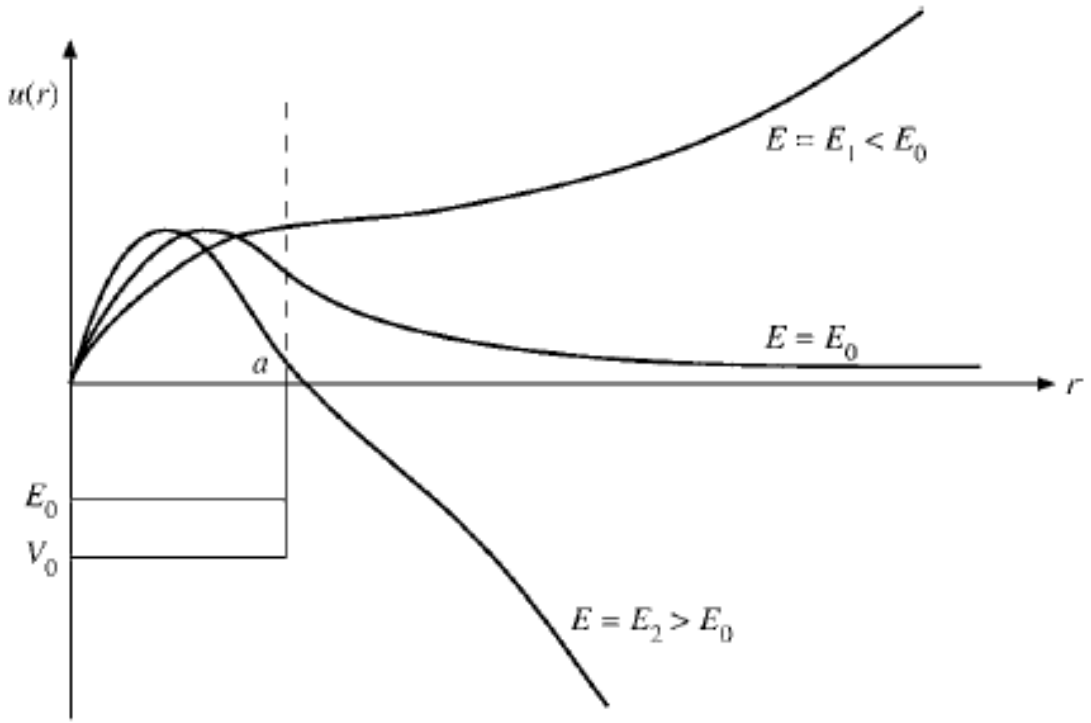


FIGURE 10.1 A deuteron eigenfunction.

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 $\exp(-k_2 a)$. 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 *uλ(x) was* required to satisfy certain imposed boundary conditions.

$$v^* pu' \Big|_{x=a} = v^* pu' \Big|_{x=b}$$

in which *u(x) and v(x) are solutions of the differential equation corresponding to the same* or to different eigenvalues.

Example 10.1.3 INTEGRATION INTERVAL $[a, b]$

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

$$\frac{d^2}{dx^2}u(x) + n^2 u(x) = 0, \tag{10.21}$$

with eigenfunctions

$$u_n = \cos nx, \qquad v_m = \sin mx.$$

Equation (10.20) becomes

$$-n \sin mx \sin nx\Big|_a^b = 0, \qquad \text{or} \qquad m \cos mx \cos nx\Big|_a^b = 0,$$

interchanging u_n and v_m. Since $\sin mx$ and $\cos nx$ are periodic with period 2π (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	$(1-x^2)^{-1/2}$
Shifted Chebyshev I	0	1	$[x(1-x)]^{-1/2}$
Chebyshev II	-1	1	$(1-x^2)^{1/2}$
Laguerre	0	∞	e^{-x}
Associated Laguerre	0	∞	$x^k e^{-x}$
Hermite	$-\infty$	∞	e^{-x^2}
Simple harmonic oscillator	0	2π	1
	$-\pi$	π	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 self-adjoint form.

Hermitian Operators in QuantumMechanics

- The operator *L is called* ***Hermitian if***

$$\int \psi_1^* \mathcal{L}\psi_2 \, d\tau = \int (\mathcal{L}\psi_1)^* \psi_2 \, d\tau.$$

So that the wave functions satisfy appropriate boundary conditions

- Clearly, if $A = A^\dagger$ ***(self-adjoint) and satisfies the aforementioned boundary*** conditions, then *A is Hermitian.*

- If we require *L to be Hermitian, it is easy to show that L is* real

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

Exercises :

9.7.7, 10.1.1, 10.1.10