Chapter 1

Orthonormal Functions

1.1 Introduction

Previous experience:

1. College-level linear algebra: expand finite-dimensional vectors in a basis
2. Quantum Mechanics: expand a wavefunction in an eigenbasis

Today: Treatment of expanding a function in terms of an orthonormal set of functions.

(You won't necessarily understand all the words used in this paragraph; that's OK). We will be thinking about expanding a function in the eigenbasis of a linear differential operator that we don't necessarily associate with the Hamiltonian. We are just touching upon the sophisticated topic of spectral decomposition of self-adjoint (more restrictive than Hermitian) operators in infinite dimensional vector spaces (see, e.g., Richtmyer's "Principles of Advanced Mathematical Physics").

Why do we want to do this? We want to solve PDEs in general, the Poisson equation in particular.

1. You will learn (today?) the very powerful technique of Separation of Variables. We will find that SoV yields complete, orthogonal sets of basis functions
2. You will learn very powerful methods for finding Green's functions using an orthonormal, complete basis of functions (see Jackson chapter 3.12).

1.2 General Notions for Expanding in a Basis

1.2.1 Finite Dimensional Vector Space

Finite number of bases.

Suppose we wish to decompose a vector $\mathbf{a}$ in terms of a set of basis vectors, say $\{\hat{e}_i\}$ (i runs from 1 to N, where N is the dimensionality of the space). Let's take as a concrete example $\mathbb{R}^2$. Then

$$\mathbf{a} = \sum_{i=1}^{2} a_i \hat{e}_i. \tag{1.1}$$

One property we'd like to have satisfied by our basis is that the decomposition is unique. Specifically

$$a_i = \hat{e}_i \cdot \mathbf{a} \tag{1.2}$$

$$= \sum_{j=1}^{2} \hat{e}_i a_j \hat{e}_j \tag{1.3}$$

$$= a_i. \tag{1.4}$$

In order to get to the last line we see that the $\hat{e}_i$ have to be *orthonormal*; i.e.,

$$\hat{e}_i \cdot \hat{e}_j = \delta_{i,j}. \tag{1.5}$$

So we see that uniqueness of the decomposition requires orthonormality of the basis vectors (really we just need orthogonality, but the normalization of orthonormality makes our lives easier).

Note that any finite dimensional vector space is *complete*; i.e. any sequence of vectors in the space converges to a vector that is still in the space.

1.2.2 Hilbert Space with a Countably Infinite Number of Basis Vectors

Let's first think about countably infinite dimensional vector spaces (really we're thinking about Hilbert spaces). Under very general conditions the solution set of differential equations (e.g. of Sturm-Liouville type) on a finite domain is a vector space with only a countably infinite number of basis functions. (The quantum mechanics of a particle in an infinite potential well is in this class of problems.) Let's think about spaces of functions, $f(x)$, with a set of basis vectors, $\{u_n\}$ with $n \in \mathbb{N}$. For definiteness let's take $x \in [a, b]$. Then we will have

$$f(x) = \sum_{n=1}^{\infty} a_n u_n(x), \tag{1.6}$$

$$a_n = \int_a^b f(x) u_n^*(x) dx. \tag{1.7}$$

What properties of the basis vectors, $\{u_n\}$, do we want? First, uniqueness of decomposition. Then

$$a_n = \int_a^b \sum_{m=1}^{\infty} a_m u_m(x) u_n^*(x) dx \tag{1.8}$$

$$= \sum_m a_m \int_a^b u_m(x) u_n^*(x) dx \tag{1.9}$$

$$= a_n. \tag{1.10}$$

Again, in order to get to the last line we require orthonormality of our basis functions:

$$\int_a^b u_m(x) u_n^*(x) dx = \delta_{m,n} \tag{1.11}$$

We also want an additional condition on the basis functions, namely that we can recover our function. Specifically

$$f(x) = \sum_n a_n u_n(x) = \sum_n \int_a^b f(x') u_n^*(x') dx' u) n(x) \tag{1.12}$$

$$= \int_a^b f(x') \sum_n u_n^*(x') u_n(x) dx' \tag{1.13}$$

$$= f(x). \tag{1.14}$$

In order to get to the last line we require *completeness* of our basis:

$$\sum_n u_n^*(x') u_n(x) = \delta(x - x'). \tag{1.15}$$

Completeness guarantees that I can decompose in my basis any function that is continuous almost everywhere.

1.2.3 Hilbert Space with Uncountably Infinite Number of Bases

Often the solution set of differential equations whose domain is unbounded is an uncountably infinitly dimensional Hilbert space. (From QM think wavepackets $\exp(ikx)$.) Now our set of basis functions is $\{u_k\}$ with $k \in \mathbb{R}$:

$$f(x) = \int_{-\infty}^{\infty} dk a_k u_k^*(x), \tag{1.16}$$

$$a_k = \int_{-\infty}^{\infty} dx f(x) u_k^*(x), \tag{1.17}$$

where we're now integrating over the index,k. Let's see what uniqueness of coefficients nets us.

$$\begin{aligned} a_k &= \int_{-\infty}^{\infty} dx f(x) u_k^*(x) && (1.18)\\ &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dk' a_{k'} u_{k'}(x) u_k^*(x) && (1.19)\\ &= \int_{-\infty}^{\infty} dk' a_{k'} \int_{-\infty}^{\infty} dx u_{k'}(x) u_k^*(x) && (1.20)\\ &= a_k. && (1.21) \end{aligned}$$

So in the case of an uncountably infinite number of basis functions we see that orthogonality now requires a Dirac as opposed to a Kronecker delta function:

$$\int_{-\infty}^{\infty} dx u_{k'}(x) u_k^*(x) = \delta(k - k'). \tag{1.22}$$

As for uniqueness of functions we have that

$$\begin{aligned} f(x) &= \int_{-\infty}^{\infty} dk a_k u_k(x) = \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dx' f(x') u_k^*(x') u_k(x) && (1.23)\\ &= \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dk u_k^*(x') u_k(x) && (1.24)\\ &= f(x). && (1.25) \end{aligned}$$

We still need a Direc delta function for completeness:

$$\int_{-\infty}^{\infty} dk u_k^*(x') u_k(x) = \delta(x - x'). \tag{1.26}$$

Notice the symmetry between the orthonormality and completeness relations. We will come back to this later.

1.3 Specific Examples of Expanding in a Basis

1.3.1 Finite Dimensional Vector Space Example

Orthonormality

Suppose we're again in $\mathbb{R}^2$, and we choose our basis vectors to be

$$\hat{e}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \hat{e}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{1.27}$$

It's clear that our basis vectors are orthonormal,

$$\hat{e}_i \cdot \hat{e}_j = \delta_{i,j}. \tag{1.28}$$

Decomposition Example

Suppose I have some vector $\mathbf{a}$. I can find its decomposition:

$$\hat{e}_1 \cdot \mathbf{a} = 3 \tag{1.29}$$

$$\hat{e}_2 \cdot \mathbf{a} = 4. \tag{1.30}$$

Then I know that I can write

$$\mathbf{a} = 3\hat{e}_1 + 4\hat{e}_2. \tag{1.31}$$

1.3.2 Countably Infinite Dimensionality Example

Orthonormality and Completeness

We will prove that on the domain of $(-a/2, a/2)$ the set of functions

$$\{u_n(x)\} = \left\{\sqrt{\frac{2}{a}}\sin\frac{2m\pi x}{a}, \sqrt{\frac{2}{a}}\cos\frac{2m\pi x}{a} \middle| m \in \mathbb{N}\right\} \bigcup \left\{\frac{1}{\sqrt{a}}\right\} \tag{1.32}$$

is a complete, orthonormal basis.

First, to make our lives easier, let's take $a \to 2$. Let's do orthnormality:

$$\int_{-1}^{1} dx \sin(\pi m x)\sin(\pi n x) = \frac{1}{2}\int_{-1}^{1}\left[\cos\big(\pi x(m-n)\big) - \cos\big(\pi x(m+n)\big)\right] \tag{1.33}$$

$$= \frac{1}{2}\left[\frac{\sin\big(\pi x(m-n)\big)}{\pi(m-n)} - \frac{\sin\big(\pi x(m+n)\big)}{\pi(m+n)}\right]_{x=-1}^{1}. \tag{1.34}$$

The first term is clearly 0 for $m \neq n$. Since m, $n > 0$ the second term is always 0. When $m = n$ we may return to the original integral and see that the normalization is correct. On the other hand we may also exploit l'Hôpital's rule to the same effect:

$$\lim_{m-n\to 0}\frac{\sin(\pi(m-n))}{\pi(m-n)} = 1. \tag{1.35}$$

Therefore we have that

$$\int_{-1}^{1} dx \sin(\pi m x)\sin(\pi n x) = \delta_{m,n}. \tag{1.36}$$

This argument follows in exactly the same way for the cosines. Sines and cosines are always orthogonal to each other on a domain such as this; similarly sines and cosines are also orthogonal on this domain to a constant. The constant basis funciton is clearly normalized properly.

Now let's check completeness. We want to check that

$$I_1 \equiv \frac{1}{2} + \sum_{n=1}^{\infty}\sin(n\pi x)\sin(n\pi y) + \cos(n\pi x)\cos(n\pi y) = \delta(x-y). \tag{1.37}$$

Note that the $1/2$ our front comes from the $1/\sqrt{2}$ basis function.

How would we go about proving that I_1 is a delta function? Well, what are the salient properties of a delta function? It turns out we need to show that

1. $\delta(x-y) = 0$ for $x \neq y$
2. $\int dx \delta(x-y) = 1$, where we require that y be within the region of integration

These two properties guarantee that the delta function behaves as we expect it; i.e., that $\int dx f(x)\delta(x-y) = f(y)$ for any smooth function f, and where again the region of integration is taken such that it includes y. This is because we can always Taylor expand the smooth function:

$$\int dx f(x)\delta(x-y) = \int dx\big[f(y) + f'(y)(x-y) + \ldots\big]\delta(x-y) \tag{1.38}$$

$$= f(y). \tag{1.39}$$

Let's get back to I_1. We have that

$$I_1 = \frac{1}{2} + \sum_{m=1}^{\infty} \cos\big(m\pi(x-y)\big) = -\frac{1}{2} + \frac{1}{2}\sum_{m=0}^{\infty} e^{im\pi(x-y)} + e^{-im\pi(x-y)}. \tag{1.40}$$

Examine

$$\sum_{m=0}^{\infty}\left[e^{i\pi(x-y)}\right]^m = \lim_{\varepsilon\to 0}\sum_{m=0}^{\infty}\left[e^{i\pi(x-y+i\varepsilon)}\right]^m \tag{1.41}$$

$$= \lim_{\varepsilon\to 0}\frac{1}{1-e^{i\pi(x-y+i\varepsilon)}} \tag{1.42}$$

$$= \frac{1}{1-e^{i\pi(x-y)}}. \tag{1.43}$$

Therefore

$$I_1 = -\frac{1}{2} + \frac{1}{2}\left[\frac{1}{1-e^{i\pi(x-y)}} + \frac{1}{1-e^{-i\pi(x-y)}}\right] \tag{1.44}$$

$$= -\frac{1}{2} + \frac{1}{2}\left[\frac{1-e^{-i\pi(x-y)}+1-e^{i\pi(x-y)}}{1-e^{i\pi(x-y)}-e^{-i\pi(x-y)}+1}\right] \tag{1.45}$$

$$= 0 \text{ for } x \neq y \tag{1.46}$$

So we know that the function is 0 everywhere that $x \neq y$. Now we just have to show that it has the right normalization to prove that it's a delta function. To make our lives easier, let's take $y = 0$. Then we need to integrate I_1 over a region in x that contains 0. We could integrate from $-\varepsilon$ to ε; it turns out our lives will be even easier still if we simply integrate from -1 to 1:

$$\int_{-1}^{1} I_1 dx = \int_{-1}^{1} \frac{1}{2} + \frac{1}{2}\sum_{m=1}^{\infty}\cos(m\pi x)dx \tag{1.47}$$

$$= 1 + \frac{1}{2}\sum_{m=1}^{\infty}\frac{\sin(m\pi x)}{m\pi}\Bigg|_{-1}^{1} \tag{1.48}$$

$$= 1. \tag{1.49}$$

Note that with the integration region we chose the entire weight of the delta function came from the constant 1/2; if we decided to shrink the integration region down the contribution from the constant would decrease with the contribution from the infinite sum compensating exactly.

Check notes online for a hint for HW problem 2.15.

Decomposition Example

Let's do an example where we explicitly determine the coefficients for a specified function using the previous basis. Suppose we have the function

$$f(x) = 1 - |x| \tag{1.50}$$

on the domain $x \in (-1, 1)$. Since f is an even function the coefficients of the sines are identically 0. The coefficient of the constant function is

$$a_0 = \int_{-1}^{1}\big(1-|x|\big)\frac{1}{\sqrt{2}}dx = \frac{2}{\sqrt{2}}\int_0^1 (1-x)dx \tag{1.51}$$

$$= \frac{1}{\sqrt{2}}\big(2x - x^2\big)\big|_0^1 = \frac{1}{\sqrt{2}}. \tag{1.52}$$

The coefficients a_n, $n > 0$ are found from

$$a_n = 2\int_0^1 (1-x)\cos(n\pi x)dx. \tag{1.53}$$

The 1 of the $1-x$ is identically 0 after integration over the cosine. For the contribution from the x, I don't like doing integration by parts so I'll use Feynman's trick. Consider

$$g(\alpha) \equiv \int_0^1 \sin(\alpha x) dx. \tag{1.54}$$

Note that by differentiating under the integral sign

$$\partial_\alpha g(\alpha) = \int_0^1 dx \partial_\alpha \big(\sin(\alpha x)\big) \tag{1.55}$$

$$= \int_0^1 x \cos(\alpha x) dx \tag{1.56}$$

gives us exactly the definite integral we wish to evaluate. Simple integration yields

$$g(\alpha) = -\left.\frac{\cos(\alpha x)}{\alpha}\right|_0^1 = \frac{1-\cos(\alpha)}{\alpha}. \tag{1.57}$$

The value of the definite integral is then

$$\partial_\alpha g(\alpha) = -\frac{1}{\alpha^2} - \frac{\sin(\alpha)}{\alpha} + \frac{\cos(\alpha)}{\alpha^2} \tag{1.58}$$

$$= \frac{\cos(n\pi)-1}{(n\pi)^2} = \frac{(-1)^n - 1}{(n\pi)^2}, \text{ for } \alpha = n\pi. \tag{1.59}$$

Plugging in the factor of -2 in the original integral we find then that

$$a_n = \begin{cases} \frac{4}{(n\pi)^2}, \ n \text{ odd} \\ 0, \ n \text{ even} \end{cases} \tag{1.60}$$

Putting everything together we find that

$$1 - |x| = \frac{1}{2} + \frac{4}{\pi^2} \sum_{m=1}^{\infty} \frac{\cos\big((2m+1)\pi x\big)}{(2m+1)^2}. \tag{1.61}$$

1.3.3 Uncountably Infinite Basis Example

Orthonormality and Completeness

An example of a set of basis functions for the unbound interval of $x \in (-\infty, \infty)$ is

$$u(x,k) = \left\{ \frac{1}{\sqrt{2\pi}} e^{ikx} \big| k \in \mathbb{R} \right\}. \tag{1.62}$$

These are so important we call the coefficients we find using u Fourier Transforms. Specifically

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} dx \tag{1.63}$$

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dk \tag{1.64}$$

One can think of Fourier Transforms as the continuum limit of Discrete Fourier Transforms, in which the (countably) infinite complete orthonormal basis is taken to be

$$u_m(x) = \left\{ \frac{1}{\sqrt{a}} e^{i2\pi m x/a} \big| m \in \mathbb{Z} \right\}. \tag{1.65}$$

This DFT basis is intimately related to the basis example given in the previous section; unlike the previous section the use of exponentials the nonconstant basis functions here have the same normalization as the constant basis function.

Let's check orthonormality.

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dx e^{ix(k-k')} = \frac{1}{2\pi}\lim_{\varepsilon\to 0}\left[\int_{0}^{\infty} dx e^{ix(k-k'+i\varepsilon)} + \int_{-\infty}^{0} dx e^{ix(k-k'-i\varepsilon)}\right] \tag{1.66}$$

$$= \frac{1}{2\pi}\lim_{\varepsilon\to 0}\left[\left.\frac{e^{ix(k-k'+i\varepsilon)}}{i(k-k'+i\varepsilon)}\right|_{0}^{\infty} + \left.\frac{e^{ix(k-k'+i\varepsilon)}}{i(k-k'+i\varepsilon)}\right|_{-\infty}^{0}\right] \tag{1.67}$$

$$= \frac{1}{2\pi}\lim_{\varepsilon\to 0}\left[-\frac{1}{i(k-k'+i\varepsilon)} + \frac{1}{i(k-k'-i\varepsilon)}\right] \tag{1.68}$$

$$= 0, \text{ for } k \neq k'. \tag{1.69}$$

Now let's check the normalization to finish the proof that it's a delta function. We can do this quite easily using contour integration (see, e.g., Brown and Churchill's "Complex Variables and Applications"). Let's set $k' = 0$ again. Then by choosing to close the contour above (we can just as easily close below),

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dx e^{ixk} = \frac{1}{2\pi i}\oint dk \lim_{\varepsilon\to 0}\left[\frac{1}{k-i\varepsilon} - \frac{1}{k+i\varepsilon}\right] = 1. \tag{1.70}$$

A less sophisticated, but no less correct, derivation uses common denominators:

$$\frac{1}{2\pi i}\lim_{\varepsilon\to 0}\int_{-\infty}^{\infty} dk \frac{2i\varepsilon}{k^2+\varepsilon^2} = \frac{1}{\pi}\lim_{\varepsilon\to 0}\tan^{-1}\left.\left(\frac{k}{\varepsilon}\right)\right|_{k=-\infty}^{\infty} = 1. \tag{1.71}$$

Symmetry between x and k demands that the completeness relation also holds; i.e.

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ik(x-x')} = \delta(x-x'). \tag{1.72}$$

This symmetry between x and k means there's a complete equivalence between working with $f(x)$ and $\tilde{f}(k)$.

Note that in the process above we've found two (very) useful expressions for the delta function:

$$\delta(x) = \begin{cases} \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ikx} \\ \frac{1}{2\pi}\lim_{\varepsilon\to 0}\left[\frac{1}{x-i\varepsilon} - \frac{1}{x+i\varepsilon}\right]. \end{cases} \tag{1.73}$$

Decomposition Example

Let

$$f(x) = e^{-x^2}. \tag{1.74}$$

Then

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx e^{-ikx} e^{-x^2} = \frac{1}{\sqrt{2\pi}}\sqrt{\pi} e^{-k^2/4}. \tag{1.75}$$

Therefore we can write

$$f(x) = \int_{-\infty}^{\infty} dk \frac{1}{\sqrt{2\pi}} e^{ikx} \frac{1}{\sqrt{2}} e^{-k^2/4} = \frac{1}{2\sqrt{\pi}}\int_{-\infty}^{\infty} dk e^{ikx} e^{-k^2/4}. \tag{1.76}$$

Note that, as must be true, performing the last integral returns $f(x) = \exp(-x^2)$.

1.4 Aside

In higher dimensions

$$\delta^{(n)}(\mathbf{x}-\mathbf{x}') = \delta(x_1 - x_1')\cdots\delta(x_n - x_n') \tag{1.77}$$

$$= \int \frac{dk_1}{2\pi} e^{ik_1(x_1-x_1')} \cdots \int \frac{dk_n}{2\pi} e^{ik_n(x_n-x_n')} \tag{1.78}$$

$$= \int \frac{d^n k}{(2\pi)^n} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}. \tag{1.79}$$

1.5 Fourier Transforms for Solving ODEs and PDEs

As an example, let's use FT to find the Green's function for the Laplacian in Cartesian coordinates in 3 dimensions:

$$\nabla^2_{\mathbf{x}} G(\mathbf{x},\mathbf{x}') = -4\pi\delta^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{1.80}$$

Let's begin by Fourier transforming G. Ordinarily we'd have to perform a double FT:

$$G(\mathbf{x},\mathbf{x}') = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}} \int \frac{d^3k'}{(2\pi)^{3/2}} e^{i\mathbf{k}'\cdot\mathbf{x}'} \tilde{G}(\mathbf{k},\mathbf{k}'). \tag{1.81}$$

However we notice that the RHS of Eq. (1.80) is symmetric with respect to $\mathbf{x}-\mathbf{x}'$; therefore G must respect this symmmetry: $G(\mathbf{x},\mathbf{x}') = G(\mathbf{x}-\mathbf{x}')$. Therefore we can get away with only a single FT:

$$G(\mathbf{x},\mathbf{x}') = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \tilde{G}(\mathbf{k}). \tag{1.82}$$

Plugging this expression for G back in to Eq. (1.80) and simultaneously expressing the delta function in the wavepacket basis yields

$$\nabla^2_{\mathbf{x}} \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \tilde{G}(\mathbf{k}) = -4\pi \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \tag{1.83}$$

$$\int \frac{d^3k}{(2\pi)^{3/2}} \tilde{G}(\mathbf{k}) \nabla^2_{\mathbf{x}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} = \int \frac{d^3k}{(2\pi)^{3/2}} \big[-\mathbf{k}^2 \tilde{G}(\mathbf{k})\big] = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \big[\frac{-4\pi}{(2\pi)^{3/2}}\big]. \tag{1.84}$$

In finite-dimensional vector spaces you know that for two vectors to be equal, their components in an orthnormal basis *must* be the same. Similarly, we showed that in infinite dimensional vector spaces the components of a function are *unique*. Therefore we can simply set the integrands in the last equation equal.

$$-\mathbf{k}^2 \tilde{G}(\mathbf{k}) = \frac{-4\pi}{(2\pi)^{3/2}} \quad \Rightarrow \quad \tilde{G}(\mathbf{k}) = \frac{4\pi}{(2\pi)^{3/2}} \frac{1}{\mathbf{k}^2}. \tag{1.85}$$

Therefore

$$G(\mathbf{x},\mathbf{x}') = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \frac{4\pi}{(2\pi)^{3/2}} \frac{1}{\mathbf{k}^2} \qquad \big(+F(\mathbf{x},\mathbf{x}') \text{ with } \nabla^2_{\mathbf{x}} F = 0\big). \tag{1.86}$$

We have exchanged a nasty PDE for an unpleasant integral, which we'll now evaluate.

$$G(\mathbf{x},\mathbf{x}') = \frac{1}{2\pi^2}\int k^2 dk \sin\theta d\theta d\phi \frac{1}{k^2} e^{ik|\mathbf{x}-\mathbf{x}'|\cos\theta} \tag{1.87}$$

$$= \frac{1}{2\pi^2} 2\pi \int_0^\infty dk \left[-\frac{e^{ik|\mathbf{x}-\mathbf{x}'|\cos\theta}}{ik|\mathbf{x}-\mathbf{x}'|} \right]_{\theta=0}^{\pi} \tag{1.88}$$

$$= \frac{1}{\pi}\int_0^\infty dk \frac{1}{ik|\mathbf{x}-\mathbf{x}'|} \left[e^{ik|\mathbf{x}-\mathbf{x}'|} - e^{-ik|\mathbf{x}-\mathbf{x}'|} \right] \tag{1.89}$$

$$= \frac{2}{\pi}\int_0^\infty dk \frac{\sin\left(k|\mathbf{x}-\mathbf{x}'|\right)}{k|\mathbf{x}-\mathbf{x}'|} \tag{1.90}$$

$$= \frac{2}{\pi}\frac{1}{|\mathbf{x}-\mathbf{x}'|}\int_0^\infty dt \frac{\sin t}{t} \tag{1.91}$$

$$= \frac{1}{|\mathbf{x}-\mathbf{x}'|}. \tag{1.92}$$

Note that in the first line we use the physicist's trick of choosing to align the z axis along the direction of $\mathbf{x}-\mathbf{x}'$, and in the last line we used a definite integral derived in HW1 (after changing variables to $t = k|\mathbf{x}-\mathbf{x}'|$.

Chapter 2

Separation of Variables

Separation of variables is a very powerful tool for solving PDEs (e.g. Poisson's Equation). Generically the method is as follows. Once you have your PDE, choose a coordinate system (e.g. Cartesian coordinates in 3D, x, y, z; there are generally 11 different coordinate systems which permit the use of Separation of Variables for the Poisson Equation). Assume the solution factorizes into functions that depend on only one coordinate (e.g. $\phi(x, y, z) = X(x)Y(y)Z(z)$). Then the PDE turns into a system of ODEs. The differential operators that one finds are usually of the Sturm-Liouville type; more generally speaking they are usually self-adjoint, which is in fact more restrictive in infinite dimensional spaces than Hermitian (see, e.g. Richtmyer's "Principles of Advanced Mathematical Physics," Hassani's "Mathematical Physics," or www.math.ohio-state.edu/~gerlach/math/BVtypeset for information on Sturm-Liouville theory, Hermitian, and self-adjointness). As a result the eigenfunctions of these differential operators, which are themselves solutions to the ODEs, will form a complete, orthonormal set. Therefore we will be able to describe any separable solution with boundary conditions consistent with the PDE.

2.1 Example: Poisson's Equation in 3D Cartesian Coordinates

This will often provide a very good means for solving box problems.

The partial differential equation we wish to solve is

$$\nabla^2_{\mathbf{x}}\phi(x, y, z) = \partial^2_x\phi(x, y, z) + \partial^2_y\phi(x, y, z) + \partial^2_z\phi(x, y, z). \tag{2.1}$$

Now suppose that the solution is separable. Then

$$\phi(x, y, z) = X(x)Y(y)Z(z). \tag{2.2}$$

Pluggin this back in to the original PDE yields

$$\Delta\phi(x, y, z) = Y(y)Z(z)X''(x) + X(x)Z(z)Y''(y) + X(x)Y(y)Z''(z). \tag{2.3}$$

Dividing by ϕ gives us

$$\frac{1}{X(x)}X''(x) + \frac{1}{Y(y)}Y''(y) + \frac{1}{Z(z)}Z''(z) = 0. \tag{2.4}$$

Since each of these terms depends only on x, y, or z, and these coordinates are all allowed to vary freely, each term must be equal to a constant. If a term, say the x one, was not equal to a constant, then in order for the whole to sum to zero the other terms would have to have some dependence on x, too; we assumed this not to be the case so it is not a possibility. Let's choose these constanst such that

$$\frac{1}{X(x)}X''(x) = -\alpha^2 \tag{2.5}$$

$$\frac{1}{Y(y)}Y''(y) = -\beta^2 \tag{2.6}$$

$$\frac{1}{Z(z)}Z''(z) = \alpha^2 + \beta^2 \equiv \gamma^2. \tag{2.7}$$

Note that α, $\beta \in \mathbb{C}$ are at this point completely arbitrary. We will find that their values become restricted once we impose boundary conditions (for instance if the box is of finite volume then they take on only discrete values). The solutions of these differential equations are trivially

$$X(x) = A_\alpha e^{i\alpha x} + B_\alpha e^{-i\alpha x} \tag{2.8}$$

$$Y(y) = A_\beta e^{i\beta y} + B_\beta e^{-i\beta y} \tag{2.9}$$

$$Z(z) = A_\gamma e^{\gamma z} + B_\gamma e^{-\gamma z}, \tag{2.10}$$

where the A_μ and B_ν will be set uniquely by the boundary conditions. The general solution to our problem is

$$\phi(x,y,z) = \text{“}\int d\alpha d\beta\text{”} \left(A_\alpha e^{i\alpha x} + B_\alpha e^{-i\alpha x}\right)\left(A_\beta e^{i\beta y} + B_\beta e^{-i\beta y}\right)\left(A_\gamma e^{\gamma z} + B_\gamma e^{-\gamma z}\right), \tag{2.11}$$

where the integration is in quotes because it's meant to represent a sum over all possibilities for the constants α and β; in some cases this will result in an integral, in others a discrete sum. Technically, then, it's a Stieltjes integral (without the quotes), which allows one to incorporate both summation over discrete terms and integration over the continuous terms in a single formula (see Richtmyer).

Example of Determining A_μ and B_μ for a Specific Box

Suppose we take our box problem and assume that it is of finite extent—$x \in [0,a]$, $y \in [0,b]$, and $z \in [0,c]$—and we set all sides to have potential 0 except for the top, for which we take $V(x,y,z=c) = V(x,y)$ and leave $V(x,y)$ unspecified. What is the solution? Immediately we know that

$$X(0) = 0 \;\Rightarrow\; X(x) \sim \sin(\alpha x) \tag{2.12}$$

$$X(a) = 0 \;\Rightarrow\; X(x) \sim \sin\left(\frac{n\pi x}{a}\right) \tag{2.13}$$

$$Y(0) = 0 \;\Rightarrow\; Y(y) \sim \sin(\beta y) \tag{2.14}$$

$$Y(b) = 0 \;\Rightarrow\; Y(y) \sim \sin\left(\frac{m\pi y}{b}\right) \tag{2.15}$$

$$Z(0) = 0 \text{ and } \alpha,\beta \in \mathbb{R} \;\Rightarrow\; Z(z) \sim \sinh(\gamma_{n,m} z), \tag{2.16}$$

where

$$\gamma_{n,m} = \sqrt{\alpha_n^2 + \beta_m^2} = \sqrt{\left(\frac{n\pi}{a}\right)^2 + \left(\frac{m\pi}{b}\right)^2} > 0. \tag{2.17}$$

The general solution is then

$$\phi(x,y,z) = \sum_{n,m=1}^{\infty} A_{n,m} \sin(\alpha_n x)\sin(\beta_m y)\sinh(\gamma_{n,m} z). \tag{2.18}$$

We need to solve for $A_{n,m}$. We will have one boundary condition left:

$$\phi(x,y,z=c) = \sum n,m=1^\infty A_{n,m} \sin(\alpha_n x)\sin(\beta_m y)\sinh(\gamma_{n,m} c) = V(x,y). \tag{2.19}$$

Let's use the orthonormality of sines. Integrate both sides by

$$\int_0^a dx \left(\frac{2}{a}\right) \sin\left(\frac{n'\pi x}{a}\right) \int_0^b dy \left(\frac{2}{b}\right) \sin\left(\frac{m'\pi y}{b}\right). \tag{2.20}$$

Then we will have that

$$A_{n',m'} \sinh(\gamma_{n,m} c) = \frac{4}{ab} \int_0^a dx \int_0^b dy \sin\left(\frac{n'\pi x}{a}\right) \sin\left(\frac{m'\pi y}{b}\right) V(x,y) \tag{2.21}$$

$$\therefore A_{n',m'} = \frac{4}{ab \sinh(\gamma_{n,m} c)} \int_0^a dx \int_0^b dy \sin\left(\frac{n'\pi x}{a}\right) \sin\left(\frac{m'\pi y}{b}\right) V(x,y). \tag{2.22}$$