# P231: Mathematical Methods in Graduate Physics

## Flip Tanedo

flip.tanedo@ucr.edu

Department of Physics & Astronomy, University of California, Riverside, CA 92521

#### Abstract

This is a crash course on mathematical methods necessary to succeed in the first-year physics graduate curriculum at UC Riverside. The focus is how to solve differential equations using Green's functions.

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## 1 Introduction: Why mathematical methods?

Physics 231: Methods of Theoretical Physics is a course for first-year physics and astronomy lec 01 graduate students. It is a 'crash course' in mathematical methods necessary for graduate courses in electrodynamics, quantum mechanics, and statistical mechanics. It is a *boot camp* rather than a rigorous theorem–proof mathematics class. Where possible, the emphasis is on physical intuition rather than mathematical precision.

#### 1.1 Green's functions

Our primary goal is to solve linear differential equations:

$$\mathcal{O}f(x) = s(x) \ . \tag{1.1}$$

In this equation,  $\mathcal{O}$  is a differential operator that encodes some kind of physical dynamics<sup>1</sup>, s(x) is the source of those dynamics, and f(x) is the system's physical response that we would like to determine. The solution to this equation is:

$$f(x) = \mathcal{O}^{-1}s(x) . (1.2)$$

Simply writing that is deeply unsatisfying! In this course, we think carefully about what  $\mathcal{O}^{-1}$  actually *means* and how we can calculate it. As you may have guessed,  $\mathcal{O}^{-1}$  is the **Green's function** for the differential operator  $\mathcal{O}$ .

We approach problem by analogy to linear algebra, where a linear transformation  $^2$  A acts on a vector to give equations like

$$A\mathbf{v} = \mathbf{w} , \qquad (1.3)$$

<sup>&</sup>lt;sup>1</sup>A differential operator is just something built out of derivatives that can act on a function. The differential operator may contain coefficients that depend on the variable that we are differentiating with respect to; for example,  $\mathcal{O} = (d/dx)^2 + 3x(d/dx)$ . Pop quiz: is this operator linear? The first term is squared...

<sup>&</sup>lt;sup>2</sup>Recall that as physicists, 'linear transformation' is a fancy way of saying 'matrix.'

$$\mathbf{v} = A^{-1}\mathbf{w} \ . \tag{1.4}$$

We connect the notion of a linear differential operator to a matrix in an infinite dimensional space to give a working definition of  $\mathcal{O}^{-1}$ . We then pull out a bag of tricks from complex analysis to actually solve  $\mathcal{O}^{-1}s(x)$  given  $\mathcal{O}$  and s(x).

### 1.2 This is not what I expected from a math methods course

This is a course in mathematical methods for *physicists*. We will not solve *every* class of differential equation that is likely to pop up in your research careers<sup>3</sup>—that's neither feasible nor particularly enjoyable. This is also not a course in formal proofs—there are plenty of excellent textbooks for you to learn those formal proofs to your heart's content<sup>4</sup>. The goal of this course is to weave together ideas that are not often connected explicitly in undergraduate physics courses in the United States: linear algebra, differential equations, complex analysis. These ideas are not necessarily new—in fact, I *expect* you have seen many them often—but rather we will take a big view of how the interconnection of these ideas come up over and over again in our description of nature.

Do not be surprised if we only mention Bessel functions in passing. Do not think less of our efforts if we do not determine Wronksians or go beyond a single Riemann sheet. As graduate students, it is *your* responsibility to be able to grab your favorite textbook to apply mathematics as needed to your research. *This course* is about the larger narrative that is not often shared explicitly in those books. It is the 'knack for math' that physicists are, as a culture, rather proud of. It is what tends to make us employable in Silicon Valley while simultaneously terrible at splitting the bill at a restaurant.

## 1.3 The totally not-mathematical idea of mathematical niceness

I find it useful to appeal to the notion of a **nice** mathematical situation. This is not a formal idea, and it is one many things mathematicians find ridiculous about me. But as a physicist, the concept of mathematical *niceness* is helpful.

The physical systems that we spend the most time thinking about are all *nice*. While our mathematical cousins may spend years proving every exceptional case to a theorem, we tend to be happy to push onward as long as mathematical results are true for the *nice* cases. Nice mathematical models make tidy predictions. Then we can Taylor expand about these nice predictions to make better predictions. When doing this, we sometimes say *perturbation theory* multiple times in case someone watching us does not think are being rigorous enough.

This is not to say that nature cares at all about our physical models. Every once in a while, we do have to worry about the exceptional cases because our models fail to accommodate what is actually happening in nature. Those scenarios are the most interesting of all. That's when our mathematical formalism grabs us by the collar and says, listen to me—something

<sup>&</sup>lt;sup>3</sup>That would be a course on mathematical methods for *engineers*.

<sup>&</sup>lt;sup>4</sup>... and as a graduate student, you should feel well equipped and encouraged to learn all of the necessary material *you* need for *your* research and interests—whether or not they show up in your coursework.

important is happening and it probably has to do with nature! This often happens when a calculation tells us that a physical result is infinite.

Exercise 1.1 Consider the potential that an electron feels in the hydrogen atom:

$$V(r) = -\frac{\alpha}{r} \ . \tag{1.5}$$

As the electron-proton separation goes to zero,  $r \to 0$ , the potential goes to infinity. Classical electrodynamics is telling us that something curious is happening. What actually happens? (And why didn't you ask this question when you were in high school?)

In this course we focus on *nice* functions and *nice* operators and *nice* boundary conditions, etc. For the most part, this is what we need to make progress on our physical models and it's worth spending our time learning to work with *nice* limits. Leave the degenerate cases to the mathematicians for now. Eventually, though, you may find yourself in a situation where physics demands *not nice* mathematics. In that case—and only when the physics demands it—you will be ready to poke and prod at the mathematical curiosity until the underlying *physics* reason for the not-niceness is apparent.

### 1.4 Physics versus Mathematics

Let's make one point clear:

lec 02

Physics 
$$\neq$$
 Mathematics . (1.6)

This is a truth in many different respects<sup>5</sup>:

- Physicists are rooted in experimental results<sup>6</sup>.
- Physicists Taylor expand to their hearts' content—sometimes even when the expansion is not formally justified<sup>7</sup>.
- Physicists use explicit coordinates, mathematicians abhor this. Even worse, we pick a basis and decorate every tensor with indices<sup>8</sup>.
- Physicists seek to uncover a truth about this universe.

## 1.5 The most important binary relation

When we write equations, the symbol that separates the left-hand side from the right-hand side is a binary relation. We use binary relations like = or  $\neq$ . Sometimes to make a point we'll write  $\cong$  or  $\equiv$  or  $\stackrel{.}{=}$  to mean something like 'definition' or 'tautologically equivalent to' or some other variant of even more equal than equal.

As physicists the most important binary relation is none of those things<sup>9</sup>. Usually what we really care about is in  $\sim$ .<sup>10</sup> This tells how how something *scales*. If I double a quantity

<sup>&</sup>lt;sup>5</sup>The astronomer Fritz Zwicky would perhaps call this a *spherical truth*; no matter how you look at it, the statement is still true.

<sup>&</sup>lt;sup>6</sup>Even theorists? *especially* theorists.

<sup>7</sup>https://johncarlosbaez.wordpress.com/2016/09/21/struggles-with-the-continuum-part-6/

<sup>&</sup>lt;sup>8</sup>Those who are not trained may be intimidated by physics because of all the indices we use. Ironically, physicists are often intimidated by mathematics because of the conspicuous absence of any indices.

<sup>9</sup>https://xkcd.com/2343/

<sup>&</sup>lt;sup>10</sup>I use this the same way as  $\propto$ , which is completely different from 'approximately,'  $\approx$ .

on the right-hand side, how does the quantity on the left-hand side scale? Does it depend linearly? Quadratically? Non-linearly? The answer encodes something important about the underlying physics of the system. It's the reason why *imagine the cow is a sphere* is a popular punchline in a joke about physicists.

By the way, implicit in this is the idea that in this class, we will not care about stray factors of 2. As my adviser used to say, if you're worried about a factor of 2, then your additional homework is to figure out that factor of 2.<sup>11</sup>

#### 1.6 Units

There is another way in which physics is different from mathematics. It is far more prosaic. *Quantities in physics have units*. We don't just deal with numbers, we deal with kilograms, electron volts, meters. It turns out that dimensional analysis is a big part of what we do as physicists.

## 2 Dimensional Analysis

You may be be surprised how far you can go in physics by thinking deeply about dimensional lec 03 analysis. Here we'll only get you started. To go one step further, you may read more about the Buckingham Pi theorem<sup>12</sup> or dive into neat applications<sup>13</sup>.

## 2.1 Converting Units

Imagine that you have three apples. This is a number (three) an a unit (apple). The meaning of the unit depends on what you're using it to measure. For example, if apples are \$1 each, then you could use an apple as a unit of currency. The way to do this is to simply multiply by one:

$$(3 \text{ apples}) \times \left(\frac{\$ 1}{\text{apple}}\right) = \$3. \tag{2.1}$$

We have used the fact that the exchange rate is simply the statement that

$$1 \text{ apple} = \$1 \qquad \Rightarrow \qquad 1 = \frac{\$1}{1 \text{ apple}} \,. \tag{2.2}$$

You can do a similar thing for [kilo-]calories or any other conversion rate.

All that matters is that the conversion is constant. Indeed, the constants of nature make very good 'exchange rates.' For example, in high-energy physics we like to use **natural units**. This is the curious statement that

$$\hbar = c = 1 . \tag{2.3}$$

<sup>&</sup>lt;sup>11</sup>That being said, you're reading these notes and find an error, do let me know about it.

<sup>12</sup>https://aapt.scitation.org/doi/10.1119/1.1987069

<sup>13</sup>https://aapt.scitation.org/doi/full/10.1119/1.3535586, http://inspirehep.net/record/153032?ln=en

At face value, this doesn't make sense.  $\hbar$  has units of action, c is a speed, and 1 is dimensionless. However, because nature gives us a *fundamental* unit of action and a *fundamental* unit of speed, we may use them as conversion factors (exchange rates),

$$c = 3 \times 10^{10} \text{ cm/s}$$
 (2.4)

If c = 1, then this means

$$1 \text{ s} = 3 \times 10^{10} \text{ cm}$$
 (2.5)

This, in turn, connects a unit of time to a unit of distance. By measuring time, the constant c automatically gives us an associated distance. The physical relevance of the distance is tied to the nature of the fundamental constant: one second (or 'light-second') is the distance that a photon travels in one second. Observe that this only works because c is a constant.

### 2.2 Quantifying units

We use the notation that a physical quantity Q has **dimension** [Q] that can be expressed in terms of units of length, mass, and time:

$$[Q] = L^a M^b T^c . (2.6)$$

The dimension is the statement of the powers a, b, and c. You may want to also include units of, say, electric charge. Sticklers may pontificate about whether electric charge formally carries a new unit or not.

**Example 2.1** What are the units of force? We remember that  $\mathbf{F} = m\mathbf{a}$ , so

$$[\mathbf{F}] = [m][\mathbf{a}] = M \times LT^{-2} = L^1 M^1 T^{-2}$$
 (2.7)

Life is even easier in **natural units**, where c=1 means that units of length and time are 'the same' and  $\hbar=1$  means that units of time and energy (mass) are inversely related. In natural units, one typically write [Q] to mean the mass-dimension of a quantity. To revert back to conventional units, one simply multiplies by appropriate factors of 1=c and  $1=\hbar$ .

**Example 2.2** What are the units of force in natural units? From (2.7) we multiply by one to convert length and time into mass dimensions:

$$[\mathbf{F}] = [c^{-3}\hbar\mathbf{F}] = M^2$$
 (2.8)

In natural units we say  $[\mathbf{F}] = 2$ . Recall that energy and mass have the same dimension, which you may recall from the Einstein relation  $E^2 = m^2c^4 + p^2c^2$ .

## 2.3 Usage: Sanity Check

The simplest use of dimensional analysis is to check your work. The following expression is obviously wrong:

$$1 + (3 \text{ cm})$$
 (2.9)

This does not make sense. You cannot sum terms with different dimensions. Similarly,  $\sin(3 \text{ cm})$  does not make sense. What about  $e^{5 \text{ cm}}$ ? This doesn't make sense because

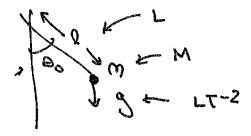
$$e^x = 1 + x + \frac{1}{2!}x^2 + \dots {2.10}$$

Since each term comes with a different power of x, the argument of the exponential must be dimensionless.

Exercise 2.1 Consider the energy spectrum of light emitted from some constant source—a distant star, the ongoing annihilation of dark matter in the galactic center, a laser in the Hemmerling lab. The spectrum encodes how many photons are emitted per unit time. We can plot this spectrum as a curve on a graph. We can even normalize the curve so that it integrates to one photon. This means we only care about the distribution of energy, not the absolute amount. The horizontal axis of such a plot is the photon energy. What are the units of the vertical axis?

## 2.4 Usage: Solving problems

Here's a common problem in introductory physics. Assume you have a pendulum with some [sufficiently small] initial displacement  $\theta_0$ . What's the period,  $\tau$  of the pendulum? We draw a picture like this:



From dimensional analysis, we know that the period has dimensions of time,  $[\tau] = T$ . The problem gives us a length  $[\ell] = L$  and the gravitational acceleration,  $[g] = LT^{-2}$ . Note that  $[\theta_0] = 1$  is dimensionless. This means that the only way to form a quantity with dimensions of time is to use  $g^{-1/2}$ . This leaves us with a leftover  $L^{-1/2}$ , which we can fix by inserting a square root of  $\ell$ :

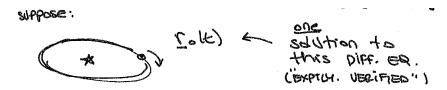
$$\tau \sim q^{-1/2} \ell^{1/2} \ . \tag{2.11}$$

If we wanted to be fancy, we can make this an equal sign by writing a function of the other dimensionless quantities in the problem:

$$\tau = f(\theta_0) \sqrt{\frac{\ell}{g}} \ . \tag{2.12}$$

## 2.5 Scaling

A large part of physics has to do with scaling relations. Here's a somewhat contrived example of how this works<sup>14</sup>. Suppose you have some static, central potential  $U(\mathbf{r})$ . Maybe it's some planet orbiting a star.



The force law gives:

$$m\ddot{\mathbf{r}} = -\frac{\partial U}{\partial \mathbf{r}} \ . \tag{2.13}$$

Suppose we are given a solution,  $\mathbf{r}_0(t)$ . Perhaps this is a trajectory that is experimentally verified. Dimensional analysis gives a way to scale this solution into other solutions. For example, let us scale time by defining a new variable t':

$$t \equiv \alpha t' \ . \tag{2.14}$$

If the potential is static, then only the left-hand side of the force law changes. Even though the right-hand side formally has dimensions of time  $\sim T^{-2}$ , it does not transform because those units are carried in a constant, perhaps  $G_N$ , not a  $(d/dt)^2$  like the left-hand side. The left-hand side of the force law gives:

$$m\left(\frac{d}{dt}\right)^{2}\mathbf{r}_{0}(t) = m\alpha^{-2}\left(\frac{d}{dt'}\right)^{2}\mathbf{r}_{0}(\alpha t'). \qquad (2.15)$$

This begs us to define a new mass  $m' = m\alpha^{-2}$ . We thus have

$$m'\left(\frac{d}{dt'}\right)^2 \mathbf{r}_0(\alpha t') = -\frac{\partial U}{\partial \mathbf{r}_0}$$
 (2.16)

What this tells us is that  $\mathbf{r}_1(t') \equiv \mathbf{r}_0(\alpha t')$  is a solution in the same potential that traces the same trajectory but at  $\alpha$  times the speed and with mass m'. Changing labels  $t' \to t$  for a direct comparison:

$$m'\left(\frac{d}{dt}\right)^2 \mathbf{r}_1(t) = -\frac{\partial U}{\partial \mathbf{r}_1} ,$$
 (2.17)

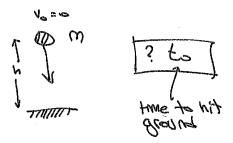
which is indeed<sup>15</sup> (2.13) with a new mass m' and a trajectory  $\mathbf{r}_1(t') \equiv \mathbf{r}_0(\alpha t')$ . For example, if  $\alpha = 2$ , then  $\mathbf{r}_1(t)$  traces the same trajectory at double the velocity with one fourth of the mass.

<sup>&</sup>lt;sup>14</sup>This is adapted from section 11 of V. I. Arnold's *Mathematical Methods of Classical Mechanics*, one of my favorite differential geometry textbooks because it's disguised as a book on mechanics.

<sup>&</sup>lt;sup>15</sup>We were able to swap  $\mathbf{r}_0$  with  $\mathbf{r}_1$  simply because U only depends on the position.

### 2.6 Error Estimates

This section is based on a lovely *American Journal of Physics* article by Craig Bohren. <sup>16</sup> Let's go back to another high school physics problem.



Suppose you drop a mass m from height h that is initially at rest. How long before this hits the ground? You can integrate the force equation to get

$$t_0 = \sqrt{\frac{2h}{g}} \ . \tag{2.18}$$

This is the *exact* answer within our model of the system. The model made several assumptions. The mass is a point mass, the gravitational acceleration is constant at all positions, there is no air resistance, etc. In fact, we know that if we do an experiment, our result will almost certainly not be  $t_0$ . All we know is that  $t_0$  is probably a good approximation of what the actual answer is.

How good of an approximation is it?

One way to do this is to do the next-to-leading order ('NLO') calculation, taking into account a more realistic (and hence more complicated) model and then compare to  $t_0$ . But this is stupid. Why do we need to do a *hard* calculation to justify doing an *easy* one? If we're going to do the hard calculation anyway, what's the point of ever doing the easy one?

What we really want is an error estimate. The error is

$$\epsilon = \frac{t_1 - t_0}{t_0} \ . \tag{2.19}$$

This is a dimensionless quantity that determines how far off  $t_0$  is from a more realistic calculation,  $t_1$ . Ideally we don't actually have to do work to get  $t_1$ .

Let's assume that we're not completely nuts and that we're in a regime where the error is small<sup>17</sup>. Then the error is a function of some dimensionless parameters,  $\xi$ , in the system. We define these  $\xi$  so that as  $\xi \to 0$ ,  $\epsilon(\xi) \to 0$ . In other words, the approximation gets better as the  $\xi$  are made smaller. By Taylor expansion:

$$\epsilon(\xi) = \epsilon(0) + \epsilon'(0)\xi + \mathcal{O}(\xi^2) . \tag{2.20}$$

<sup>&</sup>lt;sup>16</sup>https://doi.org/10.1119/1.1574042

<sup>&</sup>lt;sup>17</sup>Note the error has to be dimensionless in order for us to be able to call it 'small,' otherwise it begs the question of 'small with respect to what;

By assumption  $\epsilon(0) = 0$  and  $\mathcal{O}(\xi^2)$  is small. We can then make a reasonable assumption that the dimensionless value  $\epsilon'(0)$  is  $\mathcal{O}(1)$ . This tells us that the error goes like  $\epsilon(\xi) \sim \xi$ .

By the way  $\mathcal{O}(1)$  is read "order one" and is fancy notation for the order of magnitude. Numbers like 0.6, 2, and  $\pi$  are all  $\mathcal{O}(1)$ . A number like  $4\pi^2$ , on the other hand, is  $\mathcal{O}(10)$ . The assumption that a dimensionless number is  $\mathcal{O}(1)$  is reasonable. When nature gives you a dimensionless parameter that is both (a) important and (b) very different from  $\mathcal{O}(1)$ , then there's a good chance that it's trying to tell you something about your model. Good examples of this are the cosmological constant, the strong CP phase, and the electroweak hierarchy problem<sup>18</sup>.

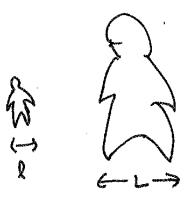
Here's how it works in practice. One effect that we miss in our toy calculation of  $t_0$  is that the earth is round with radius R. This means that assuming a constant g is an approximation. We have two choices for a dimensionless parameter  $\xi$ :

$$\xi = \frac{h}{R} \qquad \text{or} \qquad \qquad \xi = \frac{R}{h} \,. \tag{2.21}$$

There is an obvious choice:  $\xi = h/R$ , because we know that as h is made smaller (drop the ball closer to the ground) or R becomes bigger (larger radius of Earth) then the constant g approximation gets better. We thus expect that the corrections from the position-dependence of g go like  $\mathcal{O}(h/R)$ .

### 2.7 Bonus: Allometry

There's a fun topic called **allometry**. This is basically dimensional analysis applied to biology. A typical example is to consider two people who have roughly the same shape but different characteristic lengths,  $\ell$  and L:



Exercise 2.2 If both people exercised at the same rate, which one loses more absolute weight? By how much? Let's assume that weight loss is primarily from the conversion of organic molecules into carbon dioxide.

<sup>&</sup>lt;sup>18</sup>There are also 'bad' examples. The ratio of the angular size of the moon to the angular size of the sun is unity to very good approximation. This is quite certainly a coincidence. Our universe appears to be in an epoch where the density of matter, radiation, and dark energy all happen to be in the same ballpark. Our cosmological models imply that this is purely a coincidence. It would be very curious if this were not the case. As an exercise, you can explore (and critique) the appearance of the anthropic principle in physics.

Exercise 2.3 David Hu won his first IgNobel prize for determining that mammals take about 21 seconds to urinate, largely independently of their size<sup>19</sup>. Can you use dimensional analysis to argue why this would be the case? It may be helpful to refer to the paper<sup>20</sup>; as you read this, figure out which terms are negligible (and in what limits), identify the assumptions of the mathematical model (scaling of the bladder and urethra), and prove the approximate scaling relation. Make a note to yourself of which steps were non-trivial and where one may have naively mis-modeled the system. By the way, David Hu won a second IgNobel prize for understanding how wombats poop.

## 3 Linear Algebra Review

As physicists, linear algebra is part of our DNA, from the vector calculus in our first electrodynamics course to quantum mechanics. So why should we patronize ourselves with yet another review of linear algebra? We want to understand Green's functions the inverse of a matrix. The 'matrix' in question is the differential operator  $\mathcal{O}$  in (1.1). This is important:

differential operator = 
$$\infty$$
-dimensional matrix. (3.1)

If differential operators are matrices, what vector space do these matrices act on? These matrices act on a space of functions, which turns out to be a vector space:

function space = 
$$\infty$$
-dimensional vector space. (3.2)

Don't be intimidated by terminology like function space; this is just an abstract place where functions live. Just recall back to your intuition from 3D Euclidean vector space,  $\mathbb{R}^3$ : any 3-vector  $\mathbf{v}$  lives in the vector space  $\mathbb{R}^3$ . If we transform  $\mathbf{v}$  by a linear transformation A, you get a new vector  $\mathbf{w} = A\mathbf{v} \in \mathbb{R}^3$  that is also in the vector space.

Weird things can happen when we extend our intuition from finite things to infinite things<sup>21</sup>, but for this course we'll try to draw as much intuition as we can from finite dimensional linear algebra to apply it to infinite dimensional function spaces.

#### 3.1 The basics

A linear transformation A acts on a vector  $\mathbf{v}$  as  $A\mathbf{v}$ . This transformation satisfies

$$A(\alpha \mathbf{v} + \beta \mathbf{w}) = \alpha A \mathbf{v} + \beta A \mathbf{w} . \tag{3.3}$$

Here  $\alpha$  and  $\beta$  are numbers. This is conventionally matrix multiplication. The result is also a vector. One way that we like to think about vectors is as columns of elements:

$$\begin{pmatrix} v^1 \\ v^2 \\ \vdots \\ v^N \end{pmatrix} , \tag{3.4}$$

<sup>&</sup>lt;sup>19</sup>I learned about this in his excellent popular science book, *How To Walk on Water and Climb Up Walls*.

<sup>&</sup>lt;sup>20</sup>https://doi.org/10.1073/pnas.1402289111

<sup>&</sup>lt;sup>21</sup>For example, the Hilbert Hotel puzzle.

where N is the **dimension** of the vector space. Our notation is that  $v^i$  refers to the  $i^{th}$  component of  $\mathbf{v}$ . Sometimes—as physicists—we refer to  $v^i$  as the vector itself, which is a slight abuse of notation that occasionally causes confusion.

In this course we always assume a nice orthonormal basis. In this case,  $(\mathbf{v} + \mathbf{w})^i = v^i + w^i$ .

**Exercise 3.1** Convince yourself that adding vectors becomes more complicated in polar coordinates. Namely,  $(\mathbf{v} + \mathbf{w})^i \neq v^i + w^i$ .

Because the linear transformation of a vector is another vector, we know that the sequential application of linear transformations is itself a linear transformation. This is a bombastic way of saying that you can multiply matrices to produce a matrix. Here's how it works in two dimensions. A transformation that takes vectors into vectors takes the following form:

$$A = \begin{pmatrix} A_1^1 & A_2^1 \\ A_1^2 & A_2^2 \end{pmatrix} . {3.5}$$

We have introduced upper and lower indices; for now treat this as a definition. This sometimes causes confusion. So here are some guidelines:

- Treat the upper and lower indices as a definition. The components of the linear transformation A are defined by  $A^{i}_{j}$  where i is the row number and j is the column number.
- We have not yet explained the significance of the heights, but for now we mandate that the first index is always upper and the lower index is always lower. The following objects do not (yet) make sense:  $A_2^1$  and not  $A_{12}$ ,  $A_{12}^{12}$ , or  $A_{12}^{2}$ .
- We will soon define *additional machinery* to raise and lower indices shortly. This is takes us from a vector space to a metric space.
- The heights of the indices are a convenient shorthand notation that we will elucidate shortly; it is related to the choice of upper indices in (3.4).
- All of this may be familiar from special relativity. Extra credit if you realize that this should also be familiar from quantum mechanics.

If you're squeamish about the indices, don't worry: the elements of A have two indices, the first one is written a little higher than the second one. This notation is neither mathematics nor physics, it's a convention that we use for future convenience.

The action of a linear transformation A on a vector  $\mathbf{v}$  is:

$$A\mathbf{v} = \begin{pmatrix} A_1^1 & A_2^1 \\ A_1^2 & A_2^2 \end{pmatrix} \begin{pmatrix} v^1 \\ v^2 \end{pmatrix} = \begin{pmatrix} A_1^1 v^1 + A_2^1 v^2 \\ A_1^2 v^1 + A_2^2 v^2 \end{pmatrix} . \tag{3.6}$$

Look at this carefully. The components of the new vector  $(A\mathbf{v})^i$  are sums. In each term, the second/lower index of an A element multiplies the component of  $\mathbf{v}$  with the same index. The first/upper index of A tells you whether that term should is in  $(A\mathbf{v})^1$  or  $(A\mathbf{v})^2$ .

A generic component of  $(A\mathbf{v})$  is

$$(A\mathbf{v})^i = \sum_j A^i_{\ j} v^j = A^i_{\ j} v^j \quad \text{(Einstein convention)} \ . \tag{3.7}$$

On the right-hand side we use Einstein notation: we implicitly sum over repeated upper/lower indices. We will use this notation from now on. If you are at all in doubt about this, please work out the  $2 \times 2$  case carefully and compare to the succinct notation above.

**Exercise 3.2** Consider three-dimensional Euclidean space,  $\mathbb{R}^3$ . A linear transformation A on this space is a  $3 \times 3$  matrix with elements of the form  $A^i{}_j$ . Explicitly write out the second component of the vector  $A\mathbf{v}$ . This is a sum of three terms.

If A and B are linear transformations, then A + B is a linear transformation. The components of A + B are simply the piecewise sum of the corresponding components of A and B:

$$(A+B)^{i}_{j} = A^{i}_{j} + B^{i}_{j} . {3.8}$$

## 3.2 Linear Transformations and Vector Spaces

Let's be a little more pedantic. We need to move past the idea that a vector  $\mathbf{v}$  is some *column* of numbers. A vector space is abstract and we need to to start thinking of vector spaces more generally. The layer of abstraction is encoded in the basis vectors, which we write as  $\mathbf{e}_{(i)}$ . For a space of dimension N, there are N such vectors indexed by the subscript. Let us more formally write the vector  $\mathbf{v}$  as

$$\mathbf{v} = v^1 \mathbf{e}_{(1)} + v^2 \mathbf{e}_{(2)} + \dots = v^i \mathbf{e}_{(i)} .$$
 (3.9)

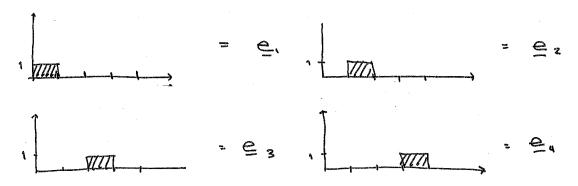
These basis vectors may be unit vectors in space. In the 'column of numbers' representation, they can be unit column vectors, e.g.

$$\mathbf{e}_{(1)} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \qquad \mathbf{e}_{(2)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad \qquad \cdots \qquad (3.10)$$

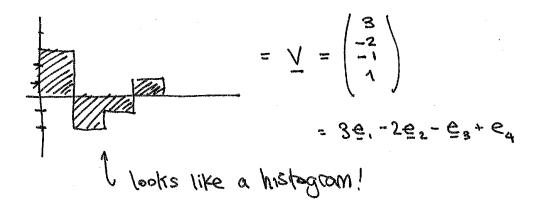
With this basis, (3.9) gives (3.4) But these may be more general objects. For example, you can specify a color of light by specifying the red/green/blue content. We could have  $\mathbf{e}_{(1)}$  be a unit amount of red light,  $\mathbf{e}_{(2)}$  be a unit amount of green light, and  $\mathbf{e}_{(3)}$  be a unit amount of blue light. Then a 3-vector  $\mathbf{v}$  would correspond to light of a particular color. This color space is a vector space.

## 3.3 A funny vector space: histogram space

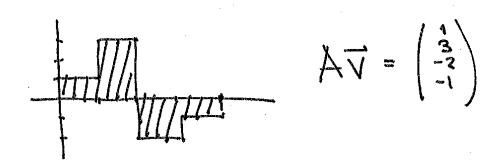
Here's a funny vector space that we're going to use as a pedagogical crutch. Imagine histogram-space. The basis vectors are:



This is a basis for a histogram over unit bins from x = 0 to x = 4. A vector in this space is, for example:



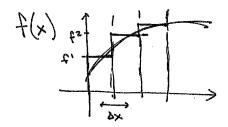
We can perform a linear transformation A on  $\mathbf{v}$  which outputs another vector. Let's say it's this:



Exercise 3.3 From the image above, can you derive what A is?

The answer to the above exercise is *no*. Please make sure you convince yourself why: there are many different transformations that convert to old histogram into the new histogram. If you're not convinced: the matrix A is  $4 \times 4$  and thus has 16 entries that we need to define. The matrix equation  $A\mathbf{v} = \mathbf{w}$  for known vectors  $\mathbf{v}$  and  $\mathbf{w}$  encodes only four equations.

The power of this admittedly strange formalism is that we can think of these histograms as approximations of continuous functions:



Thus a vector in this approximate (discretized) function space is

$$\mathbf{f} = \begin{pmatrix} f^1 \\ f^2 \\ \vdots \\ f^N \end{pmatrix} . \tag{3.11}$$

### 3.4 Derivative Operators

Our discretized function space allows us to define a [forward] derivative<sup>22</sup>:

$$\mathbf{f}' = \frac{1}{\Delta x} \begin{pmatrix} f^2 - f^1 \\ f^3 - f^2 \\ \vdots \\ f^{i+1} - f^i \\ \vdots \end{pmatrix} . \tag{3.12}$$

This is familiar if you've ever had to manually program a derivative into a computer program. Note that the right-hand side looks like a linear transformation of  $\mathbf{f}$ . In other words, we expect to be able to write a matrix D so that

$$\mathbf{f}' = D\mathbf{f} \ . \tag{3.13}$$

One problem is apparent: what happens at the 'bottom' of the vector? What is the last component of the derivative,  $\mathbf{f'}^N$ ? Formally, this is

$$(f')^{N} = \frac{1}{\Delta x} (f^{N+1} - f^{N})$$
(3.14)

but now we have no idea what  $f^{N+1}$  is. That was never a component in our vector space. There is no  $\mathbf{e}_{(N+1)}$  basis vector. This demonstrates and important lesson that we'll need when we move more formally to function spaces:

### Boundary conditions are part of the definition of the function space.

That was so important that I put the whole damn sentence in boldface and set it in the middle of the line. The significance of boundary conditions may be a bit surprising—but think of this as part of the definition of which functions we allow into our function space.

**Example 3.1** When one first learns about Fourier series with Dirichlet boundary conditions, one finds that the Fourier expansion only contains sines. The solution to the wave equation in such a system is some function that is zero at each endpoint. So the function space relevant to the system is composed only of functions that are zero at each endpoint.

One could have also defined a backward derivative where  $(f')^i \sim f^i - f^{i-1}$ . Note that you cannot try to make this symmetric by defining a 'centered' derivative like  $(f')^i \sim f^{i+1/2} - f^{i-1/2}$  because there's no such thing as a fractional index. If you tried to write  $(f')^i \sim f^{i+1} - f^{i-1}$  you're making a worse approximation. If you're like me, the fact that there's some asymmetry in how we define the first derivative is deeply unsettling. There's something to this intuition!

For now let's assume **Dirichlet boundary conditions**. A convenient way to impose this is to define what happens to all functions outside the domain of the function space:

$$f^{i>N} = f^{i<1} = 0 (3.15)$$

This solves the problem of the derivative on the last component:

$$(f')^N = \frac{1}{\Delta x}(f^{N+1} - f^N) = \frac{-f^N}{\Delta x}$$
 (3.16)

Alternatively, we could have also imposed **periodic boundary conditions**:

$$f^i = f^{i+kN} k \in \mathbb{Z} . (3.17)$$

This would then give

$$(f')^{N} = \frac{1}{\Delta x} (f^{N+1} - f^{N}) = \frac{1}{\Delta x} (f^{1} - f^{N}) . \tag{3.18}$$

Periodic boundary conditions amount to wrapping the x-axis into a circle. Older folks sometimes call this Asteroids boundary conditions. I'd also accept  $Star\ Control$  boundary conditions. Periodic boundary conditions show up all the time in physics. Sometimes they show up in obvious places, like the Brillouin zone of a crystal lattice. Other times they show up in not-so-obvious places like the boundary conditions of the known universe. In addition to being crucial for a well-defined function space, the boundary conditions of a system establish its topology<sup>23</sup>.

Exercise 3.4 We don't know anything about the universe outside the Hubble radius. Why do you think it would be reasonable in a physical model to assume that it has periodic boundary conditions? Hint: what would happen to the x-momentum of an asteroid in the classic arcade game Asteroids if the game did not have periodic boundary conditions?

The second derivative may be defined symmetrically:

$$(f'')^{i} = \frac{(f^{i+1} - f^{i}) - (f^{i} - f^{i-1})}{\Delta x^{2}} . \tag{3.19}$$

You may pontificate about the reason why the first derivative does have a symmetric discretization while the second derivative does.

<sup>&</sup>lt;sup>23</sup>I cannot over-emphasize the importance of topology in contemporary physics. Most of the physics you will learn in your first year graduate courses are intrinsically *local* because the laws of physics are causal. Topological quantities are *global*, they are integrals over an entire space. Because winding numbers (and their higher-dimensional cousins) are quantized, they are robust against perturbations. The number of holes in a donut is one, whether or not it's been slightly squished in the box. By the way, the best donuts in Southern California are from *Sidecar Doughnuts* in Costa Mesa. Get the Basil Eggs Benedict donut before 11am; you can thank me later.

### 3.5 Derivatives in other function space bases

There are other ways to write a discrete basis of functions. Here's a natural one for functions that are up to second-order polynomials:

$$\mathbf{e}_{(0)} = 1$$
  $\mathbf{e}_{(1)} = x$   $\mathbf{e}_{(2)} = x^2$ . (3.20)

Let's sidestep questions about orthonormality for the moment. Clearly linear combinations of these basis functions can produce any quadratic function:

$$f(x) = ax^2 + bx + c$$
  $\Rightarrow$   $\mathbf{f} = \begin{pmatrix} c \\ b \\ a \end{pmatrix}$  (3.21)

The derivative operator has an easy representation in this space:

$$D = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 2 \\ 0 & 0 & 0 \end{pmatrix} . \tag{3.22}$$

We can see that

$$D\mathbf{f} = \begin{pmatrix} b \\ 2a \\ 0 \end{pmatrix} \qquad D^2\mathbf{f} = \begin{pmatrix} 2a \\ 0 \\ 0 \end{pmatrix} \qquad D^3\mathbf{f} = 0 . \tag{3.23}$$

The last line is, of course, the realization that the third-derivative of a quadratic function vanishes. Feel free to attach mathy words to this like *kernel*.

There are other bases that we may use for function space. A particularly nice one that we will use over and over is the Fourier basis, which we usually refer to as  $momentum\ space$ . The basis vectors are things like sines, cosines, or oscillating exponentials. These do not vanish for any power of D.

## 3.6 Locality

Notice that in the histogram basis, the derivative matrix D is sparse: it is zero everywhere away from the diagonal. The only non-zero elements on the  $i^{\text{th}}$  row are around the  $(i \pm 1)^{\text{th}}$  column. Higher powers of D sample further away, but the non-zero elements are always clustered near the diagonal.

This is simply a notion of **locality**. Remember the Taylor expansion:

$$f(x) = f(0) + f'(0)x + \frac{1}{2}f''(0)x^2 + \cdots$$
 (3.24)

If we think about the histogram as a discretization of a continuous function, then it is clear what the higher derivatives are doing. Given a function  $f(x) = \mathbf{f}$ , one might like to know about the function around some point  $x_0$  corresponding to some index i. That is:  $f^i = f(x_0)$ . If you'd like to learn more about the function around that point, one can express the derivative at  $x_0$ . Thus  $D\mathbf{f}$  says something about the slow,  $D^2\mathbf{f}$  says something about the curvature,

and so on. Because each successive power of D samples terms further away from  $f^i$ , you can tell that these higher order terms are learning about the function further and further away from  $x_0$ .

Now think about the types of differential equations that you've encountered in physics. They often include one or two derivatives. You hardly ever see three, four, or more derivatives<sup>24</sup>. There's a reason for this: at the scales that we can access experimentally, nature appears to be local. Our mathematical models of nature typically have locality built in<sup>25</sup>. Physics at one spacetime point should not depend on spacetime points that are far away.

This may be familiar from the idea of causality—the idea that A causes B therefore A must have happened before B. One of the key results in special relativity is that causality can be tricky if two events do not occur at the same spacetime point. More carefully, A can only cause B if there is a timelike separation of the appropriate sign. If we want to build causal theories of nature, then the dynamics at  $x_0$  should not rely on what is happening at  $x_1$ , a finite distance away.<sup>26</sup>

#### 3.7 Row Vectors and all that

In high school we did not distinguish between row vectors and column vectors. They both seemed to convey the same information—they were simply one-dimensional arrays of numbers. Row vectors are just 'tipped over.' Such a tipping-over is convenient since you could apply the elementary schools rules of 'matrix multiplication' have the row vector act on a column vector:

$$(w_1 \ w_2 \ \cdots) \begin{pmatrix} v^1 \\ v^2 \\ \vdots \end{pmatrix} = w_1 v^1 + w_2 v^2 + \cdots$$
 (3.25)

In fact, this is like  $\mathbf{w}^T$  is a function that acts *linearly* on its argument,  $\mathbf{v}$ :

$$\mathbf{w}^{T}(\mathbf{v}) = w_1 v^1 + w_2 v^2 + \cdots {3.26}$$

Perhaps you see why we wrote the row vector components with lower indices,  $w_i$  so that we may use Einstein summation notation:  $\mathbf{w}^T \mathbf{v} = w_i v^i$ .

Indeed, let is be a bit more formal about this. This layer of formalism is uncharacteristic of our approach in this course, but this underpins so much of the mathematical structure of our physical theories that it is worth getting right from the beginning. Let V be a vector space. It contains vectors,  $\mathbf{v}$ . Sometimes these are called contravariant vectors or kets. They have basis vectors  $\mathbf{e}_{(i)}$ .

Now introduce a related but *completely distinct* vector space called  $V^*$ . This is the space of **dual vectors** to V. A **dual vector** is what you may know as a **row vector**, a **ket**, a

 $<sup>^{24}</sup>$ With some thought, it may also be clear why spatial derivatives typically appear squared.

 $<sup>^{25} \</sup>mathrm{A}\, \mathrm{recent}\, \mathrm{counterexample:}\,\, \mathrm{https://www.quantamagazine.org/physicists-discover-geometry-underlying-particle-p$ 

<sup>&</sup>lt;sup>26</sup>This is different from saying that information cannot propagate from  $x_0$  to  $x_1$ ; such propagation could come from some causal excitation of the electromagnetic field traveling every infinitesimal distance between the two positions. This is reminiscent of the classical Zeno's paradox.

**covariant vector**, or a [differential] **one-form**. These are all words for the *same idea*. A dual vector, say  $(\mathbf{w}^T)$  is a *linear function that takes vectors and spits out numbers*:

$$\mathbf{w}^T \in V^* \Rightarrow \mathbf{w}^T : V \to \mathbb{R} \ . \tag{3.27}$$

Don't think about  $\mathbf{w}^T$  as some kind of operation on a vector  $\mathbf{w} \in V$ ; at least not yet. For now the 'T' is just part of the name of  $\mathbf{w}^T$ . The two spaces V and  $V^*$  are totally different. We haven't said anything about how to turn elements of V into elements of  $V^*$  or vice versa. It should be clear that there is a sense of 'duality' here: the vectors V are also linear functions that take a dual vector and spit out a number.

Let us call the basis of dual vectors  $\widetilde{\mathbf{e}}^{(i)}$ . This notation is cumbersome, so we'll change to something different soon. The upper index is deliberate. The defining property of  $\widetilde{\mathbf{e}}^{(i)}$  is:

$$\widetilde{\mathbf{e}}^{(i)}\left(\mathbf{e}_{(j)}\right) \equiv \mathbf{e}_{(j)}\left(\widetilde{\mathbf{e}}^{(i)}\right) \equiv \delta_{j}^{i}$$
 (3.28)

One may check that this gives

$$(w_i \widetilde{\mathbf{e}}^{(i)}) (v^j \mathbf{e}_{(j)}) = w_i v^j \delta_j^i = w_i v^i = w_1 v^1 + w_2 v^2 + \cdots$$
 (3.29)

All that we've done here is defined basis vectors that carry the intrinsic *vector-ness* or *dual-vector-ness* through their relations (3.28). We have 'derived' the contraction of a lower-index object with an upper-index object, and hence our summation convention, in terms of these basis vectors.

#### 3.8 Dual vectors as vector-eaters

It is perhaps useful to use a slightly different notation based on Pac-Man. Rather than writing  $\tilde{\mathbf{e}}^{(i)}$ , lets write the basis dual vectors as

In this notation, the action of a basis dual vector on a basis vector is simply Pac-Man eating the basis vectors:

$$G' = G'$$

$$G' = G$$

So we can write (3.26) and (3.29) as

#### 3.9 Orthonormal Bases

At this point we should take a deep breath and state explicitly that we've been assuming an orthonormal basis. In this course we will continue to use an orthonormal basis. You may object to this and say that you used to believe in orthonormal bases until you were forced to write down the gradient (or worse, the Laplacian) in spherical coordinates. In other words, in principle one could imagine a basis where (3.28) does not hold. There are many things to be said about this, none of them are particularly edifying without a full discussion. With no apologies, I'll make the following [perhaps perplexing] remarks:

- 1. There is no such thing as a 'position vector.' Positions refer to some base space, whereas vectors (like differential operators) act on the tangent space at a point of that base space.
- 2. A given tangent space is 'nice' and has a nice orthonormal basis.
- 3. That basis may not be the same for neighboring tangent spaces (perhaps due to coordinates, perhaps due to intrinsic curvature).

In this course these nuances will not come up. In the rest of your life you'll still have to deal with curvilinear coordinates. But suffice it to say that our study of function space will be nice an orthonormal. We haven't yet given an adequate definition of 'orthonormality,' so let's take (3.28) as a working definition.

#### 3.10 Bra-Ket Notation

There is neither any physics nor mathematics contained in a choice of notation. However, a convenient notation does simplify our lives. Let us introduce bra-ket notation. In this

notation, we denote vectors by kets:

$$|v\rangle = v^i|i\rangle , \qquad (3.30)$$

where  $|i\rangle = \mathbf{e}_{(i)}$  is the basis of vectors that span the vector space V. There is nothing new or different about this object,  $\mathbf{v} = |v\rangle$ .

We denote dual vectors (row-vectors, one-forms) as bras:

$$\langle w| = w_i \langle i| , \qquad (3.31)$$

where  $\langle i| = \widetilde{\mathbf{e}}^{(i)}$ . The orthonormality of this basis is encoded in

$$\langle i|j\rangle = \delta_j^i \ . \tag{3.32}$$

In bra-ket notation a linear transformation A has a basis

$$A = A^{i}_{j} |i\rangle\langle j| . {3.33}$$

The notation  $|i\rangle\langle j|$  is shorthand for the **tensor product**  $|i\rangle\otimes\langle j|$ . If the  $\otimes$  doesn't mean anything to you, that's fine. It doesn't mean much to me either. Maybe you can replace it with the word 'and' so that  $|i\rangle\otimes\langle j|$  means you have a basis ket  $|i\rangle$  and an basis bra  $\langle j|$  that are somehow stuck together but aren't acting on each other. Matrix multiplication proceeds as before:

$$A\mathbf{v} = A|v\rangle = A^{i}{}_{j}|i\rangle\langle j|v^{k}|k\rangle = A^{i}{}_{j}v^{k}|i\rangle\langle j|k\rangle = A^{i}{}_{j}v^{k}|i\rangle\delta^{j}_{k} = A^{i}{}_{j}v^{j}|i\rangle . \tag{3.34}$$

Observe that the power of the notation is clear: the object with the index  $v^i$  is just a number. It commutes with everything. All of the vector-ness is carried in the basis objects: the bras, kets, and ket-bras. Those do not commute. But they have a well defined way in which kets act on bras (or vice versa).<sup>27</sup>

## 3.11 Eigenvectors are nice

Give a sufficiently *nice* linear transformation, A, there is a particularly convenient basis: the eigenvectors of A. These are kets  $|\lambda\rangle$  such that

$$A|\lambda\rangle = \lambda|\lambda\rangle \ . \tag{3.35}$$

In other words, A acts on the eigenvector by rescaling. The rescaling coefficient is the eigenvalues. For *nice* transformations (see Section 1.3), there is a complete set of such vectors to span the vector space.

If you write a general vector  $|v\rangle$  in terms of this eigenbasis,

$$|v\rangle = v^i |\lambda_{(i)}\rangle , \qquad (3.36)$$

<sup>&</sup>lt;sup>27</sup>This is where the  $\oplus$  notation is handy. It keeps track of which kets/bras might hit which other bras/kets. This falls under the name of multi-linear algebra.

Then the action of A on this vector is easy:

$$A|v\rangle = \sum_{i} \lambda_{(i)} v^{i} |\lambda_{(i)}\rangle . \tag{3.37}$$

In fact, assuming that all of the eigenvalues are non-zero, even the matrix inverse is easy:

$$A^{-1}|v\rangle = \sum_{i} \lambda_{(i)}^{-1} v^{i} |\lambda_{(i)}\rangle . \tag{3.38}$$

The first time you see this should have brought a deep joy to your life: if you can decompose a matrix (linear transformation) into its eigenvectors and eigenvalues, then taking the inverse transformation is simple.

### 3.12 Linearity of Inverse Operators

Given a linear operator A, the inverse operator  $A^{-1}$  is defined by

$$A^{-1}A = \mathbb{1}_{N \times N} \ . \tag{3.39}$$

For an N-dimensional vector space, this represents  $N^2$  different equations: one for each element. The inverse operator, by the way, is also linear. Let's remind ourselves of what this means. A linear transformation, when written as a matrix, is simply stating what that linear transformation does to your basis vectors. If a matrix B has elements

$$B = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = B_{j}^{i} |i\rangle\langle j| , \qquad (3.40)$$

then this simply means that acting on basis vectors  $\mathbf{e}_{(1)} = |1\rangle$  and  $\mathbf{e}_{(2)} = |2\rangle$  gives

$$B|1\rangle = a|1\rangle + c|2\rangle \tag{3.41}$$

$$B|2\rangle = b|1\rangle + d|2\rangle . (3.42)$$

In column vector notation:

$$B\begin{pmatrix} 1\\0 \end{pmatrix} = \begin{pmatrix} a\\c \end{pmatrix} \qquad \qquad B\begin{pmatrix} 0\\1 \end{pmatrix} = \begin{pmatrix} b\\d \end{pmatrix} . \tag{3.43}$$

So knowing the action on basis vectors is the same as knowing the transformation itself. Suppose I told you the action of the inverse transformation  $A^{-1}$  on your basis vectors, vis-a-vis (3.42):

$$A^{-1}|1\rangle = x|1\rangle + y|2\rangle \tag{3.44}$$

$$A^{-1}2\rangle = z|1\rangle + w|2\rangle . (3.45)$$

Then you know exactly how  $A^{-1}$  acts on a general vector  $|s\rangle = s^1|1\rangle + s^2|2\rangle$ :

$$A^{-1}|s\rangle = A^{-1}\left(s^{1}|1\rangle + s^{2}|2\rangle\right) \tag{3.46}$$

$$= s^{1}A^{-1}|1\rangle + s^{2}A^{-1}|2\rangle \tag{3.47}$$

$$= (s^{1}x + s^{2}z)|1\rangle + (s^{1}y + s^{2}z)|2\rangle . (3.48)$$

You can now keep this in mind when we say we want to solve  $A|\psi\rangle = |s\rangle$ . If we knew the action of  $A^{-1}$  on some basis of the space, then the problem is simple:

$$|\psi\rangle = \psi^{i}|i\rangle = \left(A^{-1}\right)^{i}{}_{i}|i\rangle\langle j|\,s^{k}|k\rangle \tag{3.49}$$

$$= \left(A^{-1}\right)^{i}_{i} s^{k} |i\rangle\langle j||k\rangle \tag{3.50}$$

$$= \left(A^{-1}\right)^i_{\ i} s^j \left|i\right\rangle \ . \tag{3.51}$$

We can write this as an equation for each component:

$$\psi^{i} = \sum_{j} \left( A^{-1} \right)^{i}_{j} s^{j} . \tag{3.52}$$

We've restored the explicit sum over j as a convenient reminder. The quantity  $(A^{-1})^i_{\ j}$  is what we would like to identify with a Green's function.

### 3.13 The Green's Function Problem

Going back to the big picture: recall that we want to solve differential equations of the form  $\mathcal{O}f(x) = s(x)$ . If we had a sense of the *eigenfunctions* of  $\mathcal{O}$ , then we could expand s(x) in a basis of those eigenfunctions and then apply  $\mathcal{O}^{-1}$  to both sides.

The analog is this:

The operator A encodes the *physics* of the system, the underlying dynamics. This is presumably local: it is a near-diagonal matrix coming from one or two powers of derivatives. The ket  $|s\rangle$  is the source. This is the thing that *causes* the dynamics. The ket  $|\psi\rangle$  is some state that we would like to determine. (3.38) is telling us that to invert a differential operator  $\mathcal{O}$ , it may be useful to decompose it into **eigenfunctions**.

By the way, *this* is where all of the 'special functions' in your physics education show up. The reason why you would ever care about Bessel functions (of various kinds) or Legendre polynomials is simply that they are the eigenfunctions of differential operators that we care about<sup>28</sup>. Sometimes we confuse mathematical physics with 'properties of special functions.'

<sup>&</sup>lt;sup>28</sup>In fact, they're mostly the eigenfunctions of the same differential operator in different coordinate systems. Do you know which differential operator? I'll give you a guess. It's starts with a 'har-' and ends with a 'monic oscillator.'

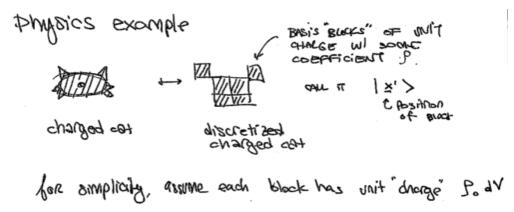
I do not care about special functions; perhaps with the notable exception of the  $\Gamma$ -function. Seriously, to screw special functions. The real intuition for what we're doing is evident in the few-dimensional harmonic oscillator. All the Bessel-schmessel function-ology that will pain you in your Jackson E&M course are just technical details.

**Example 3.2** Consider a differential operator  $A \to \mathcal{O} = (d/dx)^2$ . There's a basis of nice eigenvectors  $\xi_{(k)}$ :

$$\xi_{(k)} = \sin(kx)$$
  $\mathcal{O}\xi_{(k)} = -k^2\xi_{(k)}.$  (3.53)

I've deliberately avoided normalizing for now. From this you can see that writing a function as a **Fourier Series** is simply a change of basis to eigenfunctions of  $(d/dx)^2$ . Can you see how you would 'invert' this operator acting on a general function f(x) with a set of Fourier coefficients  $f(x) = \sum_k c_k \sin(kx)$ ?

**Example 3.3** A common example in electrostatics is the triboelectric effect. Go ahead, take a moment to look it up on Wikipedia. The image is very relevant. If you pet your cat with hard rubber<sup>29</sup>, the cat builds up some electrostatic charge. For simplicity, let's model this system as a bunch of Lego blocks arranged in a cat-shape where each block has a constant electric charge. Let's say that each block has volume dV and constant charge density  $\rho_0$  so that each block has charge  $\rho_0 dV$ . The entire cat is described by a charge density  $\rho(x)$  where  $\rho(x) = 0$  if you're outside the cat and  $\rho(x) = \rho_0$  if you're inside the cat.



You know how this problem works. You want to solve for the electrostatic potential,  $\Phi(x)$ , given the charge density  $\rho(x)$ . The relevant equation is

$$\nabla^2 \Phi(\mathbf{x}) = -\rho(\mathbf{x}) , \qquad (3.54)$$

where  $\epsilon_0 = 1$  in convenient units. This looks like a tricky differential equation to solve, but the fist week of our undergraduate electrodynamics course taught us that the potential from a unit point charge is

$$\Phi(\mathbf{x}) = \frac{-1}{4\pi} \frac{1}{|\mathbf{x} - \mathbf{x}'|} \ . \tag{3.55}$$

The relevant diagram is

<sup>&</sup>lt;sup>29</sup>I do not recommend doing this.

$$(\bar{x}, \frac{\bar{x}}{\sqrt{1\bar{x}-\bar{x}_{1}}}) \Rightarrow (\bar{x}) = \frac{\alpha \underline{x}}{\sqrt{1}} \frac{(\bar{x}-\bar{x}_{1})}{\sqrt{1}}$$

If we know the potential from a single point charge, then we can invoke linearity—specifically, the linearity of  $\nabla^2$ )—to write down the potential for two unit point charges:

$$\bar{x}$$
,  $\bar{x}$ 

At this point, you should start to see how this looks just like (3.48). The result is

$$\Phi(\mathbf{x}) = \sum_{\mathbf{x}'} \frac{1}{4\pi} \frac{1}{|\mathbf{x} - \mathbf{x}'|} \rho(\mathbf{x}') dV \rightarrow \int d^3 \mathbf{x}' \frac{1}{4\pi} \frac{1}{|\mathbf{x} - \mathbf{x}'|} \rho(\mathbf{x}') . \tag{3.56}$$

This last example is really useful. You've seen this calculation before, but please review it carefully from the perspective of the action of  $(\nabla^2)^{-1}$ . Just as we are able to build a 'Lego cat' out of unit blocks, each of those unit blocks comes with an electrostatic potential. The solution to  $\nabla^2 \Phi(x) = -\rho(x)$  is to simply sum together those point-source solutions in the same way that one sums together the point sources (assembles the blocks) to model the finite source.

#### **Exercise 3.5** In the example above, what plays the role of the basis vectors?

Compare (3.56) to (3.52). The sum over positions  $\mathbf{x}'$  that becomes an integral over  $d^3\mathbf{x}'$  is completely analogous to the sum over the index j.  $\rho(\mathbf{x}')$  plays the role of a component of the source,  $s^j$ . On the left-hand side,  $\Phi(\mathbf{x})$  plays the role of  $\psi^i$ . We note that the index i is replaced by the position  $\mathbf{x}$ . Evidently, the inverse of  $\nabla^2$  is simply

$$(\nabla^2)^{-1} \equiv G(\mathbf{x}, \mathbf{x}') = -\frac{1}{4\pi} \frac{1}{|\mathbf{x} - \mathbf{x}'|} . \tag{3.57}$$

Here we've written out  $G(\mathbf{x}, \mathbf{x}')$ , the Green's function for  $\nabla^2$ . Observe that the Green's function has two arguments in the same way that the inverse matrix  $(A^{-1})^i_{\ j}$  has two indices. The  $\mathbf{x}'$  'index' is integrated/summed over—it scans each 'building block' of the source in the same way that we sum over j in the index contraction  $(A^{-1})^i_{\ j} s^j$ . In other words, we may heuristically write (3.57) as

$$\Phi^i \sim \sum_j G^i_{\ j} \rho^j \ . \tag{3.58}$$

At this point, it's useful to point out that the Green's function is often called a **propagator**. As a function, G(x, x') propagates the information of the source at x' to the observer at x assuming some dynamics—the operator for which G is a Green's function.



Please, please, please make sure you understand this example. This will be the key starting point from which we will generalize our study of Green's functions in physics.

### 3.14 Remark: Implicit assumption of linearity

In everything we're building we're assuming that the dynamics that relates the source  $|s\rangle$  and the state  $|\psi\rangle$  is *linear*. That's why we can think of the differential operator  $\mathcal{O}$  as a matrix. If  $|\psi_0\rangle$  is the effect of source  $|s_0\rangle$ , then you know by linearity that  $2|\psi_0\rangle$  is the effect of a source that is twice as strong,  $2|s_0\rangle$ .

Linearity is *not* a truth of nature, yet we're spending all of this course developing techniques for dealing with linear dynamics! The fact of the matter is that a good chunk of physics is linear—and that's good because those are the parts that we can solve using our standard toolkit. Most of the frontier of physics has to do with how to deal with the *non*-linearities. There are a few options here: numerical solution, perturbation expansions about a linear solution (Feynman diagrams), and looking for topological invariants.

## 3.15 Metrics on Finite Dimensional Vector Spaces

Thus far we have introduced vector spaces. The dual vector space is a set of linear functions that act on elements of a vector space; these are bras/row-vectors/one-forms. Let us now introduce a new piece of machinery: a **metric**. This is also known as an **inner product** or a **dot product**. A space with a metric is called a metric space. We only state this fact to emphasize that we are *adding this structure by hand*. Vector spaces don't come with metrics—someone makes up a metric and slaps it onto the vector space.

The **metric** is a function that takes two vectors and spits out a number. It is linear in each argument. In other words, a metric g is:

$$q: V \times V \to \mathbb{R}$$
 (3.59)

Occasionally one may want a metric defined such that the output is a complex number. We thus have:

$$g(\alpha \mathbf{v} + \beta \mathbf{w}, \delta \mathbf{x} + \gamma \mathbf{y}) = \alpha \delta g(\mathbf{v}, \mathbf{x}) + \alpha \gamma g(\mathbf{v}, \mathbf{y}) + \beta \delta g(\mathbf{w}, \mathbf{x}) + \beta \gamma g(\mathbf{w}, \mathbf{y}). \tag{3.60}$$

One more special assumption about the metric is that it is **symmetric**<sup>30</sup>:

$$g(\mathbf{v}, \mathbf{w}) = g(\mathbf{w}, \mathbf{v}) . \tag{3.61}$$

<sup>&</sup>lt;sup>30</sup>Actually it is conjugate symmetric,  $g(\mathbf{v}, \mathbf{w}) = g(\mathbf{w}, \mathbf{v})^*$ . This distinction will be important for function spaces.

In indices one may write

$$g = g_{ij}\langle i| \otimes \langle j| \tag{3.62}$$

so that

$$g(\mathbf{v}, \mathbf{w}) = g_{ij} v^i w^j \ . \tag{3.63}$$

Here we see the usefulness of the  $\otimes$  notation. It tells us that the bras and kets resolve as follows:

$$g_{ij}\langle i|\otimes\langle j|\left(v^{k}|k\right)\right)\left(w^{\ell}|\ell\rangle\right) = g_{i}jv^{k}w^{\ell}\langle i|k\rangle\langle j|\ell\rangle = g_{i}jv^{k}w^{\ell}\delta_{k}^{i}\delta_{\ell}^{j} = g_{ij}v^{i}w^{j}. \tag{3.64}$$

If this is your first time seeing it, please re-read (3.64) carefully to see exactly how the bras and kets resolve themselves. For ordinary Euclidean space in flat coordinates, the metric is simply the unit matrix:  $g_{ij} = \text{diag}(1, \dots, 1)$ . In Minkowski space there's a relative minus sign between space and time. In curvilinear coordinates things get ugly.

Here's the neat thing about metrics. We can take a metric g and pre-load it with a vector  $\mathbf{v}$ :

$$g(\mathbf{v},)$$
 (3.65)

In fact, we may then define a function with respect to this pre-loaded metric:

$$f(\mathbf{w}) = g(\mathbf{v}, \mathbf{w}) \tag{3.66}$$

Observe that  $f(\mathbf{w})$  is a linear function that takes elements of V and returns a number. In other words, this is a *dual vector* (row-vector, one-form, element of  $V^*$ ). The metric has allowed us to *convert vectors into dual vectors*:

$$g(\mathbf{v}, \qquad) = g_{ij}v^i\langle j| \ . \tag{3.67}$$

Similarly, one may define an inverse metric  $g^{-1}$  such that  $g^{-1}g = 1$ . In a slight abuse of notation, the inverse metric is written with two upper indices:  $g^{ij}$ . Note that we do not write the '-1.' The inverse metric will *raise* the index on a lower-index object, while the metric *lowers* the index of an upper-index object.<sup>31</sup>

## 3.16 The dot/inner product, orthonormality

You are already familiar with the 'obvious' way to take two vectors and spit out a number. This is the dot product of two vectors, also known as the inner product. They are equivalent to each other and equivalent to the action of the metric on a pair of vectors;

$$\mathbf{v} \cdot \mathbf{w} = \langle \mathbf{v}, \mathbf{w} \rangle = g(\mathbf{v}, \mathbf{w}) . \tag{3.68}$$

<sup>&</sup>lt;sup>31</sup>Of course: what's really happening is that the metric has a basis  $\langle i|\otimes \langle j|$  while the inverse metric has a basis  $|i\rangle\otimes |j\rangle$ .

The norm of a vector  $\mathbf{v}$  is simply the square root of  $g(\mathbf{v}, \mathbf{v})$ . By the linearity of the metric, we can decompose the dot product into the action of the metric on basis vectors:

$$g(\mathbf{v}, \mathbf{w}) = g(v^1 \mathbf{e}_{(1)} + v^2 \mathbf{e}_{(2)} + \cdots, w^1 \mathbf{e}_{(1)} + w^2 \mathbf{e}_{(2)} + \cdots)$$
(3.69)

$$= v^{1}w^{1}g(\mathbf{e}_{(1)}, \mathbf{e}_{(1)}) + v^{1}w^{2}g(\mathbf{e}_{(1)}, \mathbf{e}_{(2)}) + \cdots,$$
(3.70)

where our assumption of an orthonormal basis<sup>32</sup> is the statement that

$$g(\mathbf{e}_{(i)}, \mathbf{e}_{(j)}) = \pm \delta_j^i . \tag{3.71}$$

The  $\pm$  depends on the signature of the metric. As physicists, this is the distinction between 'space' and 'time.' For Euclidean space the sign is always plus. For Minkowski spacetime, there's some choice of sign for the timelike direction and the opposite sign for the spacelike direction. The choice is a convention, there's no 'right' choice<sup>33</sup>. When (3.71) is not true the basis is not orthonormal. Sometimes this happens when your space is curvy (general relativity); other times you just have curvilinear coordinates for a flat space (e.g. polar coordinates). I'm glossing over several subtleties here, among them is the idea that position vectors do not exist<sup>34</sup>.

Exercise 3.6 Speaking of the notion of curved space: Consider a sheet of paper as an idealized two-dimensional surface. If you tape opposite edges of the paper together to make a cylinder, is the two-dimensional space curved or flat? For example, if two-dimensional beings lived on the paper like in Edwin Abbot-Abbot's novella Flatland, would they say that their space is curved?

Exercise 3.7 The cylinder from the previous exercise is an example of periodic boundary conditions. For those familiar with special relativity, this entire section has probably been a big review. Here's a fun puzzle to think about while you skim. What happens to the twin paradox if the universe were periodic in some spatial direction? The usual resolution to the twin paradox is that the twin that 'turns around' must change inertial frame. However, if there were a periodic direction, neither twin has to 'turn around' for them to meet once again and compare clocks<sup>35</sup>.

**Example 3.4** Given two vectors  $\mathbf{v}$  and  $\mathbf{w}$ , there are two equivalent ways of thinking about how they may be combined into a number. First, one can lower the index of one of the vectors with the metric  $v_i \equiv g_{ij}v^i$  and then contract the 'row vector'  $v_i$  with the 'column vector'  $w^j$ :  $v_iw^i$ . I am of course abusing notation by conflating the components  $v_i$  and  $w^j$  with the row/column vectors. The second way of doing this is taking the two vectors and contracting them directly with the metric:  $v^iw^jg_{ij}$ . Please make sure you are comfortable that these 'two ways' are exactly the same thing.

 $<sup>^{32}</sup>$ Not an 'oprhan normal' basis like Zoom's auto-transcription claims I said.

 $<sup>^{33}</sup>$ The right choice is + for timelike and - for spacelike.

<sup>&</sup>lt;sup>34</sup>Formally, vectors live in the tangent space of a manifold. They are 'intrinsically' tangent vectors (velocities) of some trajectory on the manifold with some 'time' parameter. The position on the manifold is a coordinate, but it is not a *vector*. For more on what I mean by this, I recommend hep-th/0611201, Arnold's *Mathematical Methods of Classical Mechanics*, or a graduate general relativity textbook.

<sup>&</sup>lt;sup>35</sup>For a nice solution, see: https://doi.org/10.1080/00029890.2001.11919789

### 3.17 Comment: Why physicists like indices

Einstein's summation convention tells us that we should see repeated upper/lower indices as contracted pairs—we should treat them differently. In contrast, the un-paired indices tell us something about the physical quantity to which those indices are attached. This is why—despite what our mathematician colleagues tell us—we love indices<sup>36</sup> Vectors are objects that transform in a well defined way with respect to rotations:

$$v^i \to v'^i = R^i{}_i v^j$$
,

where R is a rotation matrix. Similarly, one-forms/column vectors transform 'oppositely':

$$w_k \to w_k' = \left(R^T\right)_k^\ell w_\ell \ . \tag{3.72}$$

Observe that the rotation matrix is *transposed* when acting on an *lower* index object. This is consistent with the idea that the dot product is invariant under rotations:

$$v^{i}w_{i} \to v'^{i}w'_{i} = R^{i}_{j}v^{j} \left(R^{T}\right)^{\ell}_{i} w_{\ell} = \left[\left(R^{T}\right)^{\ell}_{i} R^{i}_{j}\right] v^{j}w_{\ell} = v^{j}w_{j} , \qquad (3.73)$$

where we've used the fact that the matrix in the square brackets is simply  $\delta_j^{\ell}$  which is evident from  $R^T R = 1$ .

**Example 3.5** We exploited something neat about the index notation in (3.73). Note that there aren't any 'vectorial' objects in (3.73)—all there is are a bunch of numbers (components of vectorial objects). We used the fact that we could re-arrange these products to make it clear how they contract. That's why we were able to move the  $(R^T)^{\ell}$ , term all the way to the left.

A neat lesson here is that

Indices tell us how an object transforms under 'rotations'.

Here 'rotations' mean whatever the appropriate symmetry is. In quantum mechanics, for example, the rotations are unitary transformations. If an object has indices, then it transforms. If an object has no indices (or is only composed of contracted indices) then it is a scalar with respect to those transformations. This 'indexology' is the backbone of how lazy physicists apply representations of symmetry groups<sup>37</sup>. It's especially useful in particle physics<sup>38</sup>.

The generalization to tensors is hopefully clear. An object with some number of upper indices and some number of lower indices transforms with several factors of the rotation matrix and its transpose:

$$T^{i_1 i_2 \cdots i_n}_{j_1 j_2 \cdots j_m} \to R^{i_1}_{k_1} R^{i_2}_{k_2} \cdots R^{i_n}_{k_n} (R^T)^{\ell_1}_{j_1} (R^T)^{\ell_2}_{j_2} \cdots (R^T)^{\ell_m}_{j_m} T^{k_1 k_2 \cdots k_n}_{\ell_1 \ell_2 \cdots \ell_m} . \tag{3.74}$$

Yes, we are so wealthy with indices that our indices have indices.

Exercise 3.8 How does the moment of inertia tensor transform under a rotation R?

<sup>&</sup>lt;sup>36</sup>Recent Nobel laureate Roger Penrose has a clever notation that replaces indices with lines; https://en.wikipedia.org/wiki/Penrose\_graphical\_notation.

<sup>37</sup>https://github.com/Tanedo/Physics262-2019

<sup>38</sup>https://sites.google.com/ucr.edu/p165/

### 3.18 Adjoints and Hermitian Conjugates

Because the metric lowers the index of a vector and produces a dual vector, you may want to think about this as 'tipping over' a column vector—almost like a transpose, right? We should be careful with this notion. Suppose we have a vector  $\mathbf{w} = A\mathbf{v}$ . How do we express the components of the dual vector  $w_i$  with respect to the elements of the dual vector  $v_i$ ?

$$w_i = g_{ij}w^j = g_{ij}A^j_{\ k}v^k = A_{jk}v^k = A_j^k v_k \equiv v_k (A^T)^k_{\ j} \ . \tag{3.75}$$

In the second-to-last step we have used  $g^{ij}g_{jk} = \delta^i_k$ . In the last step we have defined the transpose of a real matrix in the usual way: swap the first and second indices. These happen to have heights that come along for the ride. For convenience we moved the  $v_k$  to the left-side of the expression—it should be clear that this does not affect the expression at all (just write out the sum explicitly). We've gone through these gymnastics simply to motivate the notion that

$$\mathbf{w}^T = \mathbf{v}^T A^T \ . \tag{3.76}$$

Notice that the T acts on the matrix A. This is in contrast to our notation where the T in  $\mathbf{w}^T$  is simply a label to remind us that the object is a dual (row) vector.

For complex vector spaces—for example, the space of wavefunctions in quantum mechanics—we need to be a little bit more careful. We won't say much about complex vector spaces in general, but us simply state that the 'transpose' is generalized to the Hermitian conjugate. You may be most familiar with this in bra-ket notation from quantum mechanics:

$$\langle x| = |x\rangle^{\dagger} = \langle x, \rangle ,$$
 (3.77)

where  $\langle x, \rangle$  is simply the inner product on the complex space with one component preloaded<sup>39</sup>. You should now see why the Hermitian conjugate isn't just a 'transpose' but also a complex conjugation. The **norm** of a vector is  $||\mathbf{v}|| = \langle \mathbf{v}, \mathbf{v} \rangle$ . We would like the **norm** to be positive definite<sup>40</sup>, even when  $\mathbf{v}$  is complex. If  $\mathbf{v}$  has a complex phase, then there needs to be a 'complex conjugation' built into the notion of an inner product.

**Example 3.6** While this may sound like hand-waving, you already know this from quantum mechanics where the wavefunction  $\psi(x)$  is complex. You know that a nice wavefunction is normalized,  $\langle \psi, \psi \rangle = 1$ , which we interpret as:

$$\int dx \, \psi^*(x)\psi(x) = 1 \ . \tag{3.79}$$

The  $\psi^*(x)$  in the integrand is related to the complex conjugation implicit when going from a ket  $|\psi\rangle$  to a bra  $\langle\psi|$ .

$$\langle x|y\rangle = \langle x,y\rangle \ . \tag{3.78}$$

In the above equation, the left-hand side is a bra (dual vector) acting on a ket (vector), while the right-hand side is the inner product acting on two kets. This is simply repeating the statement in Example 3.4.

<sup>&</sup>lt;sup>39</sup>By the way, this motivates the bra-ket notation for vectors and dual-vectors:

<sup>&</sup>lt;sup>40</sup>The notable exception is when you have a space with nontrivial signature like Minkowski space where the relative sign between space and time is relevant.

We will work this out more carefully when we re-introduce function spaces systematically—but all of this should feel familiar.

Let us write **adjoint** to mean transpose for real spaces and Hermitian conjugate for complex spaces. The importance of the adjoint is not converting vectors into dual vectors, but rather the action on operators. Armed with a metric/inner product, the adjoint  $A^{\dagger}$  of an operator A satisfies

$$\langle A^{\dagger} w, v \rangle = \langle w, Av \rangle . \tag{3.80}$$

In a given inner product, the adjoint shifts the action from one vector to the other.

Example 3.7 From this definition, it should be clear that

$$\langle w|\mathcal{A}v\rangle = \langle A^{\dagger}w|v\rangle$$
 (3.81)

This equation does not invoke the metric in contrast to (3.80). Of course, the dual vector  $\langle w |$  is related to the vector  $|w\rangle$  by the metric.

**Exercise 3.9** If you are mathematically inclined, prove the existence, uniqueness, and linearity of the adjoint  $A^{\dagger}$  of a linear operator A. Hint: see Byron & Fuller chapter 4.4.

The adjoint/Hermitian conjugate is important because of the result that **self-adjoint operators**,  $A^{\dagger} = A$ , have real eigenvalues and a complete set of orthogonal eigenvectors. Then we can use the strategy of Section 3.11 to use eigenvectors of A to simplify the solution of  $A\mathbf{v} = \mathbf{w}$ .

## 4 Function Space

Function spaces are vector spaces where the vectors are functions. We introduced 'his- lec 04 togram space' in Section 3.3 as a crude model of a finite dimensional function spaces. An alternative finite dimensional model is the space of polynomials up to some degree, which we introduced in Section 3.5. Our models of nature are typically continuous<sup>41</sup>. This requires infinite dimensional function spaces, or Hilbert spaces.

## 4.1 The Green's Function Problem in Function Space

The Green's function can be defined by analogy to the finite-dimensional inverse transformation. The finite-dimensional linear system  $A\mathbf{v} = \mathbf{w}$  can be solved by applying the inverse transformation  $A^{-1}$  in the same way that the continuum (infinite-dimensional) system  $\mathcal{O}\psi(x) = s(x)$  can be solved with the Green's function G(x, y) of the operator  $\mathcal{O}$ :

$$v^{i} = \sum_{i} \left(A^{-1}\right)^{i}_{j} w^{j} \qquad \qquad \Rightarrow \qquad \qquad \psi(x) = \int dy \, G(x, y) s(y) \ . \tag{4.1}$$

We've explicitly written out the sum over the dummy index i to emphasize the analogy to the integration over the dummy variable y. The arguments of the functions play the role of 'continuum indices.'

<sup>&</sup>lt;sup>41</sup>This does not mean that nature is fundamentally continuous. There is a deep sense in which our models are valid whether or not nature is continuous so long as any granularity is smaller than our experimental probes.

## 4.2 Differential Operators

Linear transformations on function space are differential operators. In principle you can imagine linear transformations that are not differential operators, for example a finite translation. However, because our models of nature are typically *local* and *causal*, the linear transformations that we obtain from physical models are differential operators<sup>42</sup>.

Let's write a general differential operator as:

$$\mathcal{O} = p_0(x) + p_1(x)\frac{d}{dx} + p_2(x) + \left(\frac{d}{dx}\right)^2 + \cdots$$
(4.2)

where the  $p_i(x)$  are polynomials. Sometimes we will write this as  $\mathcal{O}_x$  to make it clear that the argument of the polynomials is x and the variable with which we are differentiating is x.

Exercise 4.1 Explain why (4.2) is a linear operator acting on function spaces.

**Exercise 4.2** A confused colleague argues to you that (4.2) cannot possibly be 'linear.' Just look at it, your colleague says: the functions  $p_i(x)$  are polynomials—those aren't linear! There are also powers of derivatives—how is that possibly linear? Explain to your colleague why the  $p_i(x)$  does not have to be linear nor is one restricted to finite powers of derivatives for the operator  $\mathcal{O}$  to be a linear operator acting on function space.

Technically (4.2) is called a **formal operator** because we haven't specified the boundary conditions of the function space. Recall in our discretized 'histogram space' in Section 3.3 that we had to be careful about how to define the derivative acting on the boundaries of the space. A differential operator along with boundary conditions is called a **concrete operator**.

## 5 Inner Product

There's a convenient inner product that you may be familiar with from quantum mechanics. For two functions f(x) and g(x) in your function space, define the inner product to be

$$\langle f, g \rangle = \int dx \, f^*(x) g(x) .$$
 (5.1)

**Example 5.1** Wave functions in 1D quantum mechanics obey this norm. For an infinite domain, we typically restrict to square-integrable functions meaning that  $|f|^2$  goes to zero fast enough at  $\pm \infty$  so that the integral  $\langle f, f \rangle$  is finite.

<sup>&</sup>lt;sup>42</sup>This is not to say that finite transformations are somehow not permitted. The dynamics that govern our models of nature, however, only dictate how information is transmitted infinitesimally in space and time. Propagation forward in time by some finite interval is described by the exponentiation of infinitesimal forward time translations. This is, of course, why the time-translation operator in quantum mechanics is  $e^{i\hat{H}t}$ , where the Hamiltonian H is described as a local function with perhaps one or two derivative operators.

Sometimes the inner product is defined with respect to a weight function w(x):

$$\langle f, g \rangle_w = \int dx \, w(x) \, f^*(x) g(x) . \qquad (5.2)$$

There's nothing mysterious about inner products with weights. They typically boil down to the fact that one is not using Cartesian coordinates.

**Example 5.2** Have you met the Bessel functions? If not, you're in for a treat in your electrodynamics course. The Bessel functions satisfy a funny orthogonality relation with weight  $w(x) \sim x$  because they show up as the radial part of a solution when using polar coordinates. When you separate variables,  $d^2x = rdr d\theta$ , we see that the measure over the radial coordinate r carries a weight r.

We will assume unit weight until we go to higher spatial dimensions<sup>43</sup>.

#### 5.1 Dual Vectors

What are the 'dual functions' (dual vectors, bras) in function space? These are linear functions on act on functions and spit out numbers. Taking inspiration from (3.67), these are integrals that are pre-loaded with some factors. Assuming unit weight:

$$\langle f| = \langle f, \rangle = \int dx \, f^*(x) \, [\text{ insert ket here }] .$$
 (5.3)

### 5.2 Adjoint operators

What is the adjoint of a differential operator? The definition of the adjoint (3.80) and the function space inner product (5.1) give us a hint. We define  $\mathcal{O}^{\dagger}$  by the property

$$\int dx \left[ \mathcal{O}f(x) \right]^* g(x) = \int dx f^*(x) \left[ \mathcal{O}^{\dagger}g(x) \right] . \tag{5.4}$$

The strategy is: given an inner product (integral) over  $f^*$  and g where there is some stuff  $(\mathcal{O})$  acting on g, can we re-write this as an integral with no stuff acting on g and some other stuff acting on  $f^*$ ? If so, then the 'other stuff' is the adjoint  $\mathcal{O}^{\dagger}$ .

**Example 5.3** What is the adjoint of the derivative operator,  $\mathcal{O} = d/dx$ ? Assume an interval  $x \in [a,b]$  and Dirichlet boundary conditions, f(a) = f(b) = 0. There's a simple way to do this: integrate by parts.

$$\int dx \left[ \frac{d}{dx} f(x) \right]^* g(x) = -\int dx f^*(x) \left[ \frac{d}{dx} g(x) \right] + \left[ f^*(x) g(x) \right]_a^b = -\int dx f^*(x) \left[ \frac{d}{dx} g(x) \right]. \tag{5.5}$$

From this we deduce that

$$\left(\frac{d}{dx}\right)^{\dagger} = -\frac{d}{dx} \ . \tag{5.6}$$

<sup>&</sup>lt;sup>43</sup>My dissertation focused on theories of extra dimensions. I also noticed that my weight increased in my final year of graduate school as I spent most of my time writing about extra dimensions and eating cafe pastries.

We will be especially interested in **self-adjoint** (Hermitian) operators for which

$$\mathcal{O}^{\dagger} = \mathcal{O} \ . \tag{5.7}$$

This is, as we mentioned for the finite-dimensional case, because self-adjoint operators are *nice*: they have real eigenvalues and orthogonal eigenvectors. Since most physical values are real eigenvalues of some operator, one may expect that the differential operators that show up in physics are typically self-adjoint.

Exercise 5.1 We saw above that the derivative operator is not self-adjoint. What is an appropriate self-adjoint version of the derivative operator? Hint: what is the momentum operator in quantum mechanics?

**Example 5.4** Consider  $\mathcal{O} = -\partial_x^2$  defined on the domain  $x \in [0,1]$  with the boundary conditions f(0) = f(1) = 0. Is this operator self-adjoint? We want to check of  $\langle f, \mathcal{O}g \rangle = \langle Of, g \rangle$ . We have one trick: integration by parts. Let's see how this works.

$$\langle f, \mathcal{O}g \rangle = -\int dx \, f^*(x) \partial^2 g(x) \ .$$
 (5.8)

This is compared to

$$\langle \mathcal{O}f, g \rangle = -\int_0^1 dx \left[ \partial^2 f(x) \right] * g(x)$$
 (5.9)

$$= - (\partial f(x))^* g(x)|_0^1 + \int_0^1 dx \ [\partial f(x)]^* \partial g(x)$$
 (5.10)

$$= f^*(x)\partial^2 g(x)\Big|_0^1 - \int_0^1 dx \, f^*(x)\partial^2 g(x)$$
 (5.11)

$$= -\int_0^1 dx \, f^*(x) \partial^2 g(x) . \tag{5.12}$$

And so we see that indeed  $(-\partial^2)^{\dagger} = -\partial^2$ .

Exercise 5.2 In the previous example, what is the significance of the overall sign of the operator? Hint: the sign doesn't matter, it's because we typically think of  $-\partial^2$  and its higher-dimensional derivatives as the square of the momentum operator.

**Example 5.5** The eigenfunctions  $f_n$  of  $-\partial^2$  defined on  $x \in [0,1]$  with Dirichlet boundary conditions are simply

$$f_n(x) = A_n \sin(n\pi x) \qquad \lambda_n = -n^2 \pi^2 , \qquad (5.13)$$

where  $\lambda_n$  is the associated eigenvalue and  $A_n$  is some normalization that. These eigenfunctions are orthonormal in the following sense:

$$\langle f_n, f_m \rangle = \int_0^1 dx \, \sin(n\pi x) \sin(m\pi x) = \frac{A_n A_m}{2} \delta_{nm} , \qquad (5.14)$$

from which we deduce that the normalization is  $A_n = \sqrt{2}$ . That's basically all there is to know about Fourier series.

**Exercise 5.3** A function g(x) defined on an interval  $x \in [0,1]$  with Dirichlet boundary conditions can be written with respect to the Fourier basis (5.13). In ket notation, the  $n^{th}$  component of q with respect to this basis is

$$g^n = \langle f_n | g \rangle . (5.15)$$

Confirm that this is precisely what you know from Fourier series. In other words, we can decompose q(x) as

$$g(x) = \sum_{n} \langle f_n | g \rangle f_n(x) . \qquad (5.16)$$

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## 5.3 Completeness in Function Space

We rarely have much to say about the unit matrix in linear algebra. However, much like when we discussed units, we can squeeze a lot out of inserting the identity in our mathematical machinations. In order to help with translate this to function space, let's review how it works in finite dimensional vector spaces. The unit matrix is 1 and may be written:

$$1 = \sum_{i} |i\rangle\langle i| , \qquad (5.17)$$

where  $|i\rangle$  and  $\langle j|$  are basis (dual-)vectors.

**Exercise 5.4** Take a moment and convince yourself that (5.17) is true and obvious. It may be helpful to explicitly write out  $|i\rangle\langle j|$  as a matrix.

Exercise 5.5 Suppose you have a two-dimensional Euclidean vector space. Show that (5.17) is true for the basis

$$|1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\1 \end{pmatrix} \qquad |2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\-1 \end{pmatrix} \qquad (5.18)$$

$$\langle 1| = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \end{pmatrix}$$
  $\qquad \langle 2| = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \end{pmatrix}$  (5.19)

In fact, (5.17) defines what it means that a set of basis vectors is **complete**. You can write any vector  $|v\rangle$  with respect to the basis  $|i\rangle$ —the components are simply

$$v^i = \langle i|v\rangle \tag{5.20}$$

so that

$$|v\rangle = \sum_{i} |i\rangle\langle i|v\rangle , \qquad (5.21)$$

which we recognize as nothing more than 'multiplying by the identity.'

What does completeness look like in function space?

Let  $e_{(n)}(x)$  be a set of basis functions. The basis is **complete** if

$$\sum_{n} \left[ e_{(n)}(x) \right]^* e_{(n)}(y) = \delta(x - y) . \tag{5.22}$$

Compare this very carefully with the completeness relation (5.17). The sum over i in the finite-dimensional case has been relabeled into a sum over n in the function space—this is just my preference<sup>44</sup>. The  $\mathbbm{1}$  has been replaced by a Dirac  $\delta$ -function,  $\delta(x-y)$ . Let's confirm that this makes sense. The multiply by one completeness relation (5.21) in function space is

$$|g\rangle = \sum_{n} |e_{(n)}\rangle\langle e_{(n)}|g\rangle \qquad \langle e_{(n)}|g\rangle = \int dy \, [e_{(n)}(y)]^* g(y) . \qquad (5.23)$$

We have deliberately changed the name of the integration variable to y to avoid confusion; since this variable is integrated over it's simply a *dummy variable* and it doesn't matter what we name it—the quantity  $\langle e_{(n)}|g\rangle$  is independent of y because y is integrated over<sup>45</sup>. Writing this out explicitly as functions:

$$g(x) = \sum_{n} \left[ \int dy \, e_{(n)}^*(y) g(y) \right] e_{(n)}(x) . \tag{5.24}$$

The factor in the square brackets is simply  $\langle e_{(n)}|g\rangle$ , which is just a *number*—it has no functional dependence on x. If this seems unusual, please refer back to Example 5.5 and Exercise 5.3.

By the way, you'll often hear people (perhaps even me) say that the Dirac  $\delta$  function is not strictly an function but rather a **distribution**—this means that it only makes sense when it is integrated over. As physicists we'll sometimes be sloppy and talk about physical quantities that could be Dirac  $\delta$ -functions. There is never an appropriate, measurable physical quantity that is described by a  $\delta(x)$ . Anything with a  $\delta(x)$  is an object that was meant to be integrated over. When you imagine that a point charge density is a  $\delta$ -function, this is only because you will eventually integrate over it to determine the total charge. This is precisely what we saw in the charged cat in Example 3.3. If you ever calculate a measurable quantity to be  $\delta(x)$  check your work. If you ever find  $\delta(x)^2$ , then go home, it's past your bed time.

## 5.4 Orthonormality in Function Space

One should contrast the notion of completeness of a a basis this with that of **orthonormality** of the basis. Orthonormality is the statement that

$$\langle i|j\rangle = \delta_i^j \ . \tag{5.25}$$

 $<sup>^{44}</sup>$ I think this is because we will deal with complex functions and I want to avoid using i as an index. But if we're being honest, it's just become a habit.

<sup>&</sup>lt;sup>45</sup>By the way, this should ring a bell from our summation convention. When an upper and lower tensor index are contracted, the resulting object behaves as if it didn't have those indices:  $A^{i}_{j}v^{j}$  behaves as a vector with one upper index.

Completeness has to do with the 'outer product'  $|i\rangle\langle i|$  while orthonormality has to do with the 'inner product'  $\langle i|i\rangle = \langle i,i\rangle$ . The function space generalization of orthonormality is<sup>46</sup>

$$\langle e_{(n)}|e_{(m)}\rangle = \int dx \, e_{(n)}^*(x)e_{(m)}(x) = \delta_{nm} .$$
 (5.26)

**Exercise 5.6** Why does (5.26) have a Kronecker  $\delta$  with discrete indices when (5.22) has a Dirac  $\delta$ ? Please make sure you can answer this; it establishes the conceptual foundation of the analogy between finite- and infinite-dimensional vector spaces.

For the completeness relation, we sum over the same eigenfunction label n for a function and its conjugate evaluated at different continuous positions. For the orthonormality relation, we integrate over the positions of two different eigenfunction indices, n and m.

Do not confuse the eigenfunction label with the index of a vector. If this is confusing, please refer back to Exercise 5.5. You may be stuck thinking about basis vectors in the Cartesian basis—this is the analog of thinking about basis functions in the 'histogram basis' of Section 3.3. What we want to do is generalize to more convenient bases, like the eigenfunctions of differential operators (e.g. the Fourier basis for  $-\partial^2$ ).

### 5.5 Completeness and Green's Functions

The utility of the completeness relation should be clear. If you happen to have a nice (self-adjoint) linear differential operator  $\mathcal{O}$  with a nice (complete, orthogonal) eigenfunctions  $e_{(n)}$  and eigenvalues  $\lambda_n$ , then we can expand any function  $\psi(x)$  with respect to these eigenfunctions. Then it is easy to invert the differential equation  $\mathcal{O}\psi(x) = s(x)$  to determine the response  $\psi(x)$  to a source s(x):

$$\psi(x) = \mathcal{O}^{-1} \sum_{n} \langle e_{(n)} | s \rangle e_{(n)}(x) = \sum_{n} \frac{\langle e_{(n)} | s \rangle}{\lambda_n} e_{(n)}(x) , \qquad (5.27)$$

where we've simply used (3.38). The inner product  $\langle e_{(n)}|s\rangle$  is an overlap integral between known functions:

$$\psi(x) = \int dy \sum_{n} \frac{e_{(n)}^{*}(y)e_{(n)}(x)}{\lambda_{n}} s(y) , \qquad (5.28)$$

where we have rearranged terms rather suggestively. This is now in the same form as our prototype Green's function example (3.56).

Referring back to (4.1), we see that our completeness relation—that is, our trick of inserting unity—in (5.28) tells us an explicit form for the Green's function of a differential operator  $\mathcal{O}$  if you know the eigenfunctions and eigenvalues of that operator:

$$G(x,y) = \sum_{n} \frac{e_{(n)}^{*}(y)e_{(n)}(x)}{\lambda_{n}} .$$
 (5.29)

<sup>&</sup>lt;sup>46</sup>If you're a purist, you'll note that  $\delta_{nm}$  should really be written as  $\delta_m^n$  because the dual basis vector has an upper index. While this may be true, I'm making the present notational choice because the object that we would call  $\tilde{\mathbf{e}}^{(n)}$  really does contain  $e_{(n)}^*(x)$ , the complex conjugate of  $e_{(n)}(x)$ .

This is formally an infinite sum and so is only practically useful if each term is successively smaller.

# Acknowledgements

P.T. the students of Physics 231 for their patience and feedback on on this course.