Chapter 10

Linear Operators, Eigenvalues, and Green's Operator

We begin with a reminder of facts which should be known from previous courses.

10.1 Inner Product Space

A *vector space* V is a collection of objects $\{x\}$ for which addition is defined. That is, if $x, y \in V$, $x + y \in V$, which addition satisfies the usual commutative and associative properties of addition:

$$x + y = y + x, \quad x + (y + z) = (x + y) + z. \tag{10.1}$$

There is a zero vector 0, with the property

$$0 + x = x + 0 = x, \tag{10.2}$$

and the inverse of x, denoted $-x$, has the property

$$x - x \equiv x + (-x) = 0. \tag{10.3}$$

Vectors may be multiplied by complex numbers ("scalars") in the usual way. That is, if λ is a complex number, and $x \in V$, then $\lambda x \in V$. Multiplication by scalars is distributive over addition:

$$\lambda(x + y) = \lambda x + \lambda y. \tag{10.4}$$

Scalar multiplication is also associative: If λ and μ are two complex numbers,

$$\lambda(\mu x) = (\lambda\mu)x. \tag{10.5}$$

An *inner product space* is a vector space possessing an inner product. If x and y are two vectors, the inner product

$$\langle x, y \rangle \tag{10.6}$$

is a complex number. The inner product has the following properties:

$$\langle x, y + \alpha z \rangle = \langle x, y \rangle + \alpha \langle x, z \rangle, \tag{10.7a}$$
$$\langle x + \beta y, z \rangle = \langle x, z \rangle + \beta^* \langle y, z \rangle, \tag{10.7b}$$
$$\langle x, y \rangle = \langle y, x \rangle^*, \tag{10.7c}$$
$$\langle x, x \rangle > 0 \quad \text{if} \quad x \neq 0, \tag{10.7d}$$

where α and β are scalars. Because of the properties (10.7a) and (10.7b), we say that the inner product is linear in the second factor and antilinear in the first. Because of the last property (10.7d), we define the *norm* of the vector by

$$\|x\| = \sqrt{\langle x, x \rangle}. \tag{10.8}$$

10.2 The Cauchy-Schwarz Inequality

An important result is the Cauchy-Schwarz inequality,[1] which has an obvious meaning for, say, three-dimensional vectors. It reads, for any two vectors x and y

$$|\langle x, y \rangle| \leq \|x\| \|y\|, \tag{10.9}$$

where equality holds if and only if x and y are linearly dependent.

Proof: For arbitrary λ we have

$$0 \leq \langle x - \lambda y, x - \lambda y \rangle = \|x\|^2 - \lambda \langle x, y \rangle - \lambda^* \langle y, x \rangle + |\lambda|^2 \|y\|^2. \tag{10.10}$$

Because the inequality is trivial if $y = 0$, we may assume $y \neq 0$, and so we may choose

$$\lambda = \frac{\langle y, x \rangle}{\|y\|^2}. \tag{10.11}$$

The the inequality (10.10) read

$$\begin{aligned} 0 &\leq \|x\|^2 - \frac{2}{\|y\|^2} |\langle x, y \rangle|^2 + \frac{|\langle y, x \rangle|^2}{\|y\|^2} \\ &= \|x\|^2 - \frac{|\langle x, y \rangle|^2}{\|y\|^2}, \end{aligned} \tag{10.12}$$

from which Eq. (10.9) follows. Evidently inequality holds in Eq. (10.10) unless

$$x = \lambda y. \tag{10.13}$$

[1] The name Bunyakovskii should also be added.

From the Cauchy-Schwarz inequality, the triangle inequality follows:

$$\|x + y\| \leq \|x\| + \|y\|. \tag{10.14}$$

Proof:

$$\begin{aligned} \|x + y\|^2 &= \langle x + y, x + y\rangle \\ &= \|x\|^2 + \|y\|^2 + 2\mathrm{Re}\,\langle x, y\rangle \\ &\leq \|x\|^2 + \|y\|^2 + 2|\langle x, y\rangle| \\ &\leq \|x\|^2 + \|y\|^2 + 2\|x\|\|y\| = (\|x\| + \|y\|)^2. \end{aligned} \tag{10.15}$$

QED

10.3 Hilbert Space

A *Hilbert space* $\mathcal{H}$ is an inner product space that is *complete*. Recall from Chapter 2 that a complete space is one in which any Cauchy sequence of vectors has a limit in the space. That is, if we have a Cauchy sequence of vectors, i.e., for any $\epsilon > 0$,

$$\{x_n\}_{n=1}^{\infty}: \quad \|x_n - x_m\| < \epsilon \quad \forall\ n, m > N(\epsilon), \tag{10.16}$$

then the sequence has a limit in $\mathcal{H}$, that is, there is an $x \in \mathcal{H}$ for which for any $\epsilon > 0$ there is an $N(\epsilon)$ so large that

$$\|x - x_n\| < \epsilon \quad \forall\ n > N(\epsilon). \tag{10.17}$$

We will mostly be talking about Hilbert spaces in the following.

Suppose we have a countable set of orthonormal vectors $\{e_i\}$, $i = 1, 2, \dots,$ in $\mathcal{H}$. Orthonormality means

$$\langle e_i, e_j\rangle = \delta_{ij}. \tag{10.18}$$

The set is said to be *complete* if any vector x in $\mathcal{H}$ can be expanded in terms of the e_is:[2]

$$x = \sum_{i=1}^{\infty} \langle e_i, x\rangle e_i. \tag{10.19}$$

Here convergence is defined in the sense of the norm as described above. Geometrically, the inner product $\langle e_i, x\rangle$ is a kind of direction cosine of the vector x, or a projection of the vector x on the basis vector e_i.

[2] If the space is finite dimensional, then the sum runs up to the dimensionality of the space.

Example

Consider the space of all functions that are square integrable on the closed interval $[-\pi, \pi]$:

$$\int_{-\pi}^{\pi} |f(x)|^2 \, dx < \infty. \tag{10.20}$$

The functions (not the values of the functions) are the vectors in the space, and the inner product is defined by

$$\langle f, g \rangle = \int_{-\pi}^{\pi} f(x)^* g(x) \, dx. \tag{10.21}$$

It is evident that this definition of the inner product satisfies all the properties (10.7a)–(10.7d). This space, called $\mathcal{L}_2(-\pi, \pi)$, is in fact a Hilbert space. A complete set of orthonormal vectors is

$$\{f_n\}: \quad f_n(x) = \frac{1}{\sqrt{2\pi}} e^{inx}, \quad n = 0, \pm 1, \pm 2, \dots . \tag{10.22}$$

whose inner products satisfy

$$\langle f_n, f_m \rangle = \delta_{n,m}. \tag{10.23}$$

The expansion

$$f = \sum_{n=-\infty}^{\infty} \langle f_n, f \rangle f_n \tag{10.24}$$

is the Fourier expansion of f:

$$\langle f_n, f \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-inx} \, dx = a_n, \tag{10.25}$$

where in terms of the Fourier coefficient a_n

$$f(x) = \sum_{n=-\infty}^{\infty} a_n \frac{1}{\sqrt{2\pi}} e^{inx}. \tag{10.26}$$

This Fourier series does not, in general, converge pointwise, but it does converge "in the mean:"

$$\left\| f(x) - \frac{1}{\sqrt{2\pi}} \sum_{n=-N}^{N} a_n e^{inx} \right\| \to 0 \quad \text{as} \quad N \to 0, \tag{10.27}$$

that is,

$$\lim_{N \to \infty} \int_{-\pi}^{\pi} dx \left| f(x) - \frac{1}{\sqrt{2\pi}} \sum_{n=-N}^{N} a_n \, e^{inx} \right|^2 = 0. \tag{10.28}$$

10.4 Linear Operators

A linear operator T on a vector space V is a rule assigning to each $f \in V$ a unique vector $Tf \in V$. It has the linearity property,

$$T(\alpha f + \beta g) = \alpha T f + \beta T g, \tag{10.29}$$

where α, β are scalars. In an inner product space, the *adjoint* (or *Hermitian conjugate*) of T is defined by

$$\langle f, Tg\rangle = \langle T^\dagger f, g\rangle, \quad \forall\ f, g \in V. \tag{10.30}$$

T is *self-adjoint* (or *Hermitian*) if

$$T^\dagger = T. \tag{10.31}$$

10.4.1 Sturm-Liouville Problem

Consider the space of twice continuously differentiable real functions defined on a segment of the real line

$$x_0 \le x \le x_1, \tag{10.32}$$

an incomplete subset of the Hilbert space $\mathcal{L}_2(x_0, x_1)$. Under what conditions is the differential operator

$$L = p(x)\frac{d^2}{dx^2} + q(x)\frac{d}{dx} + r(x), \tag{10.33}$$

where p, q, and r are real functions, self-adjoint?

Let u, v be functions in the space. In terms of the $\mathcal{L}_2$ inner product

$$\begin{aligned}
\langle u, Lv\rangle &= \int_{x_0}^{x_1} dx\, u(x) L v(x) \\
&= \int_{x_0}^{x_1} dx\, u(x)\left[p(x)\frac{d^2}{dx^2}v(x) + q(x)\frac{d}{dx}v(x) + r(x)v(x)\right] \\
&= u(x)p(x)v'(x)\bigg|_{x_0}^{x_1} - \int_{x_0}^{x_1} dx\, \left[u(x)p(x)\right]' v'(x) \\
&\qquad + u(x)q(x)v(x)\bigg|_{x_0}^{x_1} - \int_{x_0}^{x_1} dx\, \left[u(x)q(x)\right]' v(x) \\
&\qquad + \int_{x_0}^{x_1} dx\, u(x)r(x)v(x) \\
&= \left\{u(x)p(x)v'(x) + u(x)q(x)v(x) - \left[u(x)p(x)\right]' v(x)\right\}\bigg|_{x_0}^{x_1} \\
&\qquad + \int_{x_0}^{x_1} dx\, \left\{\left[u(x)p(x)\right]'' v(x) - \left[u(x)q(x)\right]' v(x) + u(x)r(x)v(x)\right\}
\end{aligned}$$

$$= \{p(x)\left[u(x)v'(x) - u'(x)v(x)\right] + \left[q(x) - p'(x)\right]u(x)v(x)\}\Big|_{x_0}^{x_1}$$
$$+ \int_{x_0}^{x_1} dx\,\big\{p(x)u''(x) + \left[2p'(x) - q(x)\right]u'(x)$$
$$+ \left[p''(x) - q'(x) + r(x)\right]u(x)\big\}v(x). \tag{10.34}$$

The last integral here equals, for all v, v,

$$\langle Lu, v\rangle = \int_{x_0}^{x_1} dx\ \left[Lu(x)\right]v(x) \tag{10.35}$$

if and only if

$$2p' - q = q, \quad p'' - q' + r = r, \tag{10.36}$$

which imply the single condition

$$p'(x) = q(x). \tag{10.37}$$

If this condition holds for all x in the interval $[x_0, x_1]$, the integrated term is

$$p(x)\left[u(x)v'(x) - u'(x)v(x)\right]\Big|_{x_0}^{x_1}. \tag{10.38}$$

Only if this is zero is L Hermitian:

$$\langle u, Lv\rangle = \langle Lu, v\rangle. \tag{10.39}$$

The vanishing of the integrated term may be achieved in various ways:

1. The function p may vanish at both boundaries:

$$p(x_0) = p(x_1) = 0, \quad \text{and} \quad u, v \quad \text{bounded for} \quad x = x_0, x_1. \tag{10.40}$$

   Thus, for example, the Legendre differential operator

$$(1 - x^2)\frac{d^2}{dx^2} - 2x\frac{d}{dx} \tag{10.41}$$

   is self-adjoint on the interval $[-1, 1]$.

2. The functions in the space satisfy *homogeneous* boundary conditions:

   (a) The functions vanish at the boundaries,

$$u(x_0) = u(x_1) = 0, \quad v(x_0) = v(x_1) = 0. \tag{10.42}$$

   These are called homogeneous *Dirichlet* boundary conditions.

   (b) The derivatives of the functions vanish at the boundaries,

$$u'(x_0) = u'(x_1) = 0, \quad v'(x_0) = v'(x_1) = 0. \tag{10.43}$$

   These are called homogeneous *Neumann* boundary conditions.

(c) Homogeneous mixed boundary conditions are a linear combination of these conditions,

$$u'(x_0) + \alpha(x_0)u(x_0) = 0, \tag{10.44a}$$
$$u'(x_1) + \alpha(x_1)u(x_1) = 0, \tag{10.44b}$$

where α is some function, the same for all functions u in the space.

3. A third possibility is that the solutions may satisfy *periodic* boundary conditions,

$$u(x_0) = u(x_1) \quad \text{and} \quad u'(x_0) = u'(x_1). \tag{10.45}$$

This only works when the function p is also periodic,

$$p(x_0) = p(x_1). \tag{10.46}$$

Conditions such as the above, which insure the vanishing of the integrated term (or, in higher dimensions, surface terms) are called *self-adjoint boundary conditions.* When they hold true, the differential equation

$$\frac{d}{dx}\left[p(x)\frac{d}{dx}u(x)\right] + r(x)u(x) = 0 \tag{10.47}$$

is self-adjoint. This equation is called the *Sturm-Liouville* equation.

10.5 Eigenvectors

If T is a (linear) operator and $f \neq 0$ is a vector such that

$$Tf = \lambda f, \tag{10.48}$$

where λ is a complex number, then we say that f is a *eigenvector* ("characteristic vector") belonging to the operator T, and λ is the corresponding *eigenvalue.*

The following theorem is most important. *The eigenvalues of a Hermitian operator are real, and the eigenvectors belonging to distinct eigenvalues are orthogonal.* The proof is quite simple. If

$$Tf = \lambda f, \quad Tg = \mu g, \tag{10.49}$$

then

$$\langle g, Tf\rangle = \lambda\langle g, f\rangle = \langle Tg, f\rangle = \mu^*\langle g, f\rangle. \tag{10.50}$$

Thus if g and f are the same, we conclude that

$$\lambda = \lambda^*, \tag{10.51}$$

i.e., the eigenvalue λ is real, while then if $\lambda \neq \mu$, we must have

$$\langle g, f\rangle = 0. \tag{10.52}$$

10.5.1 Bessel Functions

The Bessel operator is

$$B_\nu = \frac{d^2}{dx^2} + \frac{1}{x}\frac{d}{dx} - \frac{\nu^2}{x^2}. \tag{10.53}$$

where ν is a real number. This is Hermitian in the space of real functions satisfying homogeneous boundary conditions (Dirichlet, Neumann, or mixed), where the inner product is defined by

$$\langle u, v\rangle = \int_a^b x\,dx\,u(x)v(x). \tag{10.54}$$

Proof: Note that

$$xB_\nu = \frac{d}{dx}x\frac{d}{dx} - \frac{\nu^2}{x} \tag{10.55}$$

is of the Sturm-Liouville form, (10.47), with $p(x) = x$, which is Hermitian with the $\mathcal{L}_2(a, b)$ inner product. Then

$$\langle u, B_\nu v\rangle = \int_a^b dx\,u(x)xB_\nu v(x) = \int_a^b dx\,xB_\nu u(x)v(x) = \langle B_\nu u, v\rangle. \tag{10.56}$$

When $a = 0$, the lower limit of the integrated term is zero automatically if the functions are finite at $x = 0$—See Eq. (10.38). Suppose we demand that Dirichlet conditions hold at $x = b$, i.e., that the functions must vanish there. Then we seek solutions to the following Hermitian eigenvalue problem,

$$B_\nu\psi_{\nu n} = \lambda_{\nu n}\psi_{\nu n}, \tag{10.57}$$

with the boundary conditions

$$\psi_{\nu n}(b) = 0, \quad \psi_{\nu n}(0) = \text{finite}. \tag{10.58}$$

Here n enumerates the eigenvalues. The solutions to this problem are the *Bessel functions*, which satisfy the differential equation

$$\left(\frac{d^2}{dz^2} + \frac{1}{z}\frac{d}{dz} + 1 - \frac{\nu^2}{z^2}\right)J_\nu(z), \tag{10.59}$$

which are finite at the origin, $z = 0$.[3] This is the same as the eigenvalue equation (10.57) provided we change the variable $z = \sqrt{-\lambda_{\nu n}}x$. That is,

$$\psi_{\nu n}(x) = J_\nu(\sqrt{-\lambda_{\nu n}}x). \tag{10.60}$$

The solutions we seek are Bessel functions of a real variable, so the acceptable eigenvalues satisfy

$$\lambda_{\nu n} < 0, \tag{10.61}$$

[3]The second solution to Eq. (10.59), the so-called Neumann function $N_\nu(z)$ [it is also denoted by $Y_\nu(z)$ and is more properly attributed to Weber], is not regular at the origin.

so we write

$$-\lambda_{\nu n} = k_{\nu n}^2. \tag{10.62}$$

Finally, we impose the boundary condition at $x = b$:

$$0 = \psi_{\nu n}(b) = J_\nu(k_{\nu n} b), \tag{10.63}$$

that is, $k_{\nu n} b$ must be a zero of J_ν. There are an infinite number of such zeros, as Fig. 10.1 illustrates. Let the nth zero of J_ν be denoted by $\alpha_{\nu n}$, $n = 1, 2, 3, \dots$. For example, the first three zeros of J_0 are

$$\alpha_{01} = 2.404826, \quad \alpha_{02} = 5.520078, \quad \alpha_{03} = 8.653728, \tag{10.64}$$

while the first three zeros of J_1 (other than 0) are

$$\alpha_{11} = 3.83171, \quad \alpha_{12} = 7.01559, \quad \alpha_{13} = 10.17347. \tag{10.65}$$

Then the eigenvalues of the Bessel operator are

$$\lambda_{\nu n} = -\left(\frac{\alpha_{\nu n}}{b}\right)^2, \tag{10.66}$$

and the eigenfunctions are

$$J_\nu\left(\alpha_{\nu n}\frac{x}{b}\right). \tag{10.67}$$

Because of the Hermiticity of B_ν, these have the following orthogonality property, from Eq. (10.52),

$$\int_0^b dx\, x\, J_\nu\left(\alpha_{\nu n}\frac{x}{b}\right) J_\nu\left(\alpha_{\nu m}\frac{x}{b}\right) = 0, \quad n \neq m. \tag{10.68}$$

10.6 Dual Vectors. Dirac Notation

It is often convenient to think of the inner product as being composed by the multiplication to two different kinds of vectors. Thus, in 2-dimensional vector space we have column vectors,

$$\mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \tag{10.69}$$

and row vectors,

$$\mathbf{v}^\dagger = (v_1^*, v_2^*). \tag{10.70}$$

As the notation indicates, the row vector $\mathbf{v}^\dagger$ is the adjoint, the complex conjugate of the transpose of the column vector $\mathbf{v}$. The inner product is then formed by the rules of matrix multiplication,

$$\langle \mathbf{v}, \mathbf{u}\rangle = \mathbf{v}^\dagger \mathbf{u} = v_1^* u_1 + v_2^* u_2. \tag{10.71}$$

We generalize this notion to abstract vectors as follows. Denote a "right" vector (Dirac called it a "ket") by $|\lambda\rangle$ where λ is a name, or number, or set

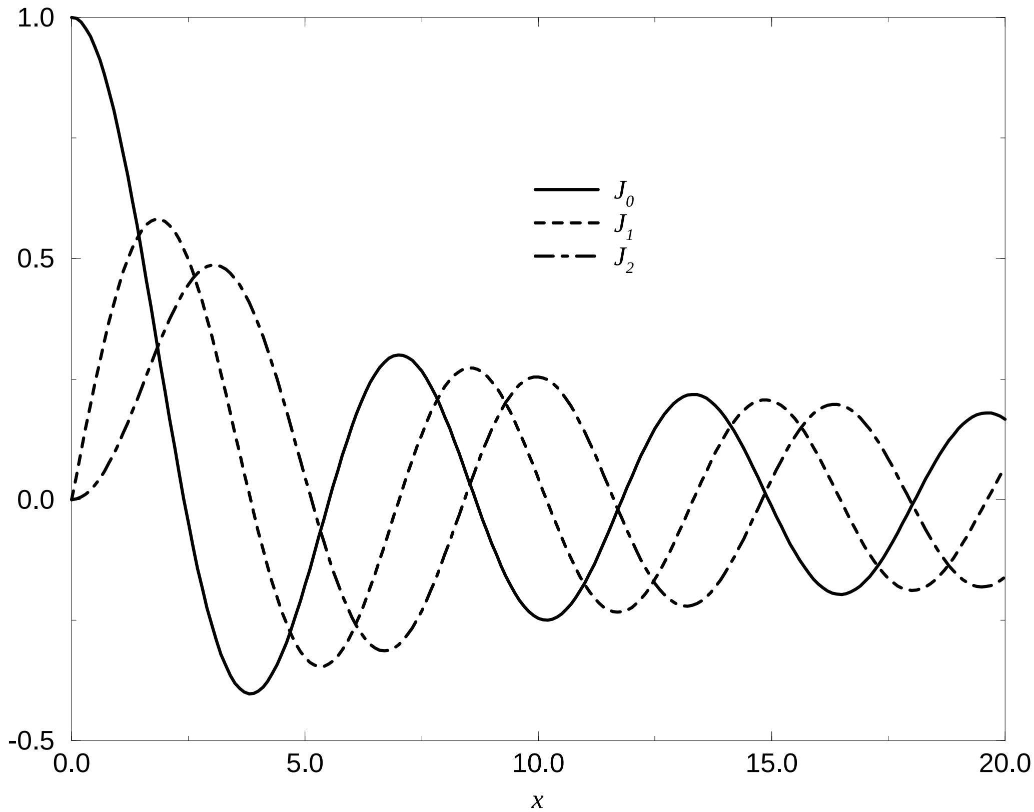

Figure 10.1: Plot of the Bessel functions of the first kind, J_0, J_1, and J_2, as functions of x.

of numbers, labeling the vector. For example, if $|\lambda\rangle$ is an eigenvector of some operator, λ might be the corresponding eigenvalue.

The *dual* (or "conjugate") vector to $|\lambda\rangle$ is

$$\langle\lambda| = (|\lambda\rangle)^\dagger, \tag{10.72}$$

which is a "left" vector or a "bra" vector. For every right vector there is a unique left vector, and vice versa, in an inner product space. The inner product of $|\alpha\rangle$ with $\langle\beta|$ is denoted $\langle\beta|\alpha\rangle$. Note that the double vertical line has coalesced into a single line. This notation is a bracket notation, hence Dirac's nomenclature.

With row and column vectors there is not only an inner product, but an *outer product* as well:

$$\mathbf{v}\mathbf{u}^\dagger = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} (u_1^*, u_2^*) = \begin{pmatrix} v_1 u_1^* & v_1 u_2^* \\ v_2 u_1^* & v_2 u_2^* \end{pmatrix}. \tag{10.73}$$

The result is a matrix or operator. So it is with abstract left and right vectors. We may define a *dyadic* by

$$|\alpha\rangle\langle\beta| \tag{10.74}$$

which is an operator. When it acts on the right vector $|\gamma\rangle$ it produces another vector,

$$|\alpha\rangle\langle\beta||\gamma\rangle = |\alpha\rangle\langle\beta|\gamma\rangle, \tag{10.75}$$

where $\langle\beta|\gamma\rangle$ is a complex number, the inner product of $\langle\beta|$ and $|\gamma\rangle$; evidently the properties of an operator are satisfied.

10.6.1 Basis Vectors

Let $|n\rangle$, $n = 1, 2, \dots$ be a complete, orthonormal set of vectors, that is, they satisfy the properties

$$\langle m|n\rangle = \delta_{mn}, \tag{10.76a}$$

and if $|\lambda\rangle$ is any vector in the space,

$$|\lambda\rangle = \sum_{n=1}^{\infty} |n\rangle\langle n|\lambda\rangle. \tag{10.76b}$$

This is just a rewriting of the statement in Eq. (10.19). Since $|\lambda\rangle$ is an arbitrary vector, we must have

$$\sum_{n=1}^{\infty} |n\rangle\langle n| = I, \tag{10.77}$$

where I is the identity operator. This operator expression is the *completeness* relation for the vectors $\{|n\rangle\}$.

10.7 $\mathcal{L}_2(V)$

As we have seen, an important example of a Hilbert space is the space of all functions square-integrable in some region. For example, suppose we consider complex-valued functions $f(\mathbf{r})$, where $\mathbf{r} = (x, y, z)$, $\mathbf{r} \in V$, where V is some volume in 3-dimensional space, such that

$$\int_V (d\mathbf{r})|f(\mathbf{r})|^2 < \infty, \tag{10.78}$$

where the volume element $(d\mathbf{r}) = dx\,dy\,dz$. We call this Hilbert space $\mathcal{L}_2(V)$. Vectors in this space are functions: The function f corresponds to $|f\rangle$, which we write as

$$f(\mathbf{r}) \longrightarrow |f\rangle. \tag{10.79}$$

The inner product is

$$\langle f|g\rangle = \int_V (d\mathbf{r}) f^*(\mathbf{r}) g(\mathbf{r}). \tag{10.80}$$

It is most convenient to define the "function" $\delta(\mathbf{r}-\mathbf{r}_0)$, the Dirac delta function, by the property

$$f(\mathbf{r}_0) = \int_V (d\mathbf{r})\, \delta(\mathbf{r}-\mathbf{r}_0) f(\mathbf{r}) \tag{10.81}$$

for all f provided $\mathbf{r}_0$ lies within V. Regarding δ as a function (it is actually a linear functional defined by the integral equation above), we denote the corresponding vector in Hilbert space by $|\mathbf{r}_0\rangle$:

$$\delta(\mathbf{r}-\mathbf{r}_0) \longrightarrow |\mathbf{r}_0\rangle. \tag{10.82}$$

(Actually, $|\mathbf{r}_0\rangle$ is not a vector in $\mathcal{L}_2(V)$, because it is not a square-integrable function.) Pictorially, $|\mathbf{r}_0\rangle$ represents a function which is localized at $\mathbf{r} = \mathbf{r}_0$, i.e., it vanishes if $\mathbf{r} \neq \mathbf{r}_0$, but with the property

$$\langle \mathbf{r}_0|f\rangle = \int_V (d\mathbf{r})\delta(\mathbf{r}-\mathbf{r}_0) f(\mathbf{r}) = f(\mathbf{r}_0); \tag{10.83}$$

the number $\langle \mathbf{r}_0|f\rangle$ is the value of f at $\mathbf{r}_0$. Also note that

$$\langle \mathbf{r}_0|\mathbf{r}_1\rangle = \int_V (d\mathbf{r})\delta(\mathbf{r}-\mathbf{r}_0)\delta(\mathbf{r}-\mathbf{r}_1) = \delta(\mathbf{r}_0-\mathbf{r}_1). \tag{10.84}$$

In the above, we always assume that $\mathbf{r}_0$ and $\mathbf{r}_1$ lie in the volume V.

It may be useful to recognize that in quantum mechanics $|\mathbf{r}_0\rangle$ is an eigenvector of the position operator. It represents a state in which the particle has a definite position, namely $\mathbf{r}_0$.

Now notice that if the completeness relation (10.77) is multiplied on the right by $|\mathbf{r}'\rangle$ and on the left by $\langle \mathbf{r}|$, it reads

$$\sum_{n=1}^{\infty} \langle \mathbf{r}|n\rangle\langle n|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}'). \tag{10.85}$$

If we define $\psi_n(\mathbf{r}) = \langle \mathbf{r}|n\rangle$ as the values of what is now a complete set of functions,

$$\sum_{n=1}^{\infty} \psi_n^*(\mathbf{r}')\psi_n(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}'). \tag{10.86}$$

Implicit in what we are saying here is the assumption that the set of vectors $|\mathbf{r}\rangle$, $\mathbf{r} \in V$, is complete:

$$\begin{aligned} \langle g|f\rangle &= \int_V (d\mathbf{r}) g^*(\mathbf{r}) f(\mathbf{r}) \\ &= \int_V (d\mathbf{r}) \langle g|\mathbf{r}\rangle\langle \mathbf{r}|f\rangle, \end{aligned} \tag{10.87}$$

which must mean, since $|g\rangle$ and $\langle f|$ are arbitrary,

$$I = \int_V (d\mathbf{r}) |\mathbf{r}\rangle\langle \mathbf{r}|. \tag{10.88}$$

(Because the vectors are continuously, not discretely, labeled, the sum in Eq. (10.77) is replaced by an integral.) This will not be true if there are other variables in the problem, such as spin, but in that case the inner product is not given in terms of an integral over $\mathbf{r}$ alone.

10.8 Green's Operator

We have now reached the taking-off point for the discussion of Green's functions. We will in this section sketch the general type of problem we wish to consider. In the next chapter we will fill in the details, by considering physical examples.

Let L be a self-adjoint linear operator in a Hilbert space. We wish to find the solutions $|\psi\rangle$ to the following vector equation

$$(L-\lambda)|\psi\rangle = |S\rangle, \tag{10.89}$$

where $|S\rangle$ is a prescribed vector, the "source," and λ is a real number not equal to any of the (real) eigenvectors of L.

Suppose the eigenvectors of L, which satisfy

$$L|n\rangle = \lambda_n|n\rangle, \tag{10.90}$$

are complete, and are orthonormalized,

$$\sum_n |n\rangle\langle n| = I. \tag{10.91}$$

We may then expand $|\psi\rangle$ in terms of these,

$$|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle. \tag{10.92}$$

When we insert this expansion into Eq. (10.89) and use the eigenvalue equation (10.90), we obtain

$$\sum_n (\lambda_n - \lambda)|n\rangle\langle n|\psi\rangle = |S\rangle. \tag{10.93}$$

Now multiply this equation on the left by $\langle n'|$, and use the orthonormality property

$$\langle n'|n\rangle = \delta_{n'n}, \tag{10.94}$$

to find ($n' \to n$)

$$(\lambda_n - \lambda)\langle n|\psi\rangle = \langle n|S\rangle, \tag{10.95}$$

or, provided $\lambda \neq \lambda_n$,

$$\langle n|\psi\rangle = \frac{\langle n|S\rangle}{\lambda_n - \lambda}. \tag{10.96}$$

Then from Eq. (10.92) we deduce

$$|\psi\rangle = \sum_n \frac{|n\rangle\langle n|}{\lambda_n - \lambda}|S\rangle, \tag{10.97}$$

which means we have solved for $|\psi\rangle$ in terms of the presumably known eigenvectors and eigenvalues of L. We write this more compactly as

$$|\psi\rangle = G|S\rangle, \tag{10.98}$$

where G, the *Green's operator*, is

$$G = \sum_n \frac{|n\rangle\langle n|}{\lambda_n - \lambda}; \tag{10.99}$$

the sum ranges over all the eigenvectors of L.

We regard Eq. (10.98) as the definition of G: the *response* of a linear system is linear in the *source*. Eq. (10.99) is the eigenvector expansion of G.

Two properties of G follow immediately from the above:

1. From Eq. (10.99), since both λ and λ_n are real, we see that G is Hermitian,

$$G^\dagger = G. \tag{10.100}$$

2. From either of Eqs. (10.98) or (10.99) we see that G satisfies the operator equation

$$(L - \lambda)G = I. \tag{10.101}$$

The case of functions is the most important one. Then if we use Eq. (10.88), the inhomogeneous equation (10.89) becomes

$$\langle \mathbf{r}|(L - \lambda)\int_V (d\mathbf{r}')|\mathbf{r}'\rangle\langle\mathbf{r}'|\psi\rangle = \langle\mathbf{r}|S\rangle. \tag{10.102}$$

Suppose

$$\langle \mathbf{r}|L|\mathbf{r}'\rangle = \hat{L}\delta(\mathbf{r}-\mathbf{r}'), \tag{10.103}$$

where $\hat{L}$ is a differential operator (the usual case), and let us further write

$$\langle \mathbf{r}'|\psi\rangle = \psi(\mathbf{r}'), \quad \langle \mathbf{r}|S\rangle = S(\mathbf{r}). \tag{10.104}$$

Then the inhomogeneous equation (10.102) reads

$$(\hat{L}-\lambda)\psi(\mathbf{r}) = S(\mathbf{r}) \tag{10.105}$$

The solution to Eq. (10.105) is given by $\langle \mathbf{r}|$ times Eq. (10.98):

$$\langle \mathbf{r}|\psi\rangle = \langle r|G\int_V (d\mathbf{r}')|\mathbf{r}'\rangle\langle \mathbf{r}'|S\rangle, \tag{10.106}$$

or

$$\psi(\mathbf{r}) = \int_V (d\mathbf{r}')\, G(\mathbf{r},\mathbf{r}')S(\mathbf{r}'), \tag{10.107}$$

where we have written the *Green's function* as

$$G(\mathbf{r},\mathbf{r}') = \langle \mathbf{r}|G|\mathbf{r}'\rangle. \tag{10.108}$$

The eigenfunction expansion of $G(\mathbf{r},\mathbf{r}')$ is

$$G(\mathbf{r},\mathbf{r}') = \sum_n \frac{\psi^*(\mathbf{r}')\psi(\mathbf{r})}{\lambda_n-\lambda}, \tag{10.109}$$

where the eigenfunctions, satisfying Eq. (10.86), are $\psi_n(\mathbf{r}) = \langle \mathbf{r}|n\rangle$. Now the properties of $G(\mathbf{r},\mathbf{r}')$ are

1. *The reciprocity relation:*

   $$G(\mathbf{r},\mathbf{r}') = G^*(\mathbf{r}',\mathbf{r}), \tag{10.110}$$

   which follows immediately from the eigenfumction expansion (10.109) or from Eq. (10.100):

   $$\langle \mathbf{r}|G^\dagger|\mathbf{r}'\rangle = \langle \mathbf{r}'|G|\mathbf{r}\rangle^* = \langle \mathbf{r}|G|\mathbf{r}'\rangle. \tag{10.111}$$

2. The differential equation satisfied by the Green's function is

   $$(\hat{L}-\lambda)G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'), \tag{10.112}$$

   which follows from Eqs. (10.107), (10.109), or (10.101).

3. Now we have an additional property. If $\psi_n(\mathbf{r})$ satisfy homogeneous boundary conditions, for example, $\psi_n(\mathbf{r}) = 0$ on the surface of V, $G(\mathbf{r},\mathbf{r}')$ satisfies the same conditions, for example it vanishes when $\mathbf{r}$ or $\mathbf{r}'$ lies on the surface of V.

Note that the eigenfunction expansion of $G(\mathbf{r},\mathbf{r}')$,

$$G_\lambda(\mathbf{r},\mathbf{r}') = \sum_n \frac{\psi_n^*(\mathbf{r}')\psi_n(\mathbf{r})}{\lambda_n - \lambda}, \tag{10.113}$$

where now the parameter λ has been made explicit in G, says that G_λ has simple poles at each of the eigenvalues λ_n, and that the residue of the pole of G_λ at $\lambda = \lambda_n$ is

$$\operatorname{Res} G_\lambda(\mathbf{r},\mathbf{r}')\big|_{\lambda=\lambda_n} = -\psi_n^*(\mathbf{r}')\psi(\mathbf{r}). \tag{10.114}$$

If the eigenvalue is degenerate, that is, there is more than one eigenfunction corresponding to a given eigenvalue, one obtains a sum over all the $\psi_n^*\psi_n$ corresponding to λ_n.

Thus, if G may be determined by other means than by an eigenfunction expansion, such as directly solving the differential equation (10.112), from it the eigenvalues and normalized eigenfunctions of $\hat{L}$ may be determined. We will illustrate this eigenfunction decomposition in the next chapter.