Massachusetts Institute of Technology
Department of Physics

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Completeness Relations

1 Introduction

Two mathematical principles underly the solution of Laplace's equation with basis function expansions such as those used in the separation of variables: orthonormality and completeness. The treatment here will be brief and non-rigorous as the aim is to give an understanding of completeness relations without proving them. The mathematical basis for completeness relations is given by Sturm-Liouville theory of second-order differential equations. The interested student may find a complete presentation in a course such as 18.075 or 18.152 at MIT.

The mathematical problem we are trying to solve is Laplace's equation $\nabla^2 V = 0$ in some volume bounded by a surface S on which boundary conditions are imposed on V or its normal gradient, $\partial V/\partial n \equiv \vec{n} \cdot \vec{\nabla} V$. In applying separation of variables, we obtain eigenvalue problems such as

$$L_2 u = -k^2 u \tag{1}$$

subject to boundary conditions. Here k^2 is a positive constant and L_2 is a second-order differential operator (ordinary or partial) that comes from separating variables in Laplace's equation. For example, in Cartesian coordinates,

$$\nabla^2 = L_2(x) + L_2(y) + L_2(z) = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \ , \tag{2}$$

while in spherical coordinates

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2} L_2(\theta, \phi) \ , \quad L_2(\theta,\phi) \equiv \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \ . \tag{3}$$

The corresponding eigenvalue problems are

$$\frac{d^2 u}{dx^2} = -k^2 u \tag{4}$$

and

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial F}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 F}{\partial\phi^2}=-l(l+1)F\ , \tag{5}$$

subject to appropriate boundary conditions in each case. The constants $-k^2$ and $-l(l+1)$ are called eigenvalues, and the corresponding solutions of the differential equations are called eigenfunctions.

Imposition of appropriate boundary conditions makes equation (4) and (5) Sturm-Liouville problems, for which orthogonality and completeness may be rigorously established. There are many more Sturm-Liouville problems than these two cases, but they arise so frequently in electromagnetism that these notes focus on them.

Equations (4) and (5) are eigenvalue problems. If one applies appropriate boundary conditions, then it turns out that these equations can only be satisfied for certain values of the constants k and l. Sturm-Liouville theory shows that the eigenfunctions form a complete, orthogonal set of functions satisfying the boundary conditions. There is a strong analogy here with ordinary vector algebra. This analogy will be exemplified in the sections that follow.

2 Orthonormality and Completeness in 1-D

We start with eigenvalue problems like equation (4) supplemented by boundary conditions. The functions $u(x)$ satisfying equation (4) form a set of basis functions for all functions satisfying the same boundary conditions. We assume that boundary conditions are imposed at $x = a$ and $x = b$ (which may be $\pm\infty$). We assume that there is a scalar product operation that takes two functions and maps them to a single number. In Sturm-Liouville theory, the inner product of two functions $f(x)$ and $g(x)$ is

$$(f, g) = \int_a^b f(x)g(x)w(x)dx\ , \tag{6}$$

where $w(x)$ is a given function that depends on the differential operator in the eigenvalue problem.

Now suppose, for simplicity, that the eigenvalues k are discrete: $k \in \{k_n\}$ with $n = 1, 2, \ldots$. Eigenvalue n has corresponding eigenfunction $u_n(x)$. Then, any function $V(x)$ satisfying the same boundary conditions as u_n may be written

$$V(x) = \sum_{n=1}^{\infty} V_n u_n(x) \tag{7}$$

where the coefficients V_n are unique constants. The functions $u_n(x)$ are akin to basis vectors; equation (7) is the expansion of a vector in basis vectors. This analogy is possible because functions define a linear vector space, albeit one with infinitely many dimensions. (Recall that the dimensionality of a vector space equals the number of linearly independent basis vectors.)

Equation (7) is useful only if two conditions are satisfied. First, we must be able to determine the coefficients V_n that solve a given problem. Second, the series expansion must converge to the solution $V(x)$.

The first condition is made possible by orthonormality of the basis functions. Now, Sturm-Liouville theory shows that eigenfunctions with different eigenvalues are orthogonal with respect to the inner product: $(u_m, u_n) = 0$ if $m \neq n$. If $m = n$, on the other hand, the Sturm-Liouville scalar product is positive-definite, so that we may normalize the eigenfunctions:

$$(u_m, u_n) = \delta_{mn} \quad \text{(Orthonormality)} \ . \tag{8}$$

Taking the scalar product of equation (7) with u_n and using orthonormality, we obtain

$$V_n = (u_n, V) \ . \tag{9}$$

The second condition expresses the completeness of the eigenfunctions. In Sturm-Liouville theory, completeness is established by showing that $(f, f) \geq 0$ for any function $f(x)$, and

$$(\delta V, \delta V) = 0 \ , \quad \text{where} \ \ \delta V(x) \equiv V(x) - \sum_{n=1}^{\infty} (u_n, v) u_n(x) \ . \tag{10}$$

This condition implies that the series given by equation (7) converges (with respect to the inner product norm) to $V(x)$ if the expansion coefficients are given by equation (9). Combining these two equations, we require

$$\begin{aligned} V(x) &= \sum_{n=1}^{\infty} \left[\int_a^b V(x') u_n(x') w(x') \, dx' \right] u_n(x) \\ &= \int_a^b \left[\sum_{n=1}^{\infty} u_n(x) u_n(x') w(x') \right] V(x') \ . \end{aligned} \tag{11}$$

It turns out that for Sturm-Liouville problems this holds for any V in the function space, which requires

$$\sum_{n=1}^{\infty} u_n(x) u_n(x') w(x') = \delta(x - x') \quad \text{(Completeness)} \ . \tag{12}$$

The following subsections give the eigenfunctions, inner product, orthonormality and completeness relations for several common 1-D cases.

2.1 Fourier Integrals

The first case is $d^2u/dx^2 = -k^2 u$ on the infinite domain $-\infty < x < \infty$ with boundary conditions $|u(x)|$ is finite as $x \to \pm\infty$. The eigenvalues k now are the set of all real numbers, so that the eigenfunctions are labelled not by a discrete index n but instead by a continuous variable k:

$$u(x; k) = e^{ikx} \ . \tag{13}$$

The inner product is defined with respect to weight $w(x) = (2\pi)^{-1}$. Because the eigenvalue is continuous rather than discrete, orthonormality is expressed with the Dirac delta function:

$$\int_{-\infty}^{\infty} u^*(x; k')u(x; k)w(x)\, dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-k')x}\, dx = \delta(k - k') \ . \tag{14}$$

Note that the eigenfunctions are complex and the inner product takes one complex conjugate. Equation (14) is the Fourier integral representation of the delta function. It is proven in math courses that discuss Fourier analysis.

The Fourier completeness relation is given by an integral rather than sum over the continuous eigenvalue:

$$\int_{-\infty}^{\infty} u^*(x'; k)u(x; k)w(x')dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')}\, dk = \delta(x - x') \ . \tag{15}$$

This follows at once from equation (14).

2.2 Fourier Sine Series

Often one has to solve boundary value problems in a finite rather than infinite domain. In this case the eigenvalues are discrete. If the boundary conditions on $d^2u/dx^2 = -k^2u$ are $u = 0$ at $x = 0$ and $x = a$, then the eigenfunctions are

$$u_n(x) = \sin(n\pi x/a) \ , \quad (n = 1, 2, \ldots) \ , \tag{16}$$

the weight function is $w(x) = 2/a$, and orthonormality is

$$(u_m, u_n) = \int_0^a u_m(x)u_n(x)w(x)\, dx = \frac{2}{a} \int_0^a \sin(m\pi x/a) \sin(n\pi x/a)\, dx = \delta_{mn} \ . \tag{17}$$

This integral is elementary and may easily be checked. However, the completeness relation is not so obvious:

$$\sum_{n=1}^{\infty} u_n(x')u_n(x)w(x) = \frac{2}{a} \sum_{n=1}^{\infty} \sin(n\pi x'/a) \sin(n\pi x/a) = \delta(x - x') \ . \tag{18}$$

Although the proof of equation (18) is beyond these notes, we can easily enough verify it numerically. If we integrate both sides over x' from $x' = 0$ to $x' = x_0$, and then exchange x and x_0, we should get the Heaviside step function:

$$\theta(x - x_0) = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[1 - \cos(n\pi x/a)\right] \sin(n\pi x_0/a) \ . \tag{19}$$

Figure 1 shows this sum evaluated with 20 and 200 terms. The series converges slowly to the correct result everywhere except at the discontinuity $x = x_0$, where there is an

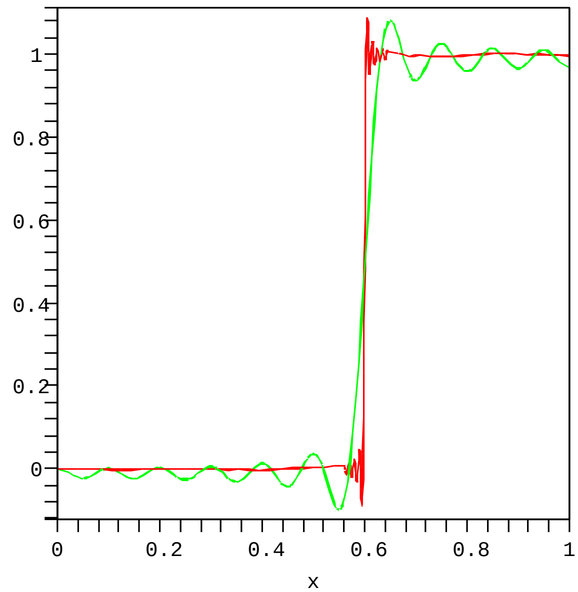

Figure 1: Numerical approximation to the Heaviside step function $\theta(x - 0.6)$ computed using 20 (green) and 200 (red) terms of the Fourier series in eq. (19). The overshoot and oscillation arise from the Gibbs phenomenon of Fourier series.

undershoot and overshoot. This phenomenon is well known with Fourier series, which converge to the correct value for continuous functions but not necessarily at discontinuities. This means that equation (18), and more generally equation (12), satisfy the delta function rule

$$f(x_0) = \int_{-\infty}^{\infty} f(x)\delta(x - x_0)\, dx \qquad (20)$$

only for smooth functions $f(x)$ without discontinuities. Fortunately, solutions of Laplace's equation are smooth, so the Gibbs phenomenon is of no concern in this case.

2.3 Fourier Cosine Series

If the boundary conditions are $u = 1$ at $x = 0$ and $x = a$, then the eigenfunctions of $d^2u/dx^2 = -k^2 u$ are

$$u_n(x) = \begin{cases} 1/\sqrt{2}\ , & n = 0\ , \\ \cos(n\pi x/a)\ , & n = 1, 1, 2, \ldots\ , \end{cases} \qquad (21)$$

the weight function is $w(x) = 2/a$, and orthonormality is

$$(u_m, u_n) = \int_0^a u_m(x)u_n(x)w(x)\,dx = \frac{2}{a}\int_0^a \cos(m\pi x/a)\cos(n\pi x/a)\,dx = \delta_{mn}\ . \tag{22}$$

The only difference with the Fourier sine series is the inclusion of the $n = 0$ term. The completeness relation is

$$\sum_{n=0}^{\infty} u_n(x')u_n(x)w(x) = \frac{2}{a}\sum_{n=0}^{\infty}\cos(n\pi x'/a)\cos(n\pi x/a) = \delta(x - x')\ . \tag{23}$$

If this relation is integrated to give the Heaviside function, and the series plotted, the results are very similar to Fig. 1.

I leave it as an exercise for the reader to write down the relations when the boundary conditions differ from the two simple cases considered here (sine and cosine series). Whatever the boundary conditions, one simply chooses the eigenfunctions of d^2u/dx^2 that obey the boundary conditions. Note that the hyperbolic functions which result when $-k^2 = \kappa^2 > 0$ do *not* form an orthonormal basis. The corresponding boundary value problem is not of Sturm-Liouville type.

2.4 Legendre Series

The Legendre differential equation arises from the equation (5) when $\partial F/\partial\phi = 0$. Defining $x = \cos\theta$, equation (5) reduces to an ordinary differential equation,

$$\frac{d}{dx}\left[(1 - x^2)\frac{du}{dx}\right] = -l(l + 1)u\ , \tag{24}$$

which is to be solved on the domain $0 \le x \le 1$. For any l there are two solutions to the differential equation, denoted $P_l(x)$ and $Q_l(x)$. For most applications, the boundary conditions are that $u(x)$ be finite everywhere in $0 \le x \le 1$. This condition is satisfied if and only if l is an integer. It is sufficient to consider non-negative integers only, because the eigenvalue $-l(l + 1)$ is invariant under $l \to -(l + 1)$.

Even with l restricted to $\{0, 1, 2, \ldots\}$, there are still two solutions to equation (24). One solution (P_l) is finite at $x = \pm 1$ while the other (Q_l) has logarithmic singularities. Only the $P_l(x)$ with integer l can satisfy the physical boundary conditions that $u(x)$ be finite everywhere. The functions $P_l(x)$ are the Legendre polynomials. The functions $Q_l(x)$ are called the Legendre functions of the second kind.

The orthonormality relation for Legendre polynomials is

$$(P_l, P_{l'}) = \frac{2l + 1}{2}\int_{-1}^{1} P_l(x)P_{l'}(x)\,dx = \delta_{ll'} \tag{25}$$

and the completeness relation is

$$\sum_{l=0}^{\infty}\frac{2l + 1}{2}P_l(x')P_l(x) = \delta(x - x')\ . \tag{26}$$

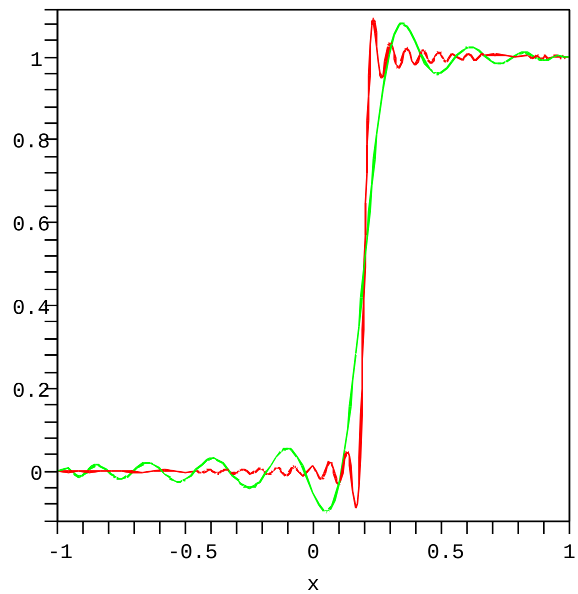

Figure 2: Numerical approximation to the Heaviside step function $\theta(x - 0.2)$ computed using 20 (green) and 90 (red) terms of the Legendre series. The Gibbs phenomenon is a general feature of Sturm-Liouville eigenfunction expansions.

Integrating the completeness relation gives a series representation of the Heaviside function. The results are shown in Figure 2.

3 Orthonormality and Completeness on the Sphere

Equation (5), with boundary conditions stating that $F(\theta, \phi)$ is finite everywhere on the sphere, defines an eigenvalue problem. The dependence on the two variables separates, and the eigenfunctions are

$$F(\theta, \phi) = Y_{lm}(\theta, \phi) \equiv \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\, P_l^m(\cos\theta) e^{im\phi} \ . \tag{27}$$

The functions $Y_{lm}(\theta, \phi)$ are called spherical harmonics. Apart from a normalization constant, they are products of the associated Legendre functions $P_l^m(\cos\theta)$ and a complex exponential. The boundary condition $F(\theta, \phi + 2\pi) = F(\theta, \phi)$ requires that m be an integer. The boundary condition that F be finite everywhere on the sphere requires that

l be an integer; as before, we can take it to be a non-negative integer without loss of generality. Finally, the boundary conditions also require $-l \leq m \leq l$. Thus, for each degree l, there are $2l+1$ values of the order m.

The spherical harmonic functions obey the following orthonormality condition:

$$\int Y_{lm}(\theta,\phi)Y^*_{l'm'}(\theta,\phi)\,d\Omega = \delta_{ll'}\delta_{mm'}\ , \tag{28}$$

where $d\Omega \equiv \sin\theta d\theta d\phi$ and the integration is taken over the sphere, $0 \leq \theta \leq \pi$, $0 \leq \phi \leq 2\pi$. The complex conjugate is necessary because of the $\exp(im\phi)$ factor just as with the complex Fourier integral. The completeness relation for spherical harmonics is

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}(\theta,\phi)Y^*_{lm}(\theta',\phi') = \frac{1}{\sin\theta}\delta(\theta-\theta')\delta(\phi-\phi')\ . \tag{29}$$

Many of the properties of spherical harmonics are presented and discussed in *Classical Electrodynamics* by J.D. Jackson. We will not use them in 8.07 but they are used extensively in advanced physics.