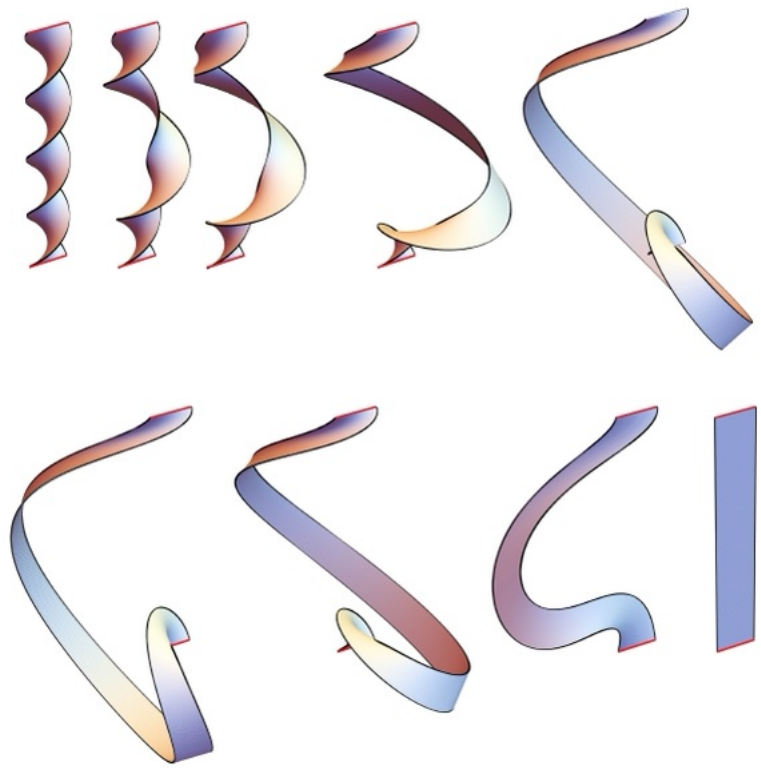

Physics Math

Linear Algebra, Fourier Analysis, Differential Equations, and *Mathematica*

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Contents

List of Tables

List of Figures

Chapter 0

Three Teasers

0.1 Abstract Algebra

Rotate a book 90° clockwise about an upward axis and then 90° clockwise about a leftward axis. Repeat the rotations in the reverse order and the book ends in a different orientation, as in Fig. 0.1! Symbolically,

$$R_1 R_2 \neq R_2 R_1. \tag{0.1}$$

What kind of numbers can represent rotations that don't **commute**?

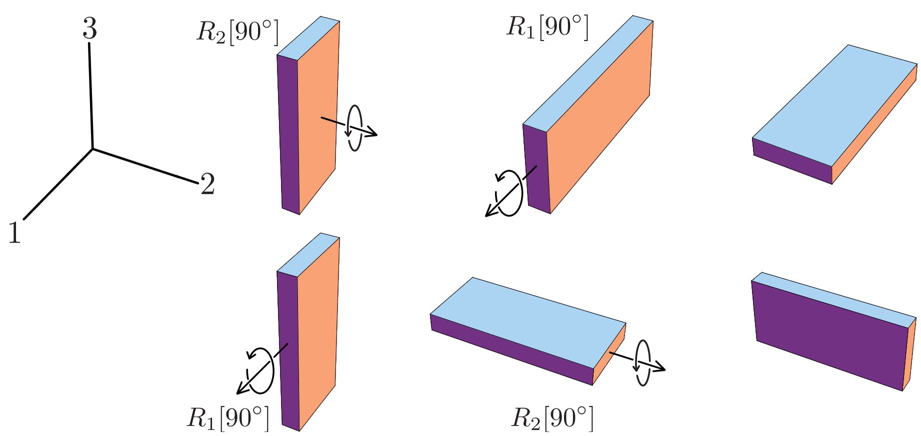


Figure 0.1: Finite rotations do not commute.

0.2 Fourier Analysis

Consider the motion of an ideal string fixed at both ends, like a guitar string. Musically, the string's motion is well-known to be a superposition of sinusoidal normal modes called **harmonics**. Symbolically,

$$y[x,t] = \sum_n a_n \sin[2\pi x/\lambda_n] \sin[2\pi f_n t]. \tag{0.2}$$

Yet the motion consists of a line segment bouncing back-and-forth inside a parallelogram envelope, as in Fig. 0.2. How can the harmonics synthesize this kinked motion and with what amplitudes?

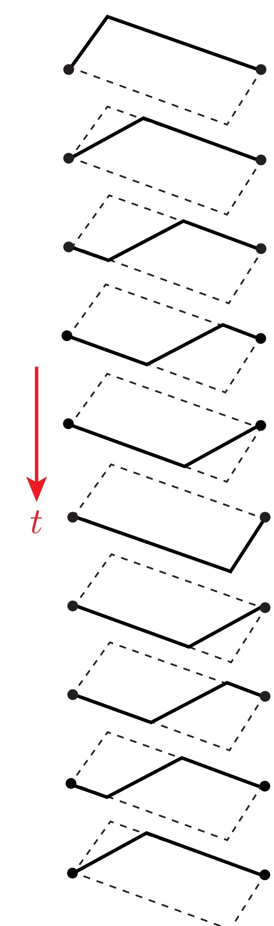


Figure 0.2: Sinusoidal normal modes synthesize kinked string dynamics.

0.3 Differential Equations

Suppose water in a bucket increases at a rate equal to the cube root of water already there. If the bucket begins empty, then symbolically

$$\frac{d}{dt}V[t] = V[t]^{1/3}, \tag{0.3a}$$

$$V[0] = 0. \tag{0.3b}$$

This **initial value problem** has *two* easily-checked solutions

$$V[t] = \left(\frac{2}{3}\right)^{3/2} t^{3/2}, \tag{0.4a}$$

$$V[t] = 0. \tag{0.4b}$$

How can the bucket both remain empty *and* fill with water? How can this evolution be nonunique?

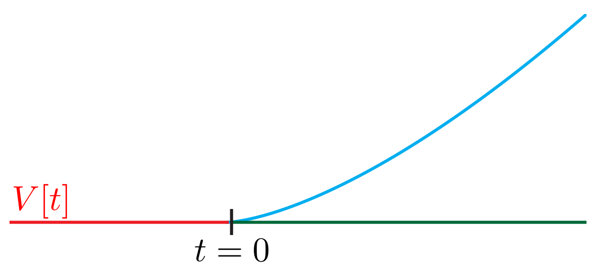


Figure 0.3: Evolution of water in the bucket has an ambiguous future.

Chapter 1

Complex Numbers

Complex numbers complete real numbers.

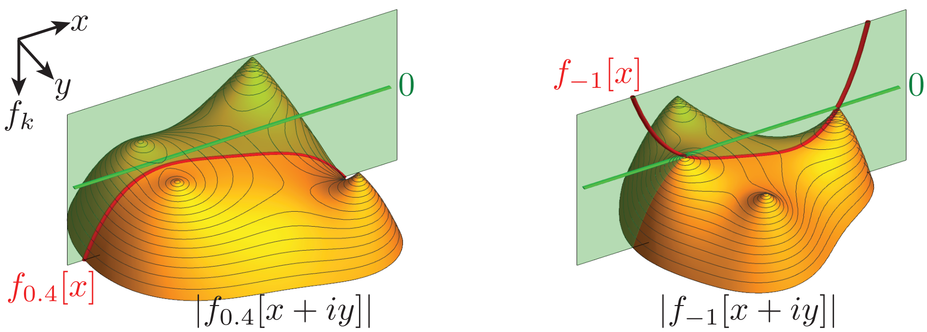


Figure 1.1: Illustrating the fundamental theorem of algebra, peaks represent 4 complex roots of the 4th-order polynomial equation $f_k[z] = kz^4 + z + 1 = 0$ for two different values of the parameter k, where $z = x + \boldsymbol{i}y$ and x and y are real.

1.1 Euler's Identity

The algebraic equation $x^2 + 1 = 0$ has no real solutions. *Imagine* that it has solutions $\pm\boldsymbol{i}$. Leverage these **imaginary solutions** to prove the **fundamental theorem of algebra**: an nth order polynomial has exactly n roots, as illustrated by Fig. 1.1. The beauty of this result convinced mathematicians of the utility of imaginary numbers.

By successive multiplication, the imaginary number $\boldsymbol{i}$ satisfies

$$\boldsymbol{i}^2 = -1, \tag{1.1a}$$

$$\boldsymbol{i}^3 = -\boldsymbol{i}, \tag{1.1b}$$

$$\boldsymbol{i}^4 = +1, \tag{1.1c}$$

$$\boldsymbol{i}^5 = +\boldsymbol{i} \tag{1.1d}$$

$$\boldsymbol{i}^6 = -1, \tag{1.1e}$$

and so on in a 4-cycle. Hence the absolutely convergent Taylor expansions of common functions, as in Fig. 1.2, dramatically reorganize when evaluated at imaginary numbers. For example, the exponential

$$\begin{aligned} e^{\boldsymbol{i}x} &= 1 + \boldsymbol{i}x + \frac{(\boldsymbol{i}x)^2}{2!} + \frac{(\boldsymbol{i}x)^3}{3!} + \frac{(\boldsymbol{i}x)^4}{4!} + \frac{(\boldsymbol{i}x)^5}{5!} + \frac{(\boldsymbol{i}x)^6}{6!} + \frac{(\boldsymbol{i}x)^7}{7!} + \frac{(\boldsymbol{i}x)^8}{8!} + \cdots \\ &= 1 + \boldsymbol{i}x - \frac{x^2}{2!} - \boldsymbol{i}\frac{x^3}{3!} + \frac{x^4}{4!} + \boldsymbol{i}\frac{x^5}{5!} - \frac{x^6}{6!} - \boldsymbol{i}\frac{x^7}{7!} + \frac{x^8}{8!} + \cdots \\ &= \left(1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \frac{x^8}{8!} - \cdots\right) + \boldsymbol{i}\left(x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots\right) \\ &= \cos x + \boldsymbol{i}\sin x, \end{aligned} \tag{1.2}$$

becomes a linear superposition of sinusoids known as **Euler's identity**. The choice $x = \pi$ generates the famously beautiful special case

$$e^{\boldsymbol{i}\pi} + 1 = 0, \tag{1.3}$$

which relates the five most important mathematical constants $e, \boldsymbol{i}, \pi, 1, 0$ in a simple formula.

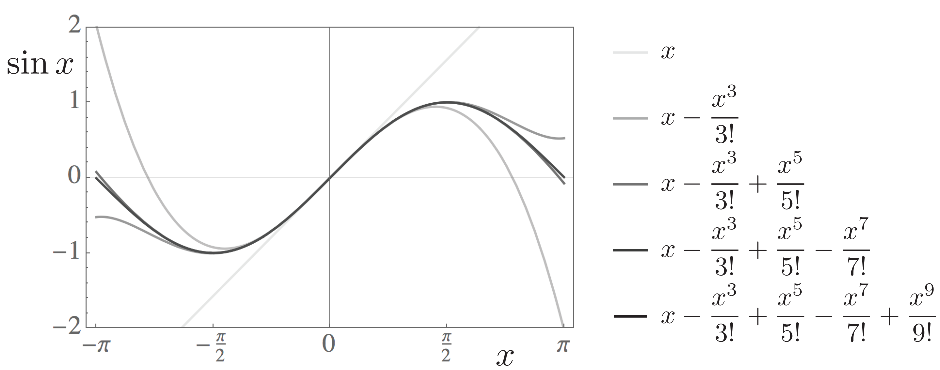


Figure 1.2: Convergent power series approximations to a sine, where the darker curves include more terms.

1.2 2D Division Algebra

A general complex number is the linear combination

$$z = z_R + z_I\boldsymbol{i} = x + \boldsymbol{i}y = \{x, y\}, \tag{1.4}$$

where the real and imaginary components $x = z_R$ and $y = z_I$ are real numbers. The product of two complex numbers

$$zz' = (x + \boldsymbol{i}y)(x' + \boldsymbol{i}y') = xx' - yy' + \boldsymbol{i}(yx' + xy') \tag{1.5}$$

is another complex number. A complex number's **conjugate**

$$z^* = \bar{z} = x - \boldsymbol{i}y \tag{1.6}$$

negates the imaginary part, so the **norm**

$$|z| = \sqrt{zz^*} = \sqrt{x^2 + y^2} \tag{1.7}$$

is the square root of the product with the conjugate, and the **inverse**

$$z^{-1} = \frac{z^*}{|z|^2} \tag{1.8}$$

is the conjugate divided by the norm squared. The inverse enables complex number division, such as

$$\frac{z'}{z} = \frac{x' + \boldsymbol{i}y'}{x + \boldsymbol{i}y} = \frac{x' + \boldsymbol{i}y'}{x + \boldsymbol{i}y}\,\frac{x - \boldsymbol{i}y}{x - \boldsymbol{i}y} = \frac{x'x + y'y}{x^2 + y^2} + \boldsymbol{i}\frac{xy' - x'y}{x^2 + y^2}. \tag{1.9}$$

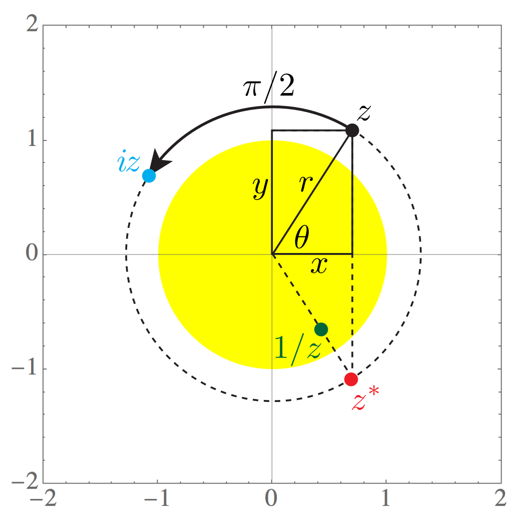


Figure 1.3: Complex number $z = re^{\boldsymbol{i}\theta} = x + \boldsymbol{i}y = \{x, y\}$. Unit disk is yellow.

1.3 2D Rotations

In the complex plane $z = \{x, y\}$, a complex numbers has the **polar representation**

$$z = x + \boldsymbol{i}y = r\cos\theta + \boldsymbol{i}\,r\sin\theta = re^{\boldsymbol{i}\theta} \tag{1.10}$$

using Euler's identity, where $r = |z|$ is the **modulus** and θ is its **phase**. The polar presentation illustrates how complex numbers can model two dimensional rotations. For example, multiplying a complex number by $e^{i\varphi}$ rotates it through an angle θ,

$$z' = ze^{i\varphi} = re^{i\theta}e^{i\varphi} = re^{i(\theta+\varphi)}. \tag{1.11}$$

Multiplying by $i = e^{i\pi/2}$ rotates a complex number through $\pi/2 = 90°$ counter clockwise, as illustrated in Fig. 1.3. Multiplying by $e^{i\pi}$ rotates a complex number through $180°$, which when applied to $+1$ produces -1, thereby providing a geometric interpretation of Euler's Eq. 1.3 identity.

1.4 Trigonometric Identities

Complex numbers facilitate the derivation of useful trigonometric identities. For real angle $a \in \mathbb{R}$, if $z = e^{ia} \in \mathbb{C}$, then

$$\begin{aligned} 1 = |z|^2 = zz^* &= e^{ia}e^{-ia} \\ &= (\cos a + i \sin a)(\cos a - i \sin a) \\ &= \cos^2 a + \sin^2 a. \end{aligned} \tag{1.12}$$

For real angles $a, b \in \mathbb{R}$,

$$\begin{aligned} e^{i(a+b)} &= e^{ia}e^{ib}, \\ \cos[a+b] + i \sin[a+b] &= (\cos a + i \sin a)(\cos b + i \sin b) \\ &= \cos a \cos b - \sin a \sin b + i(\sin a \cos b + \cos a \sin b), \end{aligned} \tag{1.13}$$

so equating real and imaginary parts generates two addition angle formulas at once,

$$\cos[a+b] = \cos a \cos b - \sin a \sin b, \tag{1.14a}$$

$$\sin[a+b] = \sin a \cos b + \cos a \sin b. \tag{1.14b}$$

Setting $a = b$ generates two double angle formulas,

$$\cos[2a] = \cos^2 a - \sin^2 a, \tag{1.15a}$$

$$\sin[2a] = 2 \sin a \cos a. \tag{1.15b}$$

1.5 Complex Functions

Complex functions map complex numbers to complex numbers. Given the complex number $z = x + iy = re^{i\theta}$, the complex function

$$f[z] = z' \tag{1.16}$$

generates the rectangular map

$$\{x, y\} \to \{x', y'\} \tag{1.17}$$

and the polar map

$$\{r, \theta\} \to \{r', \theta'\}. \tag{1.18}$$

Such mappings are best visualized in 4D. However, plotting the real part x' vertically and coloring the resulting surface by the imaginary part y' produces a faithful 3D visualization, as in the Fig. 1.4 plot of the square root function.

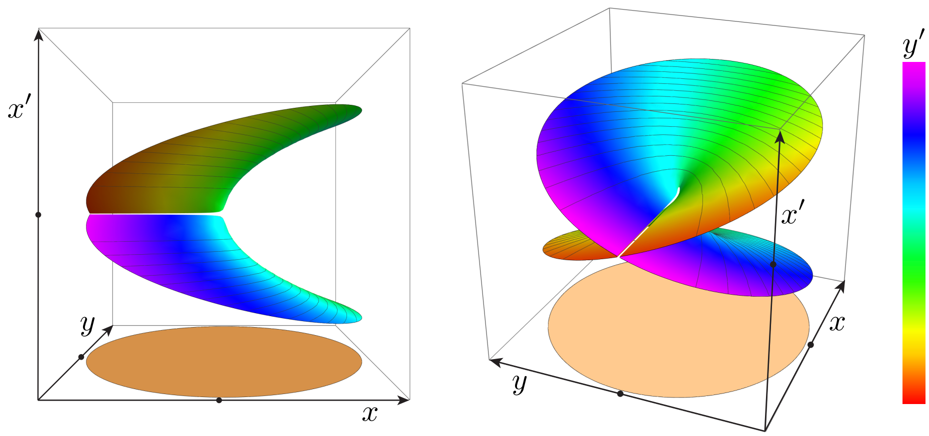


Figure 1.4: Visualize the complex square root function $z' = \sqrt{z}$ by plotting its real part x' vertically and coloring the resulting surface by its imaginary part y'. The two **branches** of the **Riemann** surface correspond to the positive and negative real square roots.

More generally, since each complex number has infinitely many polar representations

$$z = re^{i\theta} = re^{i(\theta+2\pi)} = re^{i(\theta+b2\pi)}, \tag{1.19}$$

for any integers b, then its nth root

$$z^{1/n} = r^{1/n}e^{i(\theta+b2\pi)/n} = r^{1/n}e^{i\theta/n}e^{ib2\pi/n} \tag{1.20}$$

has n distinct values or **branches** for $b = 0, 1, 2, \ldots, n-1$.

Complex functions map a complex number to a **set** of complex numbers in a multivalued relation described by 2D **Riemann surfaces** in 4D space, as in the 3D projections of Fig. 1.4 and Fig. 1.5. Differing colors at the 3D self-intersections imply no self-intersections in 4D. Define a **principle value** of a complex value by focussing on a single branch, say $b = 0$, and thereby recover a single-valued relation or function.

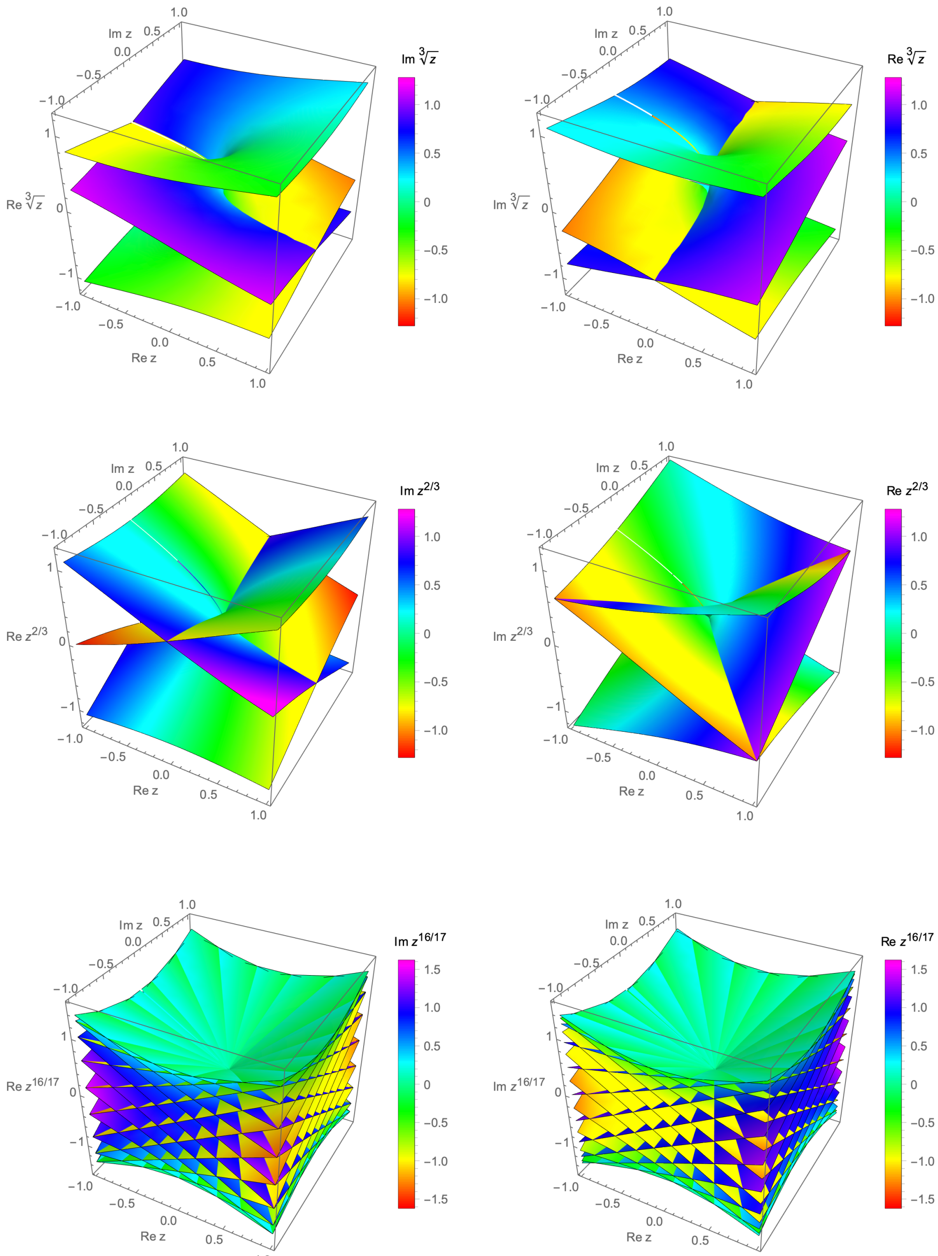


Figure 1.5: Riemann surfaces for some complex powers $z^{1/3}, z^{2/3}, z^{16/17}$, real parts colored according to imaginary parts (left) and imaginary parts colored according to real parts (right).

1.6 Hyperbolic Functions

Hyperbolic functions are intimately related to trigonometric functions. From Euler's identity

$$e^{i\theta} = \cos\theta + i\sin\theta \tag{1.21}$$

and its complex conjugate

$$e^{-i\theta} = \cos\theta - i\sin\theta, \tag{1.22}$$

add to get

$$\cos\theta = \frac{e^{i\theta} + e^{-i\theta}}{2} \tag{1.23}$$

and subtract to get

$$\sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}. \tag{1.24}$$

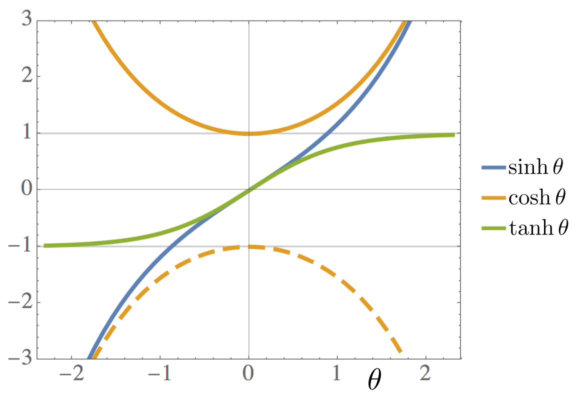


Figure 1.6: Graphs of hyperbolic functions, with $\tanh\theta = \sinh\theta/\cosh\theta$.

The substitution $\theta \to i\theta$ replaces a real angle with an imaginary angle and generates hyperbolic functions from trigonometric functions. For example,

$$\cos[i\theta] = \frac{e^{-\theta} + e^{\theta}}{2} = \cosh\theta \tag{1.25}$$

and

$$\sin[i\theta] = \frac{e^{-\theta} - e^{\theta}}{2i} = i\frac{e^{\theta} - e^{-\theta}}{2} = i\sinh\theta. \tag{1.26}$$

Cosine "swallows" the i in becoming hyperbolic cosine, while sine "passes" the i in becoming hyperbolic sine. (Similarly, cosine swallows a minus sign, $\cos[-\theta] = \cos\theta$, while sine passes a minus sign, $\sin[-\theta] = -\sin\theta$.) These functions are sometime pronounced "cosh" and "sinch".

Inversely,

$$\cosh[i\theta] = \frac{e^{-i\theta} + e^{i\theta}}{2} = \cos\theta \tag{1.27}$$

and

$$\sinh[i\theta] = \frac{e^{-i\theta} - e^{i\theta}}{2i} = i\frac{e^{i\theta} - e^{-i\theta}}{2} = i\sin\theta. \tag{1.28}$$

For every trigonometric identity there is a corresponding hyperbolic identity. For example, substitute $\theta \to i\theta$ into

$$\cos^2\theta + \sin^2\theta = 1 \tag{1.29}$$

to get

$$\cosh^2\theta - \sinh^2\theta = 1. \tag{1.30}$$

The hyperbolic functions are real, exponential, and nonrepeating, as in Fig. 1.6.

1.7 4 Division Algebras

Normed division algebras exist in dimensions 1, 2, 4, and 8 only. The algebras consist of real numbers, complex numbers or **binarions**, **quaternions**, and **octonions**. Something is lost at each dimensional doubling: While real numbers are ordered and their multiplication is both associative and commutative, complex numbers are not ordered, quaternion multiplication is not commutative, and octonion multiplication is neither associative nor commutative.

Mathematica Complex Numbers

```
1/(2 - 3 I) (* 1[CTRL]/a → 1/a, [ENTER] or [SHIFT][RET] → input *)
```

```
2/13 + 3 i/13
```

```
z = 3 + 2 i; (* [ESC]ii[ESC] → i, Set[a,b] ↔ a=b *)
```

```
z == Abs[z] e^(i Arg[z]) (* [ESC]ee[ESC] → e, a[CTRL]^b → a^b, Equal[a,b] ↔ a==b *)
```

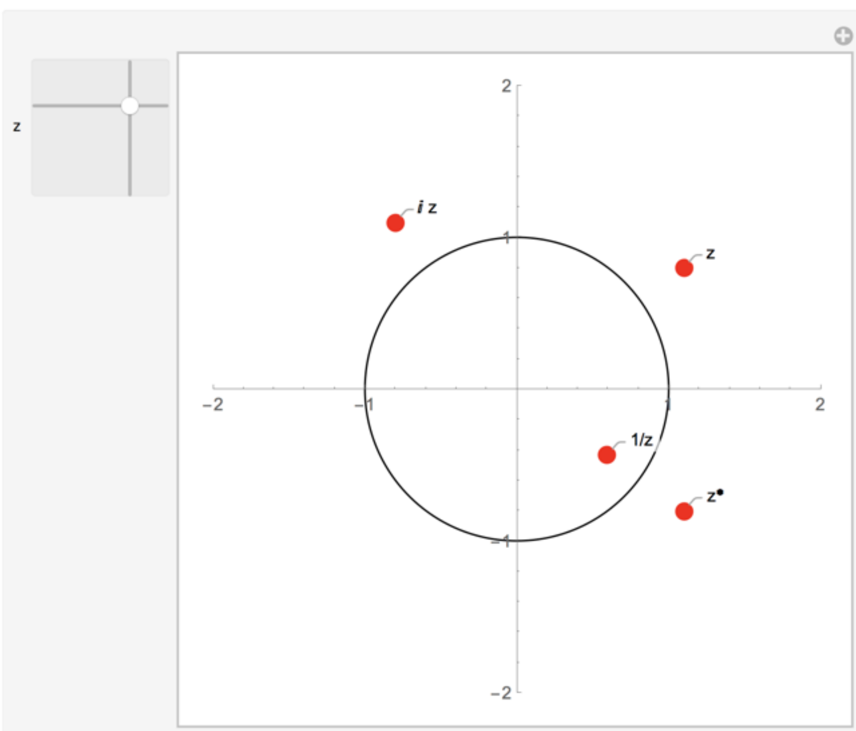
```
True
```

```
ReIm[z*] (* z[ESC]conj[ESC] → z* *)
```

```
{3, -2}
```

```
points[z_] := ReIm /@ {z, z*, 1 / z, i z} (* Map[f,expr] ↔ f/@expr *)
```

```
Manipulate[
 ListPlot[
  points[z[[1]] + i z[[2]]] → {"z", "z*", "1/z", "i z"},
  PlotRange → 2 {{-1, 1}, {-1, 1}}, (* options *)
  AspectRatio → 1,
  PlotStyle → Directive[PointSize[0.03], Red],
  Prolog → Circle[]
 ],
 {{z, {1.1, 0.8}}, {-2, -2}, {2, 2}}, ControlPlacement → Left]
```



Worked Problem

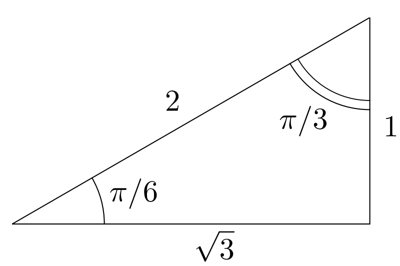
1. Rotate the vector $\vec{v} = \{\sqrt{3}, 1\}$ through an angle of $30°$.

$$\vec{v} = \{\sqrt{3}, 1\}$$

$$\begin{aligned} z &= \sqrt{3} + \boldsymbol{i} \\ &= \sqrt{3+1}\, e^{\boldsymbol{i} \arctan\left[1/\sqrt{3}\right]} \\ &= 2\, e^{\boldsymbol{i}\pi/6} \end{aligned}$$

$$\begin{aligned} z' &= z\, e^{\boldsymbol{i}\pi/6} \\ &= 2\, e^{\boldsymbol{i}\pi/6} e^{\boldsymbol{i}\pi/6} \\ &= 2\, e^{\boldsymbol{i}\pi/3} \\ &= 2\left(\cos\frac{\pi}{3} + \boldsymbol{i}\sin\frac{\pi}{3}\right) \\ &= 2\left(\frac{1}{2} + \boldsymbol{i}\frac{\sqrt{3}}{2}\right) \\ &= 1 + \boldsymbol{i}\sqrt{3} \end{aligned}$$

$$\vec{v}\,' = \{1, \sqrt{3}\}$$



Problems

1. For each complex number z, compute $\bar{z} = z^*$, $|z|^2$, $1/z$ in rectangular $x + iy$ form.

   (a) $z = 1 + i$

   (b) $z = 2 - 3i$

   (c) $z = 2e^{i\pi/3}$

2. For each pair of complex number z and z', compute $z + z'$, z/z' in rectangular form.

   (a) $z = 1 + i$, $z' = 1 - i$

   (b) $z = 2 - 3i$, $z' = 3 + 2i$

   (c) $z = 2e^{i\pi/3}$, $z' = 3e^{i\pi/2}$

3. Find the principal values of the following complex numbers in rectangular form.

   (a) $\left(\dfrac{1+i}{1-i}\right)^{2718}$ (Readily done by hand!)

   (b) $\sqrt{i}$

   (c) i^i (Eye to Eye)

   (d) $i^{i^{i^{\cdot^{\cdot^{\cdot}}}}}$ (Tower of Eyes)

4. For each complex number z, plot z, z^*, $1/z$, iz.

   (a) $z = 3 + 2i$

   (b) $z = 3e^{i\pi/4}$

5. Use complex numbers to rotate the vector $\vec{v}$ through angle θ and interpret the result graphically.

   (a) $\vec{v} = \{1, 0\}$, $\theta = 90°$.

   (b) $\vec{v} = \{1, 1\}$, $\theta = -45°$.

6. Use complex numbers to simultaneously derive the following triple angle identities.

   (a) $\sin[3\theta] = -\sin^3\theta + 3\cos^2\theta\sin\theta$

   (b) $\cos[3\theta] = +\cos^3\theta - 3\sin^2\theta\cos\theta$

7. Use complex numbers to derive the following hyperbolic identities from the corresponding trigonometric identities.

   (a) $\coth^2\theta - \mathrm{csch}^2\theta = 1$

   (b) $\tanh^2\theta + \mathrm{sech}^2\theta = 1$

8. Use *Mathematica* to visualize the complex fourth root function $z^{1/4}$ as in Fig. 1.5. (Hint: Color Plot3D functions of each branch and combine them with the Show function; compare with the ComplexPlot3D function.)

Chapter 2

Quaternions

The first abstract algebra can represent classical rotations and spin-1/2 quantum mechanics.

Figure 2.1: Plaque commemorating Hamilton's discovery of the quaternion algebra of 3D rotations. (Part of a video frame by Wayne Fitzgerald.)

2.1 Multiplication Table

In the 1840s, William Rowan Hamilton struggled to generalize complex numbers to three dimensions, but he couldn't define a generalized multiplication that was closed. On the Monday evening of 1843 October 16, while walking with his wife Helen along the Royal Canal in Dublin Ireland, he realized a fourth dimension would close the algebra, and Hamilton stopped and carved the quaternion algebra into the stone of the Brougham (Broom) Bridge, an event now commemorated by the Fig. 2.1 plaque. The noncommutativity of the quaternion product enables it to model 3D rotations. Today quaternions are used extensively in computer graphics and inertial navigation software for airplanes and spacecraft.

Hamilton's succinct summary [1] in three **quaternion (basis) units** was

$$\hat{\imath}^2 = \hat{\jmath}^2 = \hat{k}^2 = \hat{\imath}\hat{\jmath}\hat{k} = -1, \tag{2.1}$$

which implies

$$\begin{aligned} \big(\hat{\imath}\hat{\jmath}\hat{k} &= -1\big)\hat{k}, \\ -\hat{\imath}\hat{\jmath} &= -\hat{k}, \end{aligned} \tag{2.2}$$

and

$$\begin{aligned} \hat{\jmath}\hat{\imath}\big(\hat{\imath}\hat{\jmath}\hat{k} &= -1\big), \\ \hat{\jmath}\big(-\hat{\jmath}\hat{k} &= -\hat{\imath}\big), \\ \hat{k} &= -\hat{\jmath}\hat{\imath}, \end{aligned} \tag{2.3}$$

so the quaternion units **anticommute** like

$$\hat{\imath}\hat{\jmath} = \hat{k} = -\hat{\jmath}\hat{\imath} \tag{2.4}$$

and **cycle** like

$$\hat{\imath}\hat{\jmath} = \hat{k}, \tag{2.5a}$$

$$\hat{\jmath}\hat{k} = \hat{\imath}, \tag{2.5b}$$

$$\hat{k}\hat{\imath} = \hat{\jmath}. \tag{2.5c}$$

Figure 2.2 summarizes the noncommutative algebra and compares it with the familiar (but historically later) vector cross and dot products.

	b
a	ab

$\star$	1	$\hat{\imath}$	$\hat{\jmath}$	$\hat{k}$
1	1	$\hat{\imath}$	$\hat{\jmath}$	$\hat{k}$
$\hat{\imath}$	$\hat{\imath}$	-1	$\hat{k}$	$-\hat{\jmath}$
$\hat{\jmath}$	$\hat{\jmath}$	$-\hat{k}$	-1	$\hat{\imath}$
$\hat{k}$	$\hat{k}$	$\hat{\jmath}$	$-\hat{\imath}$	-1

$\times$	$\hat{\imath}$	$\hat{\jmath}$	$\hat{k}$
$\hat{\imath}$	$\vec{0}$	$\hat{k}$	$-\hat{\jmath}$
$\hat{\jmath}$	$-\hat{k}$	$\vec{0}$	$\hat{\imath}$
$\hat{k}$	$\hat{\jmath}$	$-\hat{\imath}$	$\vec{0}$

$\cdot$	$\hat{\imath}$	$\hat{\jmath}$	$\hat{k}$
$\hat{\imath}$	1	0	0
$\hat{\jmath}$	0	1	0
$\hat{k}$	0	0	1

Figure 2.2: Quaternion (star) product, vector (cross) product, and scalar (dot) product multiplication tables. For example, $\hat{\imath} \star \hat{\imath} = \hat{\imath}\hat{\imath} = -1$, $\hat{\imath} \times \hat{\imath} = \vec{0}$, and $\hat{\imath} \cdot \hat{\imath} = 1$.

2.2 4D Division Algebra

A general quaternion is the linear combination

$$\begin{aligned}\mathring{q} &= q_0 + \hat{\imath}\, q_1 + \hat{\jmath}\, q_2 + \hat{k}\, q_3 = q_0 + q_1\hat{\imath} + q_2\hat{\jmath} + q_3\hat{k} = q_0 + \vec{q} \\ &= \{q_0, q_1, q_2, q_3\} = \{q_0, \vec{q}\},\end{aligned} \tag{2.6}$$

read "q-ring equals q-sub-zero plus $\boldsymbol{i}$-hat times q-sub-one . . . ", where the components q_n are real numbers. The addition of a scalar and a vector is just a convenient notation for a list of a scalar and a vector, $q_0 + \vec{q} = \{q_0, \vec{q}\}$. A quaternion is a complex number of complex numbers,

$$\mathring{q} = q_0 + \hat{\imath}\, q_1 + \hat{\jmath}\, q_2 + \hat{k}\, q_3 = (q_0 + \hat{\imath} q_1) + \hat{\jmath}(q_2 - \hat{\imath} q_3) = z + \hat{\jmath} z'. \tag{2.7}$$

A **real quaternion** has vanishing vector part and a (pure) **imaginary quaternion** has vanishing scalar part, so abbreviate them as

$$\{q_0, \vec{0}\} = q_0, \tag{2.8a}$$

$$\{0, \vec{q}\} = \vec{q}. \tag{2.8b}$$

The product of two quaternions

$$\mathring{q} \star \mathring{p} = \mathring{q}\mathring{p} = (q_0 + q_1\hat{\imath} + q_2\hat{\jmath} + q_3\hat{k})(p_0 + p_1\hat{\imath} + p_2\hat{\jmath} + p_3\hat{k}). \tag{2.9}$$

Distribute the multiplication

$$\begin{aligned}\mathring{q}\mathring{p} = q_0p_0 &+ q_0p_1\hat{\imath} + q_0p_2\hat{\jmath} + q_0p_3\hat{k} \\ &+ q_1p_0\hat{\imath} + q_1p_1\hat{\imath}\hat{\imath} + q_1p_2\hat{\imath}\hat{\jmath} + q_1p_3\hat{\imath}\hat{k} \\ &+ q_2p_0\hat{\jmath} + q_2p_1\hat{\jmath}\hat{\imath} + q_2p_2\hat{\jmath}\hat{\jmath} + q_2p_3\hat{\jmath}\hat{k} \\ &+ q_3p_0\hat{k} + q_3p_1\hat{k}\hat{\imath} + q_3p_2\hat{k}\hat{\jmath} + q_3p_3\hat{k}\hat{k}\end{aligned} \tag{2.10}$$

and simplify with the Eq. 2.1 quaternion algebra

$$\begin{aligned}\mathring{q}\mathring{p} = q_0p_0 &+ q_0p_1\hat{\imath} + q_0p_2\hat{\jmath} + q_0p_3\hat{k} \\ &+ q_1p_0\hat{\imath} - q_1p_1 + q_1p_2\hat{k} - q_1p_3\hat{\jmath} \\ &+ q_2p_0\hat{\jmath} - q_2p_1\hat{k} - q_2p_2 + q_2p_3\hat{\imath} \\ &+ q_3p_0\hat{k} + q_3p_1\hat{\jmath} - q_3p_2\hat{\imath} - q_3p_3\end{aligned} \tag{2.11}$$

to get

$$\begin{aligned}\mathring{q}\mathring{p} = &(q_0p_0 - q_1p_1 - q_2p_2 - q_3p_3) \\ &+ (q_0p_1 + p_0q_1 + q_2p_3 - q_3p_2)\hat{\imath} \\ &+ (q_0p_2 + p_0q_2 + q_3p_1 - q_1p_3)\hat{\jmath} \\ &+ (q_0p_3 + p_0q_3 + q_1p_2 - q_2p_1)\hat{k}\end{aligned} \tag{2.12}$$

or

$$\begin{aligned}\mathring{q}\mathring{p} &= q_0p_0 - q_1p_1 - q_2p_2 - q_3p_3\\&\quad + q_0(p_1\hat{\imath} + p_2\hat{\jmath} + p_3\hat{k}) + p_0(q_1\hat{\imath} + q_2\hat{\jmath} + q_3\hat{k})\\&\quad + (q_2p_3 - q_3p_2)\hat{\imath} + (q_3p_1 - q_1p_3)\hat{\jmath} + (q_1p_2 - q_2p_1)\hat{k}\\&= q_0p_0 - \vec{q}\cdot\vec{p} + q_0\vec{p} + p_0\vec{q} + \vec{q}\times\vec{p}. \end{aligned} \tag{2.13}$$

Highlight scalar and vector parts by color coding

$$\mathring{r} = \mathring{q}\mathring{p} = (q_0 + \vec{q})(p_0 + \vec{p}) = q_0p_0 - \vec{q}\cdot\vec{p} + q_0\vec{p} + p_0\vec{q} + \vec{q}\times\vec{p} = r_0 + \vec{r} \tag{2.14}$$

or with braces

$$\mathring{r} = \mathring{q}\mathring{p} = \{q_0, \vec{q}\}\{p_0, \vec{p}\} = \{q_0p_0 - \vec{q}\cdot\vec{p},\ q_0\vec{p} + p_0\vec{q} + \vec{q}\times\vec{p}\} = \{r_0, \vec{r}\}. \tag{2.15}$$

So the product of two quaternions involves both a scalar (dot) product and a vector (cross) product. Indeed, the product of two *imaginary* quaternions

$$\mathring{q}\mathring{p} = \{0, \vec{q}\}\{0, \vec{p}\} = \{0 - \vec{q}\cdot\vec{p},\ \ \vec{0} + \vec{0} + \vec{q}\times\vec{p}\} = -\vec{q}\cdot\vec{p} + \vec{q}\times\vec{p} = \vec{q}\star\vec{p} \tag{2.16}$$

is the *difference* between the cross and dot products. In contrast, the scalar (dot) product of two quaternions

$$\begin{aligned}\mathring{q}\cdot\mathring{p} &= (q_0 + q_1\hat{\imath} + q_2\hat{\jmath} + q_3\hat{k})\cdot(p_0 + p_1\hat{\imath} + p_2\hat{\jmath} + p_3\hat{k})\\&= q_0p_0 + q_1p_1 + q_2p_2 + q_3p_3 = q_0p_0 + \vec{q}\cdot\vec{p}, \end{aligned} \tag{2.17}$$

where $1\hat{\imath} \neq 1\cdot\hat{\imath} = 0$, as real and imaginary directions are perpendicular. Thus, $\hat{\imath}\hat{\imath} = -1$ and $\hat{\imath}\hat{\jmath} = \hat{k}$ but $\hat{\imath}\cdot\hat{\imath} = 1$ and $\hat{\imath}\cdot\hat{\jmath} = 0$.

In analogy with complex numbers, a quaternion's **conjugate**

$$\mathring{q}^* = \{q_0, -\vec{q}\} = \{q_0, -q_1, -q_2, -q_3\} = q_0 - q_1\hat{\imath} - q_2\hat{\jmath} - q_3\hat{k} = q_0 - \vec{q} \tag{2.18}$$

negates the imaginary part. The conjugate of a product

$$\begin{aligned}(\mathring{q}\mathring{p})^* &= (q_0p_0 - \vec{q}\cdot\vec{p} + q_0\vec{p} + p_0\vec{q} + \vec{q}\times\vec{p})^*\\&= q_0p_0 - \vec{q}\cdot\vec{p} - q_0\vec{p} - p_0\vec{q} - \vec{q}\times\vec{p}\\&= p_0q_0 - \vec{p}\cdot\vec{q} - p_0\vec{q} - q_0\vec{p} + \vec{p}\times\vec{q}\\&= (p_0 - \vec{p})(q_0 - \vec{q})\\&= \mathring{p}^*\mathring{q}^* \end{aligned} \tag{2.19}$$

is the *reverse* of the product of the conjugates. The **norm**

$$|\mathring{q}| = \sqrt{\mathring{q}\mathring{q}^*} = \sqrt{q_0^2 + \vec{q}\cdot\vec{q}} = \sqrt{q_0^2 + q_1^2 + q_2^2 + q_3^2} = \sqrt{\mathring{q}\cdot\mathring{p}} \tag{2.20}$$

is the square root of the product with the conjugate, and the **inverse**

$$\mathring{q}^{-1} = \frac{\mathring{q}^*}{|\mathring{q}|^2} \tag{2.21}$$

is the conjugate divided by the norm squared.

Imaginary quaternions are "thick" imaginary numbers: If $\mathring{u} = \{0, \vec{u}\} = \vec{u}$ is an imaginary unit quaternion, then $\vec{u} \cdot \vec{u} = 1$ and

$$\begin{aligned}
\mathring{u}^2 &= (u_1\hat{\imath} + u_2\hat{\jmath} + u_3\hat{k})(u_1\hat{\imath} + u_2\hat{\jmath} + u_3\hat{k}) \\
&= -u_1^2 + u_1u_2\hat{k} - u_1u_3\hat{\jmath} \\
&\quad - u_2u_1\hat{k} - u_2^2 + u_2u_3\hat{\imath} \\
&\quad + u_3u_1\hat{\jmath} - u_3u_2\hat{\imath} - u_3^2 \\
&= -u_1^2 - u_2^2 - u_3^2 \\
&= -1,
\end{aligned} \tag{2.22}$$

or, more succintly with Eq. 2.16, $\mathring{u}^2 = \mathring{u}\mathring{u} = -\vec{u} \cdot \vec{u} + \vec{u} \times \vec{u} = -1 + \vec{0} = -1$.

Like complex numbers, the absolutely convergent Taylor expansions of common functions dramatically reorganize when evaluated at imaginary quaternions. Since $\mathring{u}\mathring{u} = \vec{u}\vec{u} = -1$ even though $\vec{u} \cdot \vec{u} = +1$, as in Eq. 1.2, the Euler identity

$$e^{\vec{u}\theta} = \cos\theta + \vec{u}\sin\theta \tag{2.23}$$

follows. Along with the anticommutativity of the quaternion basis units, this implies

$$\begin{aligned}
\hat{\jmath}e^{+\hat{\imath}\theta} &= \hat{\jmath}(\cos\theta + \hat{\imath}\sin\theta) \\
&= \hat{\jmath}\cos\theta + \hat{\jmath}\hat{\imath}\sin\theta \\
&= \hat{\jmath}\cos\theta - \hat{\imath}\hat{\jmath}\sin\theta \\
&= (\cos\theta - \hat{\imath}\sin\theta)\hat{\jmath} \\
&= e^{-\hat{\imath}\theta}\hat{\jmath},
\end{aligned} \tag{2.24}$$

and so on.

2.3 3D Rotations

Just as complex numbers can model 2D rotations, quaternions can model 3D rotations. For example, consider a rotation through an angle θ about a unit vector $\vec{u}$. Form the **rotation quaternion** or **rotor**

$$\mathring{q} = e^{\vec{u}\theta/2} = \cos\frac{\theta}{2} + \vec{u}\sin\frac{\theta}{2}, \tag{2.25}$$

and consider the **similarity transformation**

$$\vec{v}\,' = \mathring{q}\,\vec{v}\,\mathring{q}^* = e^{\vec{u}\theta/2}\vec{v}e^{-\vec{u}\theta/2}. \tag{2.26}$$

First consider the special case of the rotation of a vector $\vec{v} = \{a, b, 0\}$ about a perpendicular axis $\vec{u} = \{0, 0, 1\}$ through an angle θ. Form the corresponding imaginary quaternions $\mathring{v} = a\hat{\imath} + b\hat{\jmath} = \vec{v}$ and $\mathring{u} = \hat{k} = \vec{u}$ and compute

$$\vec{v}\,' = e^{\vec{u}\theta/2}\vec{v}e^{-\vec{u}\theta/2}$$

$$
\begin{aligned}
&= e^{\hat{k}\theta/2}(a\hat{\imath} + b\hat{\jmath})e^{-\hat{k}\theta/2} \\
&= e^{\hat{k}\theta/2}e^{\hat{k}\theta/2}(a\hat{\imath} + b\hat{\jmath}) \\
&= e^{\hat{k}\theta}\vec{v},
\end{aligned}
\tag{2.27}
$$

as in Eq. 2.24, which is consistent with 2D rotations of vectors using complex numbers. Next consider the generic case of the rotation of a vector $\vec{v} = \{0, 0, 1\}$ about a nonperpendicular axis $\vec{u} = \{1/\sqrt{2}, 0, 1/\sqrt{2}\}$ through an angle $\theta = \pi/4$. Form the corresponding imaginary quaternions $\mathring{v} = \hat{k} = \vec{v}$ and $\mathring{u} = (\hat{\imath}+\hat{k})/\sqrt{2} = \vec{u}$ and compute

$$
\begin{aligned}
\vec{v}\,' &= e^{\vec{u}\theta/2}\vec{v}e^{-\vec{u}\theta/2} \\
&= \exp\left[\frac{\hat{\imath}+\hat{k}}{\sqrt{2}}\frac{\pi/4}{2}\right]\hat{k}\exp\left[-\frac{\hat{\imath}+\hat{k}}{\sqrt{2}}\frac{\pi/4}{2}\right] \\
&= \left(\cos\frac{\pi}{8} + \frac{\hat{\imath}+\hat{k}}{\sqrt{2}}\sin\frac{\pi}{8}\right)\hat{k}\left(\cos\frac{\pi}{8} - \frac{\hat{\imath}+\hat{k}}{\sqrt{2}}\sin\frac{\pi}{8}\right) \\
&= \hat{k}\cos^2\frac{\pi}{8} - \hat{k}\frac{\hat{\imath}+\hat{k}}{\sqrt{2}}\cos\frac{\pi}{8}\sin\frac{\pi}{8} + \frac{\hat{\imath}+\hat{k}}{\sqrt{2}}\hat{k}\sin\frac{\pi}{8}\cos\frac{\pi}{8} - \frac{\hat{\imath}+\hat{k}}{\sqrt{2}}\hat{k}\frac{\hat{\imath}+\hat{k}}{\sqrt{2}}\sin^2\frac{\pi}{8} \\
&= \hat{k}\cos^2\frac{\pi}{8} + \frac{-\hat{\jmath}+1-\hat{\jmath}-1}{\sqrt{2}}\frac{1}{2}\sin\frac{\pi}{4} - \frac{\hat{k}-\hat{\imath}-\hat{\imath}-\hat{k}}{2}\sin^2\frac{\pi}{8} \\
&= \hat{\imath}\sin^2\frac{\pi}{8} - \hat{\jmath}\frac{1}{2} + \hat{k}\cos^2\frac{\pi}{8} \\
&= \hat{\imath}\frac{2-\sqrt{2}}{4} - \hat{\jmath}\frac{1}{2} + \hat{k}\frac{2+\sqrt{2}}{4}.
\end{aligned}
\tag{2.28}
$$

In general if $\vec{r} = r_1\hat{\imath} + r_2\hat{\jmath} + r_3\hat{k}$ and $\vec{u} = u_1\hat{\imath} + u_2\hat{\jmath} + u_3\hat{k}$, then

$$
\begin{aligned}
\vec{r}\,' &= \mathring{q}\,\vec{r}\,\mathring{q}^* \\
&= e^{\vec{u}\theta/2}\,\vec{r}\,e^{-\vec{u}\theta/2} \\
&= \left(\cos\frac{\theta}{2} + \vec{u}\sin\frac{\theta}{2}\right)\vec{r}\left(\cos\frac{\theta}{2} - \vec{u}\sin\frac{\theta}{2}\right) \\
&= \left(\vec{r}\cos\frac{\theta}{2} + \vec{u}\vec{r}\sin\frac{\theta}{2}\right)\left(\cos\frac{\theta}{2} - \vec{u}\sin\frac{\theta}{2}\right) \\
&= \vec{r}\cos^2\frac{\theta}{2} + (\vec{u}\vec{r} - \vec{r}\vec{u})\sin\frac{\theta}{2}\cos\frac{\theta}{2} - \vec{u}\vec{r}\vec{u}\sin^2\frac{\theta}{2}.
\end{aligned}
\tag{2.29}
$$

But

$$
\vec{u}\vec{r} - \vec{r}\vec{u} = (-\vec{u}\cdot\vec{r} + \vec{u}\times\vec{r}) - (-\vec{r}\cdot\vec{u} + \vec{r}\times\vec{u}) = 2\vec{u}\times\vec{r} \tag{2.30}
$$

and

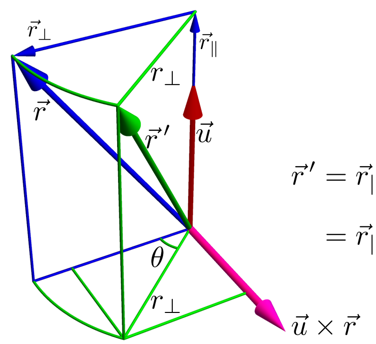
$$
\begin{aligned}
\vec{u}\vec{r}\vec{u} &= (-\vec{u}\cdot\vec{r} + \vec{u}\times\vec{r})\vec{u} \\
&= -(\vec{u}\cdot\vec{r})\vec{u} - (\vec{u}\times\vec{r})\cdot\vec{u} + (\vec{u}\times\vec{r})\times\vec{u}
\end{aligned}
$$

$$
\begin{aligned}
&= -(\vec{u}\cdot\vec{r})\vec{u} - 0 + (\vec{u}\cdot\vec{u})\vec{r} - (\vec{u}\cdot\vec{r})\vec{u} \\
&= \vec{r} - 2(\vec{u}\cdot\vec{r})\vec{u},
\end{aligned}
\tag{2.31}
$$

so

$$
\begin{aligned}
\vec{r}\,' &= \vec{r}\cos^2\frac{\theta}{2} + \vec{u}\times\vec{r}\;2\sin\frac{\theta}{2}\cos\frac{\theta}{2} - \vec{r}\sin^2\frac{\theta}{2} + (\vec{u}\cdot\vec{r})\vec{u}\;2\sin^2\frac{\theta}{2} \\
&= \vec{r}\cos\theta + \vec{u}\times\vec{r}\sin\theta + (\vec{u}\cdot\vec{r})\vec{u}(1-\cos\theta) \\
&= (\vec{u}\cdot\vec{r})\,\vec{u} + \big(\vec{r} - (\vec{u}\cdot\vec{r})\,\vec{u}\big)\cos\theta + \vec{u}\times\vec{r}\,\sin\theta \\
&= \vec{r}_{\|} + \vec{r}_{\perp}\cos\theta + \vec{u}\times\vec{r}\,\sin\theta,
\end{aligned}
\tag{2.32}
$$

which is Rodriques' formula [2] for the rotation of a vector through an angle θ about a unit vector $\vec{u}$, as in Fig. 2.3.



$$
\begin{aligned}
\vec{r}\,' &= \vec{r}_{\|} + (r_{\perp}\cos\theta)\frac{\vec{r}_{\perp}}{r_{\perp}} + (r_{\perp}\sin\theta)\frac{\vec{u}\times\vec{r}_{\perp}}{r_{\perp}} \\
&= \vec{r}_{\|} + \vec{r}_{\perp}\cos\theta + \vec{u}\times\vec{r}\,\sin\theta
\end{aligned}
$$

Figure 2.3: Decompose the vector $\vec{r}$ parallel and perpendicular to the rotation axis $\vec{u}$ and rotate the perpendicular component through the angle θ to form $\vec{r}\,'$.

2.4 Rotation Composition

Consider a positive (right-handed) rotation of $90° = \pi/2$ about $\hat{k}$ followed by a positive (right-handed) rotation of $90° = \pi/2$ about $\hat{\jmath}$, as in Fig. 2.4. The composite quaternion rotors (with the rotors concatenated right-to-left)

$$
\begin{aligned}
\mathring{q}_c = \mathring{q}_b\mathring{q}_a &= \exp\left[\hat{\jmath}\left(\frac{\pi/2}{2}\right)\right]\exp\left[\hat{k}\left(\frac{\pi/2}{2}\right)\right] \\
&= \left(\cos\frac{\pi}{4} + \hat{\jmath}\sin\frac{\pi}{4}\right)\left(\cos\frac{\pi}{4} + \hat{k}\sin\frac{\pi}{4}\right) \\
&= \frac{1}{2}(1+\hat{\jmath})(1+\hat{k}) \\
&= \frac{1}{2}(1+\hat{\imath}+\hat{\jmath}+\hat{k}) \\
&= \frac{1}{2} + \frac{\hat{\imath}+\hat{\jmath}+\hat{k}}{\sqrt{3}}\frac{\sqrt{3}}{2}
\end{aligned}
$$

$$
\begin{aligned}
&= \cos\left[\frac{\pi}{3}\right] + \frac{\hat{\imath}+\hat{\jmath}+\hat{k}}{\sqrt{3}} \sin\left[\frac{\pi}{3}\right] \\
&= \exp\left[\frac{\hat{\imath}+\hat{\jmath}+\hat{k}}{\sqrt{3}}\left(\frac{2\pi/3}{2}\right)\right],
\end{aligned} \tag{2.33}
$$

which is a single positive (right-handed) rotation of $120° = 2\pi/3$ about the coordinate diagonal $(\hat{\imath}+\hat{\jmath}+\hat{k})/\sqrt{3}$. When multiplying exponentials, the exponents add if they commute, which is not the case here. The order of the rotors is critical. For example,

$$
\begin{aligned}
\mathring{q}'_c = \mathring{q}_a\mathring{q}_b &= \exp\left[\hat{k}\left(\frac{\pi/2}{2}\right)\right]\exp\left[\hat{\jmath}\left(\frac{\pi/2}{2}\right)\right] \\
&= \left(\cos\frac{\pi}{4} + \hat{k}\sin\frac{\pi}{4}\right)\left(\cos\frac{\pi}{4} + \hat{\jmath}\sin\frac{\pi}{4}\right) \\
&= \frac{1}{2}(1+\hat{k})(1+\hat{\jmath}) \\
&= \frac{1}{2}(1-\hat{\imath}+\hat{\jmath}+\hat{k}) \\
&= \frac{1}{2} - \frac{\hat{\imath}+\hat{\jmath}+\hat{k}}{\sqrt{3}}\frac{\sqrt{3}}{2} \\
&= \cos\left[\frac{\pi}{3}\right] + \frac{-\hat{\imath}+\hat{\jmath}+\hat{k}}{\sqrt{3}}\sin\left[\frac{\pi}{3}\right] \\
&= \exp\left[\frac{-\hat{\imath}+\hat{\jmath}+\hat{k}}{\sqrt{3}}\left(\frac{2\pi/3}{2}\right)\right] \\
&\neq \mathring{q}_c
\end{aligned} \tag{2.34}
$$

which reflects the noncommutativity of rotations.

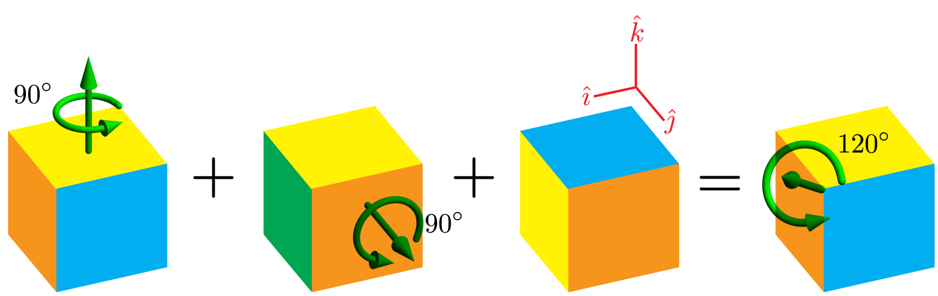


Figure 2.4: Two 90° rotations about orthogonal axis equals a 120° rotation about a diagonal axis.

2.5 Orientation-Entanglement

Unit quaternions $\mathring{q}$ lie on the surface of the hypersphere $S^3 \subset \mathbb{R}^4$ for which $\mathring{q} \cdot \mathring{q} = 1$. The quaternion

$$\mathring{q}[\vec{u}, \theta] = e^{\vec{u}\theta/2} = \cos\frac{\theta}{2} + \vec{u}\sin\frac{\theta}{2} \tag{2.35}$$

represents each 3D rotation twice, a **double cover**. Suppressing the $q_1\hat{\imath}$ direction implies

$$\mathring{q}[u_2\hat{\jmath} + u_3\hat{k}, \theta] = \cos\frac{\theta}{2} + \hat{\jmath}\, u_2\sin\frac{\theta}{2} + \hat{k}\, u_3\sin\frac{\theta}{2}, \tag{2.36}$$

as in Fig. 2.5 where the north and south poles represent the same orientation corresponding to angles of 0 and 2π.

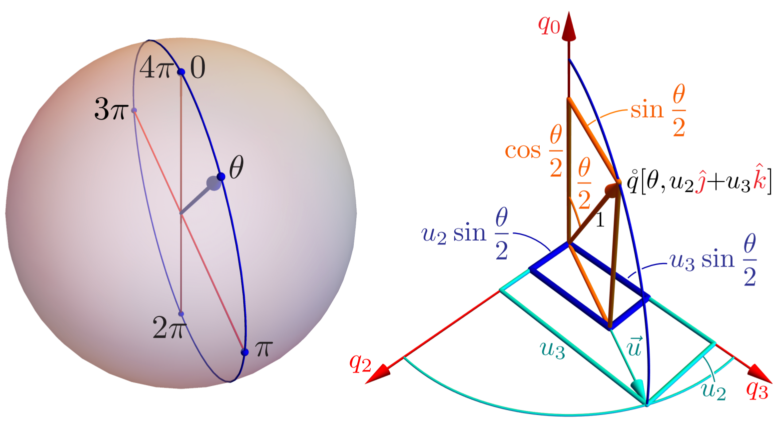


Figure 2.5: 3D projection of 4D quaternion unit sphere representing all 3D rotations twice, including the rotor $\mathring{q}[u_2\hat{\jmath} + u_3\hat{k}, \theta]$. The **rotation axis** is the rotor's projection onto the equatorial hyperplane, and the **rotation angle** is *twice* the rotor's co-latitude.

But the Feynman plate and Dirac belt tricks demonstrate that the **orientation-entanglement** of the north and south poles are different. Following Feynman, hold a dish on one hand and rotate the hand once *under* the elbow. The dish returns to the same orientation but the arm is awkwardly twisted. Now rotate once more in the same direction *over* the elbow. The dish returns again to same orientation *and* the arm is untwisted. The double 4π rotation is the true identity.

Following Dirac, twist a belt one full turn about its length. The single twist cannot be undone without changing the orientations of the belt buckles, although the twist can be changed from clockwise to counterclockwise. Now twist the belt two full turns about its length. The double twist can be undone without changing the orientations of the belt buckles by passing one buckle around the other. Again the double 4π twist is the true identity.

For a concrete model, represent twisted belts as connected paths of points in S^3. First assume the belt is extended and twisted 2π in the $\hat{k}$ direction with no twisting in the $\hat{\imath}$ direction. Then the rotors for each belt slice

$$\mathring{q}[\theta, t] = \cos\frac{\theta}{2} + \hat{\jmath}\sin[\pi t]\sin\frac{\theta}{2} + \hat{k}\cos[\pi t]\sin\frac{\theta}{2}, \tag{2.37}$$

where $0 \leq \theta < 2\pi$ parameterizes the rotation and $0 \leq t < 1$ parameterizes a transformation from clockwise to counterclockwise twist. For a 2π twist, the ends of the belt are fixed at

$$\mathring{q}[0, 0] = +1, \tag{2.38a}$$
$$\mathring{q}[2\pi, 1] = -1, \tag{2.38b}$$

and the quaternion curves joining the north and south poles of the sphere in Fig. 2.6 represent the belt.

Next assume the belt extends and twists 2π in the $\hat{k}$ direction with no twisting in the $\hat{\imath}$ direction. Then the rotors for each belt slice

$$\mathring{q}[\theta, t] = \cos\frac{\theta}{2}\cos^2\frac{\pi t}{2} + \sin^2\frac{\pi t}{2} + \hat{\jmath}\left(1 - \cos\frac{\theta}{2}\right)\sin\frac{\pi t}{2}\cos\frac{\pi t}{2} + \hat{k}\sin\frac{\theta}{2}\cos\frac{\pi t}{2}, \tag{2.39}$$

where $0 \leq \theta < 4\pi$ parameterizes the rotation and $0 \leq t < 1$ parameterizes a transformation from twisted to untwisted. For a 4π twist, the ends of the belt are fixed at

$$\mathring{q}[0, 0] = +1, \tag{2.40a}$$
$$\mathring{q}[4\pi, 1] = +1, \tag{2.40b}$$

and the quaternion curves joining the north pole of the sphere to itself in Fig. 2.7 represent the belt.

The 4π rotation is smoothly contractible to the north pole identity rotation but the 2π rotation is not. Identifying the north and south poles as the same orientation means that closed loops on the quaternion sphere represent both the 2π and 4π rotations, but only the latter is contractible to the identity. This **multiple connectivity** is reminiscent of a torus (or donut with hole), where toroidal loops (around-the-hole) are contractible but poloidal (through-the-hole) loops are not, rather than the **simple connectivity** of a sphere, where all loops are contractible.

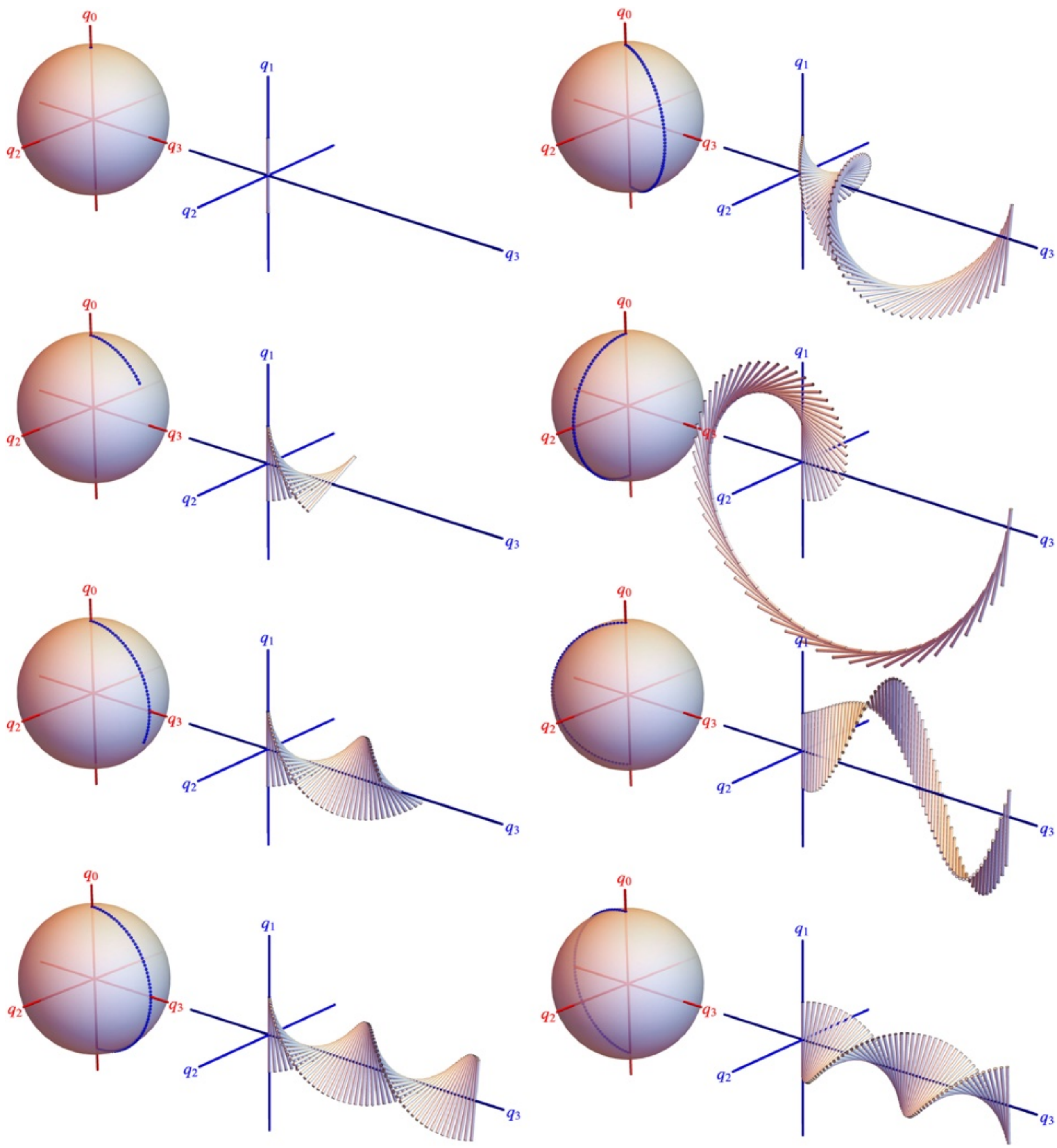


Figure 2.6: Elastic belt with a 2π twist (left column). Blue dots on quaternion sphere projection represent belt cross section rotations. Blue curve connecting dots can not be smoothly contracted to the untwisted state represented by the north pole, but without changing the orientation of the belt's ends, the twist can be changed from clockwise to counterclockwise as indicated (right column).

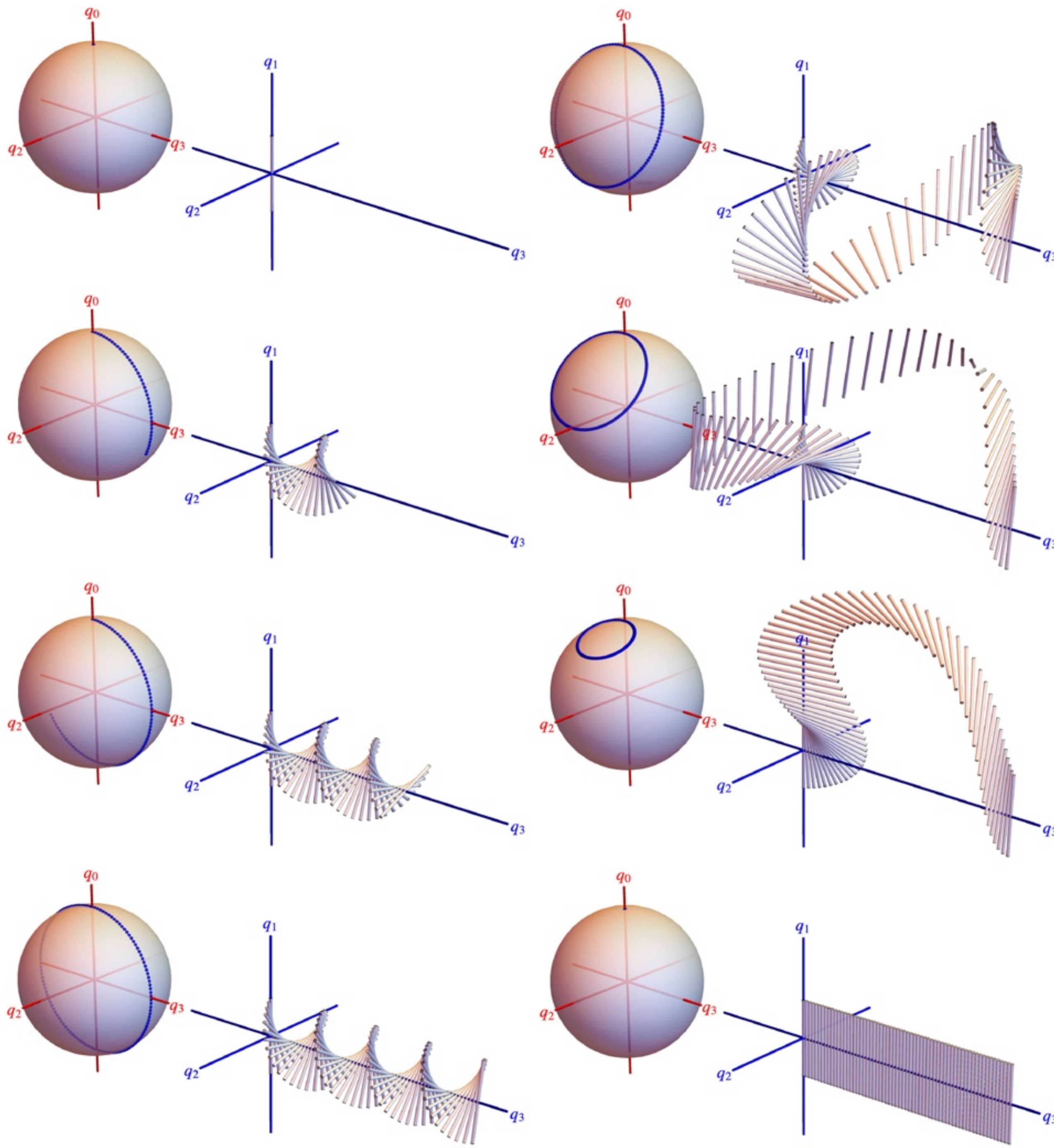


Figure 2.7: Elastic belt with a 4π twist (left column). Blue dots on quaternion sphere projection represent belt cross section rotations. Blue curve connecting dots can be smoothly contracted to the untwisted state represented by the north pole, so without changing the orientation of the belt's ends, the twist can be be undone as indicated (right column).

2.6 Fermions

1D real numbers x locate Newtonian masses. 2D complex numbers $\psi = \psi_R + \boldsymbol{i}\psi_I = \{\psi_R, \psi_I\}$ are the wave functions of nonrelativistic particles. 4D quarternions called **spinors** $\psi = \{\psi_0, \psi_1, \psi_2, \psi_3\}$ represent **fermions** like electrons. Consequently, electrons return to themselves only after $2\pi = 720°$ rotations!

Mathematica Quaternions

```
Needs["Quaternions`"] (* load file, where ` is grave accent *)

qQua = 1 - J + 2 K // ToQuaternion (* convert from symbolic entry *)

Quaternion[1, 0, -1, 2]

qVec = {1, 0, -1, 2}; (* List[a,b] ↔ {a,b} represent vectors *)

qQua = Quaternion @@ qVec (* Apply[f,List[x]] ↔ f@@List[x] ↔ f[x] *)

Quaternion[1, 0, -1, 2]

qQua* (* qQua ESC conj ESC *)

Quaternion[1, 0, 1, -2]

Conjugate[qQua] == qQua* (* Equal[a,b] ↔ a==b *)

True

Abs[qQua]^2

6

qQua ** qQua* // FromQuaternion

6

pQua = Quaternion[1, -2, -1, 0]; (* semicolon suppresses output *)

2 qQua + 3 pQua // FromQuaternion (* convert to symbolic output *)

(5 - 6 i) - 5 J + 4 K

qQua ** pQua // FromQuaternion (* quaternion multiplication *)

-6 J

pQua ** qQua // FromQuaternion (* noncommutative multiplication *)

-4 i + 2 J + 4 K

List @@ qQua.List @@ pQua (* Dot[Apply[List,qQua], Apply[List,pQua]] *)

2
```

Worked Problem

1. Combine a 90° rotation about the x-axis followed by a 60° rotation about the y-axis.

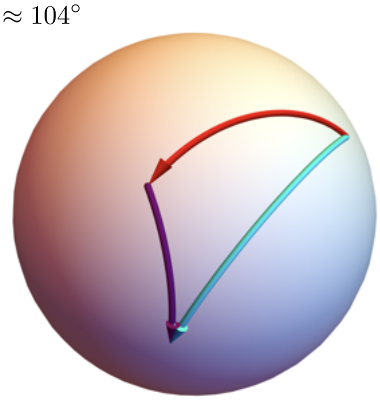
$$R_1 = e^{\vec{u}_1\theta_1/2} = e^{\hat{\imath}90^\circ/2} = e^{\hat{\imath}45^\circ}$$

$$R_2 = e^{\vec{u}_2\theta_2/2} = e^{\hat{\jmath}60^\circ/2} = e^{\hat{\jmath}30^\circ}$$

$$\begin{aligned}
R_3 &= R_2R_1 \\
e^{\vec{u}_3\theta_3/2} &= e^{\hat{\imath}30^\circ}e^{\hat{\imath}45^\circ} \\
\cos\frac{\theta_3}{2} + \vec{u}_3\sin\frac{\theta_3}{2} &= (\cos 30^\circ + \hat{\jmath}\sin 30^\circ)(\cos 45^\circ + \hat{\imath}\sin 45^\circ) \\
&= \left(\frac{\sqrt{3}}{2} + \hat{\jmath}\frac{1}{2}\right)\left(\frac{1}{\sqrt{2}} + \hat{\imath}\frac{1}{\sqrt{2}}\right) \\
&= \sqrt{\frac{3}{8}} + \hat{\imath}\sqrt{\frac{3}{8}} + \hat{\jmath}\sqrt{\frac{1}{8}} - \hat{k}\sqrt{\frac{1}{8}}
\end{aligned}$$

$$\begin{aligned}
\cos\frac{\theta_3}{2} &= \sqrt{\frac{3}{8}} \\
\sin\frac{\theta_3}{2} &= \sqrt{1 - \cos^2\frac{\theta_3}{2}} = \sqrt{1 - \frac{3}{8}} = \sqrt{\frac{5}{8}} \\
\theta_3 &= 2\arccos\sqrt{\frac{3}{8}} = 2\arcsin\sqrt{\frac{5}{8}} \approx 104^\circ
\end{aligned}$$

$$\begin{aligned}
\vec{u}_3 &= \frac{R_2R_1 - \cos[\theta_3/2]}{\sin[\theta_3/2]} \\
&= \frac{\hat{\imath}\sqrt{3/8} + \hat{\jmath}\sqrt{1/8} - \hat{k}\sqrt{1/8}}{\sqrt{5/8}} \\
&= \hat{\imath}\sqrt{\frac{3}{5}} + \hat{\jmath}\sqrt{\frac{1}{5}} - \hat{k}\sqrt{\frac{1}{5}}
\end{aligned}$$



Problems

1. Use the Fig. 2.2 multiplication tables to compute the dot and cross products of the following vectors represented as imaginary quaternions. (Do not compute a cross product as the determinant of a matrix.)
   (a) $\vec{v} = \hat{\imath} - \hat{k}$, $\vec{w} = 2\hat{\jmath} - 3\hat{k}$
   (b) $\vec{v} = 3\hat{\imath} - \hat{\jmath}$, $\vec{w} = \hat{\imath} - \hat{\jmath} + \hat{k}$

2. For each quaternion $\mathring{q}$, compute $\mathring{q}^*$, $|\mathring{q}|^2$, $1/\mathring{q}$.
   (a) $\mathring{q} = q_0 + \vec{q}$, where $q_0 = 2$, $\vec{q} = \{1, 2, 3\} = \hat{\imath} + 2\hat{\jmath} + 3\hat{k}$
   (b) $\mathring{q} = 1 + 2\hat{\jmath} + \hat{k}$
   (c) $\mathring{q} = 1 + \hat{\imath} - \hat{\jmath} + \hat{k}$

3. For each pair of quaternions $\mathring{q}, \mathring{p}$, compute $\mathring{q} + \mathring{p}$, $\mathring{q}\mathring{p}$, $\mathring{q} \cdot \mathring{p}$.
   (a) $\mathring{q} = 1 - \hat{\jmath} + \hat{k}$, $\mathring{p} = 1 - \hat{\imath} - \hat{\jmath}$
   (b) $\mathring{q} = 1 + \hat{\imath} - 2\hat{\jmath} + \hat{k}$, $\mathring{p} = 1 - 2\hat{\imath} - \hat{\jmath} + \hat{k}$

4. Use quaternions to rotate the vector $\vec{v}$ through angle θ about direction $\vec{u}$ and interpret the result graphically.
   (a) $\vec{v} = \hat{\jmath} + \hat{k}$, $\theta = 30°$, $\vec{u} = \hat{\imath}$
   (b) $\vec{v} = \{0, 0, 1\}$, $\theta = 45°$, $\vec{u} = \{1, 1, 0\}/\sqrt{2}$

5. Combine the following double rotations into single rotations and interpret the result graphically. (Hint: Normalize the rotation axis vectors if necessary.)
   (a) $90°$ about $\hat{\imath}$ and then $60°$ about $\hat{\jmath}$
   (b) $30°$ about $\{1, 1, 0\}$ and then $45°$ about $\{1, 1, 1\}/\sqrt{3}$

6. Consider the quaternions $\mathring{q} = \hat{\imath} - \hat{\jmath}$ and $\mathring{p} = \hat{\imath} + \hat{\jmath}$. Show the following.
   (a) $\mathring{q}\mathring{p} \neq \mathring{p}\mathring{q}$
   (b) $e^{\mathring{q}} e^{\mathring{p}} \neq e^{\mathring{q}+\mathring{p}}$

Chapter 3

Matrix Product

Matrices, arrays, or tableaus of numbers have been used to solve math problems for thousands of years. They combine linearly like vectors but multiply to model rotations.

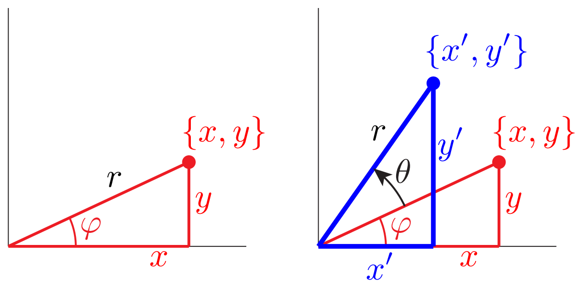


Figure 3.1: Matrices can represent the active rotation of a point through a counterclockwise angle θ in a plane.

3.1 2D Simple Rotations

Consider the active 2D rotation of a point $\vec{r} = \{x, y\}$ to a point $\vec{r}' = \{x', y'\}$ through an angle θ, as in Fig. 3.1. From the geometry,

$$\begin{aligned} x' &= r\cos[\varphi + \theta] \\ &= r\cos\varphi\cos\theta - r\sin\varphi\sin\theta \\ &= x\cos\theta - y\sin\theta, \end{aligned} \tag{3.1}$$

and

$$\begin{aligned} y' &= r\sin[\varphi + \theta] \\ &= r\sin\varphi\cos\theta + r\cos\varphi\sin\theta \\ &= y\cos\theta + x\sin\theta. \end{aligned} \tag{3.2}$$

Collect the variables in the transformation

$$x' = x\cos\theta - y\sin\theta, \tag{3.3a}$$

$$y' = x\sin\theta + y\cos\theta, \tag{3.3b}$$

into the **column matrices**

$$\boxed{\begin{matrix} x \\ y \end{matrix}} \tag{3.4}$$

and

$$\boxed{\begin{matrix} x' \\ y' \end{matrix}} \tag{3.5}$$

and collect the coefficients into the **square matrix**

$$\boxed{\begin{matrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{matrix}} \tag{3.6}$$

and form the **matrix equation**

$$\boxed{\begin{matrix} x' \\ y' \end{matrix}} = \boxed{\begin{matrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{matrix}} \boxed{\begin{matrix} x \\ y \end{matrix}}, \tag{3.7}$$

where the color guides the eye in checking the matrix multiplication, where rows are dot-producted with columns [3]. In bracket notation, write

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}, \tag{3.8}$$

and represent matrix equations symbolically as

$$\vec{r}\,' = R\,\vec{r} \tag{3.9}$$

or

$$\underline{r}' = \underline{\underline{R}}\,\underline{r} \tag{3.10}$$

or in components as

$$x_m = \sum_{n=1}^{2} R_{mn} x_n = R_{mn} x_n, \tag{3.11}$$

where $\{x_1, x_2\} = \{x, y\}$. By the **Einstein summation convention**, the sum over repeated indices n is implied in the last step.

Alternately, collect the variables in the Eq. 3.3 transformation into the **row matrices**

$$\boxed{\begin{matrix} x & y \end{matrix}} \tag{3.12}$$

and

$$\boxed{\begin{matrix} x' & y' \end{matrix}} \tag{3.13}$$

and form the matrix equation

$$\boxed{\begin{matrix} x' & y' \end{matrix}} = \boxed{\begin{matrix} x & y \end{matrix}} \boxed{\begin{matrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{matrix}}, \tag{3.14}$$

and represent it symbolically as

$$\vec{r}'^T = \vec{r}^T R^T, \tag{3.15}$$

where the transpose operation T interchanges rows and columns.

If the rotation matrix

$$R[\theta] = \boxed{\begin{matrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{matrix}}, \tag{3.16}$$

then the **inverse matrix**

$$R^{-1}[\theta] = \boxed{\begin{matrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{matrix}} = R^T[\theta] = R[-\theta], \tag{3.17}$$

and the **identity matrix**

$$R[0] = \boxed{\begin{matrix} 1 & 0 \\ 0 & 1 \end{matrix}} = I \neq \boxed{\begin{matrix} 1 & 1 \\ 1 & 1 \end{matrix}}. \tag{3.18}$$

The Eq. 3.16 square matrix $R[\theta]$ implements an **active** rotation (of a vector) counterclockwise or a **passive** rotation (of the coordinates) clockwise by pre-multiplying a column matrix of vector components, as in Eq. 3.7; the inverse Eq. 3.17 square matrix $R^T[\theta]$ implements an **active** rotation (of a vector) clockwise or a **passive** rotation (of the coordinates) counterclockwise by post-multiplying a row matrix of vector components, as in Eq. 3.14.

3.2 2D Compound Rotations

For a compound rotation first through angle a and second through angle b, write

$$x' = x\cos[b+a] - y\sin[b+a], \tag{3.19a}$$
$$y' = x\sin[b+a] + y\cos[b+a], \tag{3.19b}$$

or in matrix notation

$$\begin{aligned}\begin{bmatrix} x' \\ y' \end{bmatrix} &= \begin{bmatrix} \cos[b+a] & -\sin[b+a] \\ \sin[b+a] & \cos[b+a] \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \\ &= \begin{bmatrix} \cos b\cos a - \sin b\sin a & -\cos b\sin a - \sin b\cos a \\ \sin b\cos a + \cos b\sin a & -\sin b\sin a + \cos b\cos a \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \\ &= \begin{bmatrix} \cos b & -\sin b \\ \sin b & \cos b \end{bmatrix} \begin{bmatrix} \cos a & -\sin a \\ \sin a & \cos a \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix},\end{aligned} \tag{3.20}$$

so

$$\begin{bmatrix} \cos[b+a] & -\sin[b+a] \\ \sin[b+a] & \cos[b+a] \end{bmatrix} = \begin{bmatrix} \cos b & -\sin b \\ \sin b & \cos b \end{bmatrix} \begin{bmatrix} \cos a & -\sin a \\ \sin a & \cos a \end{bmatrix} \tag{3.21}$$

or symbolically

$$R[b+a] = R[b]R[a] \tag{3.22}$$

or in components

$$R_{rc}[b+a] = \sum_{s=1}^{2} R_{rs}[b]R_{sc}[a] = R_{rs}[b]R_{sc}[a], \tag{3.23}$$

where the indices r and c stand for row and column, so element R_{rc} of the product square matrix is the dot product of row r of the first square matrix with column c of the second square matrix.

3.3 3D Rotations

As direct 3D generalizations of 2D rotations, active counterclockwise rotations about each axis $\{x, y, z\}$ can be performed by

$$R_x[\theta] = R_{yz}[\theta] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}, \tag{3.24}$$

and

$$R_y[\theta] = R_{xz}[\theta] = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}, \tag{3.25}$$

and

$$R_z[\theta] = R_{xy}[\theta] = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{3.26}$$

which can be interconverted by cyclically permuting the rows and columns. The product

$$R = R_z[\alpha]R_y[\beta]R_x[\gamma] \tag{3.27}$$

represents a rotation with yaw α, pitch β, and roll γ. Like quaternions and the rotations they can represent, 3D rotation matrices need not commute. For example, the product

$$R_z\left[\frac{\pi}{2}\right]R_y\left[\frac{\pi}{2}\right] = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix}, \tag{3.28}$$

but reversing the factors gives

$$R_z\left[\frac{\pi}{2}\right]R_y\left[\frac{\pi}{2}\right] = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}. \tag{3.29}$$

Any linear transformation can be written as a composition of a rotation, a rescaling, and a rotation. For example,

$$\begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} \cos\frac{\pi}{8} & -\sin\frac{\pi}{8} \\ \sin\frac{\pi}{8} & \cos\frac{\pi}{8} \end{bmatrix}\begin{bmatrix} \sqrt{2}+1 & 0 \\ 0 & \sqrt{2}-1 \end{bmatrix}\begin{bmatrix} \cos\frac{3\pi}{8} & \sin\frac{3\pi}{8} \\ -\sin\frac{3\pi}{8} & \cos\frac{3\pi}{8} \end{bmatrix} \tag{3.30}$$

or symbolically

$$M = \tilde{R}SR, \tag{3.31}$$

which is an example of **singular value decomposition**.

3.4 Spacetime Rotations

By the Lorentz-Einstein transformation, if one observer records an event at spacetime coordinates $\{t, x\}$, then a second observer in relative motion at velocity $\vec{v} = \{v_x, 0, 0\}$ records the event at spacetime coordinates $\{t', x'\}$, where

$$t' = \gamma(t - v_x x/c^2), \tag{3.32a}$$
$$x' = \gamma(x - v_x t), \tag{3.32b}$$
$$y' = y, \tag{3.32c}$$
$$z' = z, \tag{3.32d}$$

where

$$\gamma = \frac{1}{\sqrt{1 - v^2/c^2}} \geq 1, \tag{3.33}$$

is the **relativistic stretch** and c is the **constant light speed**. Rewrite the transformation as

$$\boldsymbol{i}ct' = \gamma\, \boldsymbol{i}ct - \boldsymbol{i}\gamma \frac{v_x}{c}\, x, \tag{3.34a}$$
$$x' = \boldsymbol{i}\gamma \frac{v_x}{c}\, \boldsymbol{i}ct + \gamma\, x, \tag{3.34b}$$
$$y' = y, \tag{3.34c}$$
$$z' = z, \tag{3.34d}$$

and as the single matrix equation

$$\begin{bmatrix} \boldsymbol{i}ct' \\ x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \gamma & -\boldsymbol{i}\gamma v_x/c & 0 & 0 \\ \boldsymbol{i}\gamma v_x/c & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \boldsymbol{i}ct \\ x \\ y \\ z \end{bmatrix}. \tag{3.35}$$

Parameterize the relative velocity by the **rapidity** φ, where

$$-1 \leq \tanh\varphi = \frac{v_x}{c} \leq 1 \tag{3.36}$$

and

$$\gamma = \frac{1}{\sqrt{1 - \tanh^2\varphi}} = \cosh\varphi, \tag{3.37}$$

so that

$$\begin{bmatrix} \boldsymbol{i}ct' \\ x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \cosh\varphi & -\boldsymbol{i}\sinh\varphi & 0 & 0 \\ \boldsymbol{i}\sinh\varphi & \cosh\varphi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \boldsymbol{i}ct \\ x \\ y \\ z \end{bmatrix}. \tag{3.38}$$

Finally, substitute $\theta = i\varphi \in \mathbb{C}$ to get

$$\begin{bmatrix} ict' \\ x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta & 0 & 0 \\ \sin\theta & \cos\theta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} ict \\ x \\ y \\ z \end{bmatrix}. \tag{3.39}$$

The Lorentz-Einstein transformation is a rotation through a complex angle in a complex space. A change in velocity or **boost** is a 3 + 1-dimensional spacetime rotation that produces the projection effects of length contraction, time dilation, and clock desynchronization in 3-dimensional space.

3.5 Pauli Matrices & Quaternions

The **Pauli spin matrices** of quantum physics are **isomorphic** (or equivalent) to the quaternions. Specifically,

$$i\hat{\imath} = \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{3.40a}$$

$$i\hat{\jmath} = \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \tag{3.40b}$$

$$i\hat{k} = \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{3.40c}$$

where "$-i$ rides high on σ_y". Their algebra

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = -i\sigma_x\sigma_y\sigma_z = I \tag{3.41}$$

mimics the Eq. 2.1 quaternion algebra. For example,

$$\sigma_x^2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I. \tag{3.42}$$

The Pauli matrices are **self-adjoint** or **hermitian** and equal the complex conjugates of their **transposes**, where the transpose interchanges rows and columns.

That's why σ_y contains $\boldsymbol{i}$,

$$\sigma_y^\dagger = \sigma_y^{T^*} = \begin{bmatrix} 0 & -\boldsymbol{i} \\ +\boldsymbol{i} & 0 \end{bmatrix}^{T^*} = \begin{bmatrix} 0 & +\boldsymbol{i} \\ -\boldsymbol{i} & 0 \end{bmatrix}^{*} = \begin{bmatrix} 0 & -\boldsymbol{i} \\ +\boldsymbol{i} & 0 \end{bmatrix} = \sigma_y, \tag{3.43}$$

but σ_x and σ_z don't. Any complex 2D matrix is a linear combination of the Pauli matrices and the 2D identity matrix. For example, generalizing scalar multiplication of vectors to matrices,

$$\begin{aligned} \begin{bmatrix} a & b \\ c & d \end{bmatrix} &= \frac{b+c}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \boldsymbol{i}\frac{b-c}{2}\begin{bmatrix} 0 & -\boldsymbol{i} \\ \boldsymbol{i} & 0 \end{bmatrix} + \frac{a-d}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \frac{a+d}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\ &= \frac{b+c}{2}\sigma_x + \boldsymbol{i}\frac{b-c}{2}\sigma_y + \frac{a-d}{2}\sigma_z + \frac{a+d}{2}I, \end{aligned} \tag{3.44}$$

where the coefficients are the main diagonal sums or **traces** of the products of the original matrix with the Pauli matrices, such as

$$\frac{1}{2}\operatorname{tr}\left[\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} a & b \\ c & d \end{bmatrix}\right] = \frac{1}{2}\operatorname{tr}\begin{bmatrix} c & d \\ a & b \end{bmatrix} = \frac{1}{2}(c+b) = \frac{b+c}{2}. \tag{3.45}$$

3.6 Other Matrix Products

In addition to the **common matrix product**

$$M_1 M_2 = \begin{bmatrix} a_1 & b_1 \\ c_1 & d_1 \end{bmatrix}\begin{bmatrix} a_2 & b_2 \\ c_2 & d_2 \end{bmatrix} = \begin{bmatrix} a_1a_2 + b_1c_2 & a_1b_2 + b_1d_2 \\ c_1a_2 + d_1c_2 & c_1b_2 + d_1d_2 \end{bmatrix}, \tag{3.46}$$

the simple **Hadamard** or **entry-wise product**

$$M_1 \circ M_2 = \begin{bmatrix} a_1 & b_1 \\ c_1 & d_1 \end{bmatrix} \circ \begin{bmatrix} a_2 & b_2 \\ c_2 & d_2 \end{bmatrix} = \begin{bmatrix} a_1a_2 & b_1b_2 \\ c_1c_2 & d_1d_2 \end{bmatrix} \tag{3.47}$$

and **Kronecker** or **tensor product**

$$M_1 \otimes M_2 = \begin{bmatrix} a_1 & b_1 \\ c_1 & d_1 \end{bmatrix} \otimes \begin{bmatrix} a_2 & b_2 \\ c_2 & d_2 \end{bmatrix} = \begin{bmatrix} a_1M_2 & b_1M_2 \\ c_1M_2 & d_1M_2 \end{bmatrix}$$

$$= \boxed{\begin{matrix} a_1a_2 & a_1b_2 & b_1a_2 & b_1b_2 \\ a_1c_2 & a_1c_2 & b_1c_2 & b_1d_2 \\ c_1a_2 & c_1b_2 & d_1a_2 & d_1b_2 \\ c_1c_2 & c_1d_2 & d_1c_2 & d_1d_2 \end{matrix}} \tag{3.48}$$

are sometimes useful.

Nonsquare matrices can be multiplied, including the **inner product**

$$\vec{r} \cdot \vec{r}\,' = \vec{r}^{\,T} \vec{r}\,' = \boxed{\begin{matrix} x & y \end{matrix}} \boxed{\begin{matrix} x' \\ y' \end{matrix}} = \boxed{xx' + yy'} = xx' + yy' \tag{3.49}$$

and the **outer product**

$$\vec{r} \otimes \vec{r}\,' = \vec{r}\,\vec{r}\,'^T = \boxed{\begin{matrix} x \\ y \end{matrix}} \boxed{\begin{matrix} x' & y' \end{matrix}} = \boxed{\begin{matrix} xx' & xy' \\ yx' & yy' \end{matrix}}. \tag{3.50}$$

Generally, multiplication of non-square matrices is defined if the number of columns of the first matrix is the same as the number of rows of the second,

$$AB = \boxed{a \times b} \boxed{b \times c} = \boxed{a \times c}. \tag{3.51}$$

Antisymmetric matrix multiplication can mimic the cross product $\vec{u} \times \vec{v} = \vec{w}$ by

$$\boxed{\begin{matrix} 0 & -u_z & u_y \\ u_z & 0 & -u_x \\ -u_y & u_x & 0 \end{matrix}} \boxed{\begin{matrix} v_x \\ v_y \\ v_z \end{matrix}} = \boxed{\begin{matrix} u_y v_z - u_z v_y \\ u_z v_x - u_x v_z \\ u_x v_y - u_y v_x \end{matrix}} = \boxed{\begin{matrix} w_x \\ w_y \\ w_z \end{matrix}}. \tag{3.52}$$

3.7 Multidimensional Matrices

Multidimensional matrices can describe multilinear relationships of any order. For example, in General Relativity the **Lorentz transformation**

$$x'_i = \sum_j \Lambda_{ij}\, x_j \tag{3.53}$$

linearly relates the spacetime coordinates between two different references frames (by the Eq. 3.52 spacetime rotation). The **metric connection**

$$dv_i = \sum_{j,k} \Gamma_{ijk}\, v_j\, dx_k \tag{3.54}$$

linearly relates the infinitesimal changes dv_i in the components of vector v_j that is parallel transported an infinitesimal distance dx_k (due to the curved spacetime). The **Riemann curvature tensor**

$$dv_i = \sum_{j,k,l} R_{ijkl}\, v_j\, dx_k\, dx_l \tag{3.55}$$

linearly relates the infinitesimal changes dv_i in the components of vector v_j parallel transported around an infinitesimal parallelogram of sides dx_k and dx_l.

Represent these many-indexed objects by multidimensional matrices where the indices indicate rows and columns. In $1+1$ dimensional spacetime in geometrical units, the constant light speed

$$c = 1 \tag{3.56}$$

is a rank-0 scalar; an event

$$\underline{x} = \boxed{\begin{matrix} x_1 \\ x_2 \end{matrix}} \tag{3.57}$$

is a rank-1 nontensor; a Lorentz transformation

$$\underline{\underline{\Lambda}} = \boxed{\begin{matrix} \Lambda_{11} & \Lambda_{12} \\ \Lambda_{21} & \Lambda_{22} \end{matrix}} \tag{3.58}$$

is a rank-2 tensor; the metric connection

$$\underline{\underline{\underline{\Gamma}}} = \boxed{\begin{matrix} \boxed{\begin{matrix} \Gamma_{111} & \Gamma_{112} \\ \Gamma_{121} & \Gamma_{122} \end{matrix}} \\ \boxed{\begin{matrix} \Gamma_{211} & \Gamma_{212} \\ \Gamma_{221} & \Gamma_{222} \end{matrix}} \end{matrix}} \tag{3.59}$$

is a rank-3 nontensor; the Riemann curvature

$$\underline{\underline{\underline{\underline{R}}}} = \boxed{\begin{matrix} \boxed{\begin{matrix} R_{1111} & R_{1112} \\ R_{1121} & R_{1122} \end{matrix}} & \boxed{\begin{matrix} R_{1211} & R_{1212} \\ R_{1221} & R_{1222} \end{matrix}} \\ \boxed{\begin{matrix} R_{2111} & R_{2112} \\ R_{2121} & R_{2122} \end{matrix}} & \boxed{\begin{matrix} R_{2211} & R_{2212} \\ R_{2221} & R_{2222} \end{matrix}} \end{matrix}} \tag{3.60}$$

is a rank-4 tensor. (To be a **tensor**, a multidimensional matrix must also transform appropriately under a basis change.)

Mathematica Matrices 1

```
aMat = {{-1, 3}, {4, 5}}; (* matrices are lists of lists *)
bMat = {{1, 2}, {-2, 2}};
```

```
cMat = 3 aMat + 2 bMat (* matrices combine linearly like vectors *)
```

```
{{-1, 13}, {8, 19}}
```

```
cMat // MatrixForm (* not computable; for display only *)
```

$$\begin{pmatrix} -1 & 13 \\ 8 & 19 \end{pmatrix}$$

```
aMat.bMat (* . → matrix product *)
```

```
{{-7, 4}, {-6, 18}}
```

```
aMat bMat (* piecewise multiplication instead *)
```

```
{{-1, 6}, {-8, 10}}
```

```
aMat.bMat - bMat.aMat (* nonzero commutator *)
```

```
{{-14, -9}, {-16, 14}}
```

```
dMat = {{1}, {3}}; eMat = {{2, 5}};(* sublists are rows *)
MatrixForm /@ {dMat, eMat} (* /@ → Map *)
```

$$\left\{\begin{pmatrix} 1 \\ 3 \end{pmatrix}, \begin{pmatrix} 2 & 5 \end{pmatrix}\right\}$$

```
RotationMatrix[θ, {0, 0, 1}] // MatrixForm (* ESCqESC → θ *)
```

$$\begin{pmatrix} \mathrm{Cos}[\theta] & -\mathrm{Sin}[\theta] & 0 \\ \mathrm{Sin}[\theta] & \mathrm{Cos}[\theta] & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

```
PauliMatrix[1] // MatrixForm (* for display only *)
```

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Worked Problem

1. Multiply two 3×3 matrices.

$$\boxed{\begin{array}{rrr}1 & -2 & 4\\ 3 & 1 & 1\\ -2 & 4 & 1\end{array}}\boxed{\begin{array}{rrr}1 & -2 & 1\\ 2 & 1 & -3\\ 4 & -2 & 1\end{array}}$$

$$= \boxed{\begin{array}{ccc}
\boxed{\begin{array}{rrr}1 & -2 & 4\\ 3 & 1 & 1\\ -2 & 4 & 1\end{array}}\boxed{\begin{array}{rrr}1 & -2 & 1\\ 2 & 1 & -3\\ 4 & -2 & 1\end{array}} & \boxed{\begin{array}{rrr}1 & -2 & 4\\ 3 & 1 & 1\\ -2 & 4 & 1\end{array}}\boxed{\begin{array}{rrr}1 & -2 & 1\\ 2 & 1 & -3\\ 4 & -2 & 1\end{array}} & \boxed{\begin{array}{rrr}1 & -2 & 4\\ 3 & 1 & 1\\ -2 & 4 & 1\end{array}}\boxed{\begin{array}{rrr}1 & -2 & 1\\ 2 & 1 & -3\\ 4 & -2 & 1\end{array}}\\
\boxed{\begin{array}{rrr}1 & -2 & 4\\ 3 & 1 & 1\\ -2 & 4 & 1\end{array}}\boxed{\begin{array}{rrr}1 & -2 & 1\\ 2 & 1 & -3\\ 4 & -2 & 1\end{array}} & \boxed{\begin{array}{rrr}1 & -2 & 4\\ 3 & 1 & 1\\ -2 & 4 & 1\end{array}}\boxed{\begin{array}{rrr}1 & -2 & 1\\ 2 & 1 & -3\\ 4 & -2 & 1\end{array}} & \boxed{\begin{array}{rrr}1 & -2 & 4\\ 3 & 1 & 1\\ -2 & 4 & 1\end{array}}\boxed{\begin{array}{rrr}1 & -2 & 1\\ 2 & 1 & -3\\ 4 & -2 & 1\end{array}}\\
\boxed{\begin{array}{rrr}1 & -2 & 4\\ 3 & 1 & 1\\ -2 & 4 & 1\end{array}}\boxed{\begin{array}{rrr}1 & -2 & 1\\ 2 & 1 & -3\\ 4 & -2 & 1\end{array}} & \boxed{\begin{array}{rrr}1 & -2 & 4\\ 3 & 1 & 1\\ -2 & 4 & 1\end{array}}\boxed{\begin{array}{rrr}1 & -2 & 1\\ 2 & 1 & -3\\ 4 & -2 & 1\end{array}} & \boxed{\begin{array}{rrr}1 & -2 & 4\\ 3 & 1 & 1\\ -2 & 4 & 1\end{array}}\boxed{\begin{array}{rrr}1 & -2 & 1\\ 2 & 1 & -3\\ 4 & -2 & 1\end{array}}
\end{array}}$$

$$= \boxed{\begin{array}{lll}
(\ 1)(\ 1)+(-2)(\ 2)+(\ 4)(\ 4) & (\ 1)(-2)+(-2)(\ 1)+(\ 4)(-2) & (\ 1)(\ 1)+(-2)(-3)+(\ 4)(\ 1)\\
(\ 3)(\ 1)+(\ 1)(\ 2)+(\ 1)(\ 4) & (\ 3)(-2)+(\ 1)(\ 1)+(\ 1)(-2) & (\ 3)(\ 1)+(\ 1)(-3)+(\ 1)(\ 1)\\
(-2)(\ 1)+(\ 4)(\ 2)+(\ 1)(\ 4) & (-2)(-2)+(\ 4)(\ 1)+(\ 1)(-2) & (-2)(\ 1)+(\ 4)(-3)+(\ 1)(\ 1)
\end{array}}$$

$$= \boxed{\begin{array}{rrr}13 & -12 & 11\\ 9 & -7 & 1\\ 10 & 6 & -13\end{array}}$$

Problems

1. For each pair of real square matrices A, B, compute $A+B$, AB, BA.

   (a) $A = \boxed{\begin{matrix} 1 & 2 \\ 3 & 4 \end{matrix}}, B = \boxed{\begin{matrix} 0 & 1 \\ 2 & 3 \end{matrix}}$

   (b) $A = \boxed{\begin{matrix} -1 & -1 \\ 1 & 1 \end{matrix}}, B = \boxed{\begin{matrix} 1 & 2 \\ 4 & 7 \end{matrix}}$

2. For each pair of real matrices A, B, compute AB and BA.

   (a) $A = \boxed{\begin{matrix} 1 & 2 \end{matrix}}, B = \boxed{\begin{matrix} 3 \\ 4 \end{matrix}}$

   (b) $A = \boxed{\begin{matrix} 1 & 2 & -1 \end{matrix}}, B = \boxed{\begin{matrix} 3 \\ 4 \\ 5 \end{matrix}}$

3. For each pair of complex square matrices U, V, compute $2U+3V$, UV, VU.

   (a) $U = \boxed{\begin{matrix} 1 & i \\ i & 2 \end{matrix}}, V = \boxed{\begin{matrix} 0 & i \\ 2i & 3 \end{matrix}}$

   (b) $U = \boxed{\begin{matrix} -i & -1 \\ 1 & 1 \end{matrix}}, V = \boxed{\begin{matrix} 1 & 2i \\ 4 & 7 \end{matrix}}$

4. Verify the Eq. 3.30 singular value decomposition using matrix multiplication and trig identities.

5. Use quaternions to show that the rotation matrix through an angle θ about a unit vector $\vec{u} = \{u_x, u_y, u_z\}$ is

   $R[\theta, \vec{u}] =$

$$\boxed{\begin{matrix} \cos\theta + u_x^2(1-\cos\theta) & u_x u_y(1-\cos\theta) - u_z \sin\theta & u_x u_z(1-\cos\theta) + u_y \sin\theta \\ u_y u_x(1-\cos\theta) + u_z \sin\theta & \cos\theta + u_y^2(1-\cos\theta) & u_y u_z(1-\cos\theta) - u_x \sin\theta \\ u_z u_x(1-\cos\theta) - u_y \sin\theta & u_z u_y(1-\cos\theta) + u_x \sin\theta & \cos\theta + u_z^2(1-\cos\theta) \end{matrix}}. \tag{3.61}$$

6. Derive the following Pauli matrix commutator and anticommutator identities.

   (a) $[\sigma_x, \sigma_y]_- = \sigma_x\sigma_y - \sigma_y\sigma_x = 2\boldsymbol{i}\sigma_z$

   (b) $[\sigma_x, \sigma_x]_+ = \sigma_x\sigma_x + \sigma_x\sigma_x = 2I$

Chapter 4

Matrix Structure

Even before matrices had a name, determinants did. Along with traces, eigenvalues, and eigenvectors, they critically characterize matrices, as in Fig. 4.1.

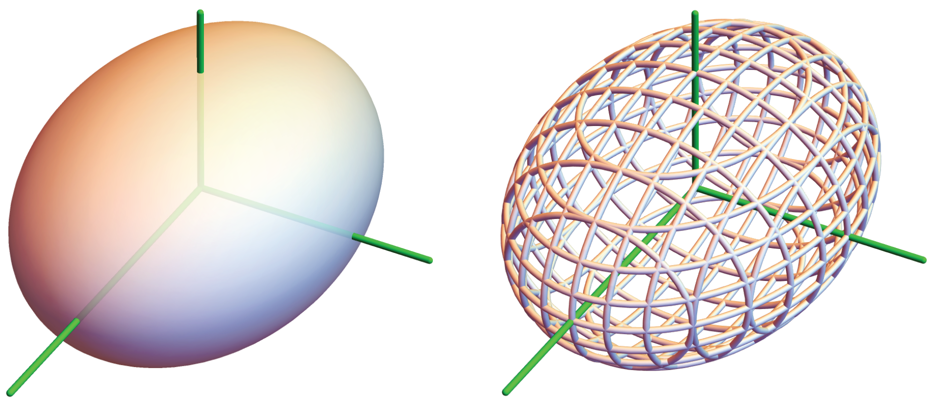


Figure 4.1: The eigenvalues and eigenvectors of a quadratic form determine the principal axes of the corresponding ellipsoid.

4.1 Determinants

Consider a generic real 2D matrix

$$M = \boxed{\begin{matrix} a & b \\ c & d \end{matrix}} = \boxed{\begin{matrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{matrix}} \tag{4.1}$$

acting on the corners of a unit square, as in Fig. 4.2. The linear transformation distorts the square into a parallelogram of vector area

$$\vec{A} = \{a, c, 0\} \times \{b, d, 0\} = (a\hat{x} + c\hat{y}) \times (b\hat{x} + d\hat{y}) = (ac - bd)\hat{z} \tag{4.2}$$

and signed area

$$A_z = ac - bd = +M_{11}M_{22} - M_{12}M_{21}. \tag{4.3}$$

This area can vanish if the initial square maps to a degenerate parallelogram consisting of just a line or a point.

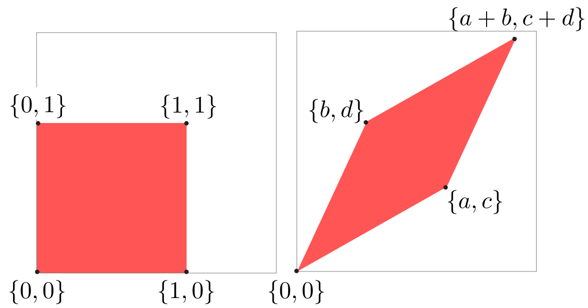


Figure 4.2: General linear transformation of a unit square is a parallelogram with vertex $\{a+b, c+d\} = \{a,c\} + \{b,d\}$.

Consider a generic real 3D matrix

$$M = \boxed{\begin{matrix} a & b & c \\ d & e & f \\ g & h & i \end{matrix}} = \boxed{\begin{matrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{matrix}} \tag{4.4}$$

acting on the corners of a unit cube, as in Fig. 4.3 (where here $i \neq \boldsymbol{i} = \sqrt{-1}$). The linear transformation distorts the cube into a parallelepiped of signed volume

$$\begin{aligned}
V &= \{a,d,g\} \times \{b,e,h\} \cdot \{c,f,i\} \\
&= (a\hat{x} + d\hat{y} + g\hat{z}) \times (b\hat{x} + e\hat{y} + h\hat{z}) \cdot (c\hat{x} + f\hat{y} + i\hat{z}) \\
&= \big((dh - eg)\hat{x} + (bg - ah)\hat{y} + (ae - bd)\hat{z}\big) \cdot (c\hat{x} + f\hat{y} + i\hat{z}) \\
&= (dh - eg)c + (bg - ah)f + (ae - bd)i \\
&= aei + cdh + bfg - ceg - afh - bdi \\
&= M_{11}M_{22}M_{33} + M_{13}M_{21}M_{32} + M_{12}M_{23}M_{31} \\
&\quad - M_{13}M_{22}M_{31} - M_{11}M_{23}M_{32} - M_{12}M_{21}M_{33}.
\end{aligned} \tag{4.5}$$

Generalize the Eq. 4.3 and Eq. 4.5 results to a square matrix of any dimension by defining the **determinant** to be the sum of all its signed elementary products. For example,

$$\det M = \begin{vmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{vmatrix} = \sum \pm M_{1i}M_{2j}M_{3k}, \tag{4.6}$$

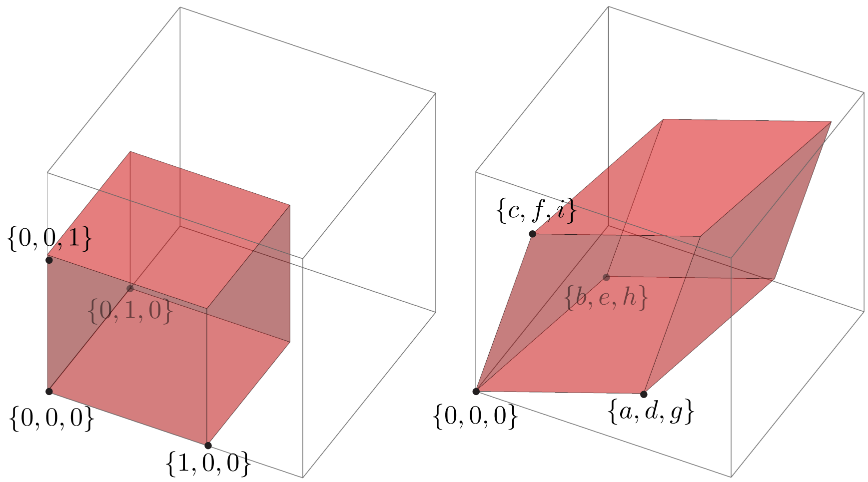


Figure 4.3: General linear transformation of a unit cube is a parallelepiped.

where each terms consists of a product of one element from each row and column and the sign is positive if the second indices ijk are an **even permutation** of the first indices 123 (like the cylic 123, 312, 231) and negative if the second indices are an **odd permutation** of the first indices (like the anti-cyclic 321, 132, 213). Alternately,

$$\det M = \sum_{i,j,k} \epsilon_{ijk} M_{1i} M_{2j} M_{3k} = \epsilon_{ijk} M_{1i} M_{2j} M_{3k}, \tag{4.7}$$

where the **Levi-Civita symbol** $\epsilon_{ijk} = (-1)^p$, where the parity p of the permutation is the number of interchanges needed to unscramble ijk to 123.

The Eq. 4.3 and Eq. 4.5 results also suggests defining the determinant as a **cofactor expansion**. Given the alternating signs and white submatrices

$$\boxed{\begin{array}{ccc} + & - & + \\ - & + & - \\ + & - & + \end{array}}, \quad \boxed{\begin{array}{ccc} a & b & c \\ d & e & f \\ g & h & i \end{array}}, \boxed{\begin{array}{ccc} a & b & c \\ d & e & f \\ g & h & i \end{array}}, \boxed{\begin{array}{ccc} a & b & c \\ d & e & f \\ g & h & i \end{array}}, \tag{4.8}$$

expand

$$\begin{aligned} \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} &= +c \begin{vmatrix} d & e \\ g & h \end{vmatrix} - f \begin{vmatrix} a & b \\ g & h \end{vmatrix} + i \begin{vmatrix} a & b \\ d & e \end{vmatrix} \\ &= c(dh - eg) - f(ah - bg) + i(ae - bd) \\ &= aei + cdh + bfg - ceg - afh - bdi \end{aligned} \tag{4.9}$$

as before, with identical results expanding about any row or column.

Because the determinant geometrically is the volume ratio induced by a transformation, the determinant of a product of matrices is simply the product of the determinants of each matrix

$$\det[MN] = \det[M]\det[N] = \det M \det N, \tag{4.10}$$

a refreshingly simple result given the complexities of matrix multiplication and determinants. Furthermore,

$$1 = \det I = \det[MM^{-1}] = \det M \det[M^{-1}], \tag{4.11}$$

so the determinate of the inverse of a matrix is the inverse of its determinant

$$\det[M^{-1}] = \frac{1}{\det M} = (\det M)^{-1}, \tag{4.12}$$

where M^{-1} is a matrix and $(\det M)^{-1}$ is a number.

4.2 Inverses

The inverse M^{-1} of the Eq. 4.1 2D matrix M satisfies

$$MM^{-1} = I \tag{4.13}$$

or more explicitly

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} a' & b' \\ c' & d' \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \tag{4.14}$$

which is equivalent to the four scalar equations

$$\begin{aligned} aa' + bc' &= 1, && (E_1) \\ ca' + dc' &= 0, && (E_2) \\ ab' + bd' &= 0, && (E_3) \\ cb' + dd' &= 1, && (E_4) \end{aligned}$$

in the four unknowns a', b', c', d'. Form the linear combinations

$$\begin{aligned} dE_1 - bE_2 \;&\rightarrow\; (da - bc)a' + (db - bd)c' = d, && (4.16a) \\ cE_1 - aE_2 \;&\rightarrow\; (ca - ac)a' + (cb - ad)c' = c, && (4.16b) \\ dE_3 - bE_4 \;&\rightarrow\; (da - bc)b' + (db - bd)d' = -b, && (4.16c) \\ cE_3 - aE_4 \;&\rightarrow\; (ca - ac)b' + (cb - ad)d' = -a, && (4.16d) \end{aligned}$$

and solve for

$$a' = \frac{+d}{ad - bc}, \tag{4.17a}$$

$$c' = \frac{-c}{ad - bc}, \tag{4.17b}$$

$$b' = \frac{-b}{ad - bc}, \tag{4.17c}$$

$$d' = \frac{+a}{ad - bc}, \tag{4.17d}$$

or in matrix form

$$M^{-1} = \frac{1}{ad - bc} \boxed{\begin{matrix} +d & -b \\ -c & +a \end{matrix}} = \begin{vmatrix} a & b \\ c & d \end{vmatrix}^{-1} \boxed{\begin{matrix} +d & -c \\ -b & +a \end{matrix}}^{T}. \tag{4.18}$$

To invert a 2D matrix, interchange the elements of the main diagonal, negate the elements of the counter diagonal, and divide by the determinant.

Similarly, the inverse M^{-1} of the Eq. 4.1 3D matrix M is

$$M^{-1} = \frac{\boxed{\begin{matrix} ei - fh & ch - bi & bf - ce \\ fg - di & ai - cg & cd - af \\ dh - eg & bg - ah & ae - bd \end{matrix}}}{cdh - ceg - fah + fbg + iae - ibd}$$

$$= \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix}^{-1} \boxed{\begin{matrix} +\begin{vmatrix} e & f \\ h & i \end{vmatrix} & -\begin{vmatrix} d & f \\ g & i \end{vmatrix} & +\begin{vmatrix} d & e \\ g & h \end{vmatrix} \\ -\begin{vmatrix} b & c \\ h & i \end{vmatrix} & +\begin{vmatrix} a & c \\ g & i \end{vmatrix} & -\begin{vmatrix} a & b \\ g & h \end{vmatrix} \\ +\begin{vmatrix} b & c \\ e & f \end{vmatrix} & -\begin{vmatrix} a & c \\ d & f \end{vmatrix} & +\begin{vmatrix} a & b \\ d & e \end{vmatrix} \end{matrix}}^{T}$$

$$= \frac{\boxed{\begin{matrix} +\begin{vmatrix} e & f \\ h & i \end{vmatrix} & -\begin{vmatrix} b & c \\ h & i \end{vmatrix} & +\begin{vmatrix} b & c \\ e & f \end{vmatrix} \\ -\begin{vmatrix} d & f \\ g & i \end{vmatrix} & +\begin{vmatrix} a & c \\ g & i \end{vmatrix} & -\begin{vmatrix} a & c \\ d & f \end{vmatrix} \\ +\begin{vmatrix} d & e \\ g & h \end{vmatrix} & -\begin{vmatrix} a & b \\ g & h \end{vmatrix} & +\begin{vmatrix} a & b \\ d & e \end{vmatrix} \end{matrix}}}{c\begin{vmatrix} d & e \\ g & h \end{vmatrix} - f\begin{vmatrix} a & b \\ g & h \end{vmatrix} + i\begin{vmatrix} a & b \\ d & e \end{vmatrix}}, \tag{4.19}$$

where in the second step the transpose M^T of a matrix M interchanges its rows and columns. Large square matrices can be inverted by similar formulas, which are implemented by computers. As Eq. 4.18 and Eq. 4.18 suggest, matrices are invertible only if their determinants are non-vanishing.

The inverse of a **sparse** matrix (of mainly zeros) can be **dense**. For example, the inverse of the 13D discrete **first difference** matrix

$$D_1 = \boxed{\begin{matrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{matrix}} \tag{4.20}$$

is the triangular matrix

$$D_1^{-1} = \boxed{\begin{matrix} 1&0&0&0&0&0&0&0&0&0&0&0&0\\ 1&1&0&0&0&0&0&0&0&0&0&0&0\\ 1&1&1&0&0&0&0&0&0&0&0&0&0\\ 1&1&1&1&0&0&0&0&0&0&0&0&0\\ 1&1&1&1&1&0&0&0&0&0&0&0&0\\ 1&1&1&1&1&1&0&0&0&0&0&0&0\\ 1&1&1&1&1&1&1&0&0&0&0&0&0\\ 1&1&1&1&1&1&1&1&0&0&0&0&0\\ 1&1&1&1&1&1&1&1&1&0&0&0&0\\ 1&1&1&1&1&1&1&1&1&1&0&0&0\\ 1&1&1&1&1&1&1&1&1&1&1&0&0\\ 1&1&1&1&1&1&1&1&1&1&1&1&0\\ 1&1&1&1&1&1&1&1&1&1&1&1&1 \end{matrix}}\,. \tag{4.21}$$

The inverse of the 13D discrete **second difference** or **discrete Laplacian** matrix

$$D_2 = \boxed{\begin{matrix} -2&1&0&0&0&0&0&0&0&0&0&0&0\\ 1&-2&1&0&0&0&0&0&0&0&0&0&0\\ 0&1&-2&1&0&0&0&0&0&0&0&0&0\\ 0&0&1&-2&1&0&0&0&0&0&0&0&0\\ 0&0&0&1&-2&1&0&0&0&0&0&0&0\\ 0&0&0&0&1&-2&1&0&0&0&0&0&0\\ 0&0&0&0&0&1&-2&1&0&0&0&0&0\\ 0&0&0&0&0&0&1&-2&1&0&0&0&0\\ 0&0&0&0&0&0&0&1&-2&1&0&0&0\\ 0&0&0&0&0&0&0&0&1&-2&1&0&0\\ 0&0&0&0&0&0&0&0&0&1&-2&1&0\\ 0&0&0&0&0&0&0&0&0&0&1&-2&1\\ 0&0&0&0&0&0&0&0&0&0&0&1&-2 \end{matrix}} \tag{4.22}$$

is the "bulging" matrix

$$D_2^{-1} = -\frac{1}{14}\begin{array}{|ccccccccccccc|}\hline 13 & 12 & 11 & 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 12 & 24 & 22 & 20 & 18 & 16 & 14 & 12 & 10 & 8 & 6 & 4 & 2 \\ 11 & 22 & 33 & 30 & 27 & 24 & 21 & 18 & 15 & 12 & 9 & 6 & 3 \\ 10 & 20 & 30 & 40 & 36 & 32 & 28 & 24 & 20 & 16 & 12 & 8 & 4 \\ 9 & 18 & 27 & 36 & 45 & 40 & 35 & 30 & 25 & 20 & 15 & 10 & 5 \\ 8 & 16 & 24 & 32 & 40 & 48 & 42 & 36 & 30 & 24 & 18 & 12 & 6 \\ 7 & 14 & 21 & 28 & 35 & 42 & 49 & 42 & 35 & 28 & 21 & 14 & 7 \\ 6 & 12 & 18 & 24 & 30 & 36 & 42 & 48 & 40 & 32 & 24 & 16 & 8 \\ 5 & 10 & 15 & 20 & 25 & 30 & 35 & 40 & 45 & 36 & 27 & 18 & 9 \\ 4 & 8 & 12 & 16 & 20 & 24 & 28 & 32 & 36 & 40 & 30 & 20 & 10 \\ 3 & 6 & 9 & 12 & 15 & 18 & 21 & 24 & 27 & 30 & 33 & 22 & 11 \\ 2 & 4 & 6 & 8 & 10 & 12 & 14 & 16 & 18 & 20 & 22 & 24 & 12 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 \\ \hline\end{array}. \tag{4.23}$$

4.3 Eigenvalues & Eigenvectors

Typically a matrix times a vector produces another vector,

$$M\vec{w} = \vec{w}\,' \neq \vec{w}. \tag{4.24}$$

But sometimes a matrix times a vector is proportional to the original vector,

$$M\vec{v} = \lambda\vec{v} \propto \vec{v}, \tag{4.25}$$

where λ and $\vec{v}$ are an **eigenvalue** and **eigenvector** of the matrix (where "eigen" is German for "own" or "self"). To solve the Eq. 4.25 eigenvalue-eigenvector equation, rewrite it as

$$\vec{0} = (M\vec{v} - \lambda\vec{v}) = (M - \lambda I)\vec{v}. \tag{4.26}$$

If $\det[M - \lambda I] \neq 0$, then the matrix $M - \lambda I$ is invertible, and so

$$\vec{0} = (M - \lambda I)^{-1}(M - \lambda I)\vec{v} = \vec{v} \tag{4.27}$$

is the trivial solution. To obtain a nontrivial solution, demand

$$0 = \det[M - \lambda I]. \tag{4.28}$$

If M is 2D, then

$$
\begin{aligned}
0 &= \det\left[\begin{bmatrix} a & b \\ c & d \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right] \\
&= \det \begin{bmatrix} a-\lambda & b \\ c & d-\lambda \end{bmatrix} \\
&= (a-\lambda)(d-\lambda) - bc \\
&= \lambda^2 - \lambda(a+d) + ad - bc \\
&= \lambda^2 - \lambda \operatorname{tr} M + \det M, \qquad (4.29)
\end{aligned}
$$

so the two eigenvalues are

$$\lambda_\pm = \frac{\tau \pm \sqrt{\tau^2 - 4\delta}}{2} = \frac{\tau \pm \mathcal{D}}{2}, \qquad (4.30)$$

where the trace, determinant, and **quadratic discriminant** are

$$
\begin{aligned}
\tau &= \operatorname{tr} M, && (4.31a) \\
\delta &= \det M, && (4.31b) \\
\mathcal{D} &= \sqrt{\tau^2 - 4\delta}. && (4.31c)
\end{aligned}
$$

The sum of the eigenvalues

$$\lambda_+ + \lambda_- = \frac{\tau + \mathcal{D}}{2} + \frac{\tau - \mathcal{D}}{2} = \tau = \operatorname{tr} M \qquad (4.32)$$

is the trace of the matrix, and the product of the eigenvalues

$$\lambda_+\lambda_- = \frac{\tau + \mathcal{D}}{2}\,\frac{\tau - \mathcal{D}}{2} = \frac{\tau^2 - \tau^2 + 4\delta}{4\delta} = \delta = \det M \qquad (4.33)$$

is the determinant of the matrix.

To find the corresponding eigenvectors $\vec{v} = \{v_x, v_y\}$, Eq. 4.26 now implies the one matrix equation

$$\begin{bmatrix} a-\lambda_\pm & b \\ c & d-\lambda_\pm \end{bmatrix} \begin{bmatrix} v_x \\ v_y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \qquad (4.34)$$

which is equivalent to the two scalar equations

$$
\begin{aligned}
(a-\lambda_\pm)v_x + bv_y &= 0, && (4.35a) \\
cv_x + (d-\lambda_\pm)v_y &= 0, && (4.35b)
\end{aligned}
$$

so that the ratio of the eigenvector components

$$\frac{v_x}{v_y} = \frac{b}{\lambda_\pm - a} = \frac{\lambda_\pm - d}{c}. \tag{4.36}$$

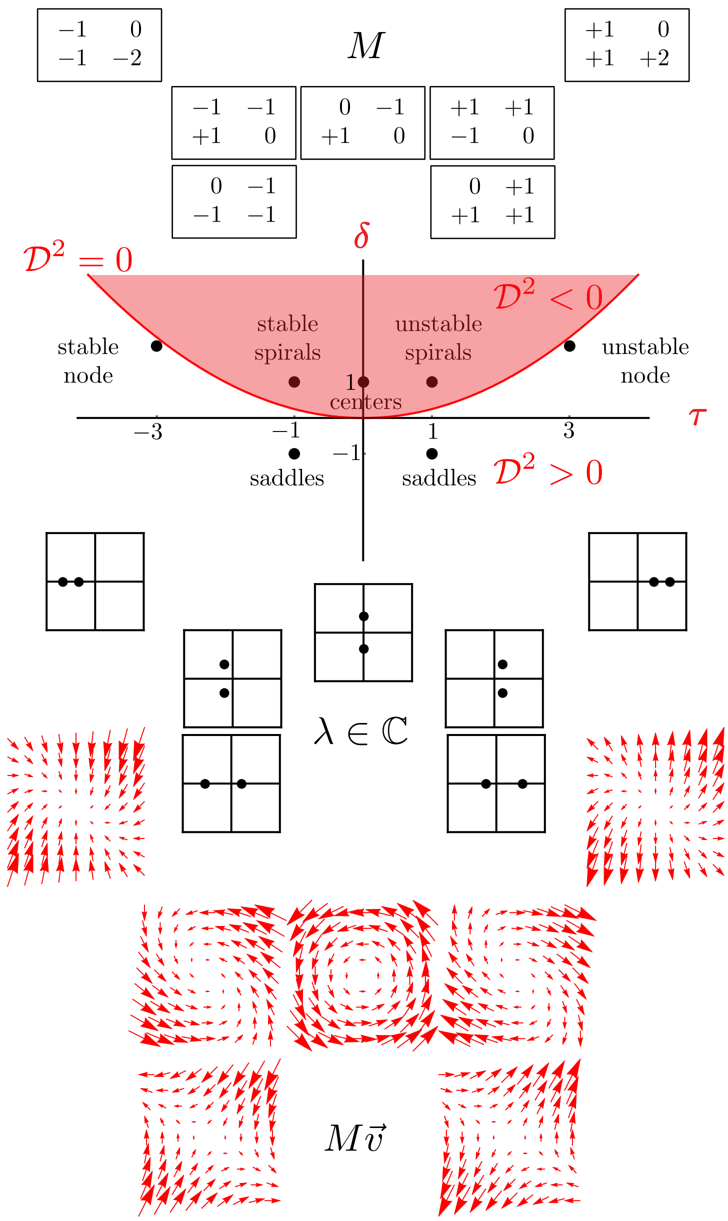


Figure 4.4: Representations of eigenvalues and eigenvectors of 2D matrices M.

The unnormalized eigenvectors

$$\vec{v}_\pm \propto \begin{bmatrix} \lambda_\pm - d \\ c \end{bmatrix} \propto \begin{bmatrix} b \\ \lambda_\pm - a \end{bmatrix} \tag{4.37}$$

and the normalized eigenvectors

$$\hat{v}_\pm = \frac{\vec{v}_\pm}{v_\pm} = \frac{1}{\sqrt{|\lambda_\pm - d|^2 + |c|^2}} \begin{bmatrix} \lambda_\pm - d \\ c \end{bmatrix} = \frac{1}{\sqrt{|b|^2 + |\lambda_\pm - a|^2}} \begin{bmatrix} b \\ \lambda_\pm - a \end{bmatrix}. \tag{4.38}$$

Figure 4.4 summarizes the 2D matrix eigenvalue-eigenvector phenomenology. Negatives determinants $\delta < 0$ correspond to **saddles** with one repelling and one attracting direction. Imaginary discriminants $\mathcal{D}^2 < 0$ correspond to **spirals**, with positive traces $\tau > 0$ rotating one way and negative traces rotating the other way.

4.4 Diagonalization

The dot product of the eigenvectors of 2D matrices

$$\begin{aligned}
\hat{v}_+ \cdot \hat{v}_- = \hat{v}_+^T \hat{v}_- \propto \begin{bmatrix} \lambda_+ - d & c \end{bmatrix} \begin{bmatrix} \lambda_- - d \\ c \end{bmatrix} \\
&= (\lambda_+ - d)(\lambda_- - d) + c^2 \\
&= \lambda_+ \lambda_- - (\lambda_+ + \lambda_-)d + d^2 + c^2 \\
&= \cancel{ad} - bc - (\cancel{a} + \cancel{d})d + \cancel{d^2} + c^2 \\
&= (c - b)c \;\propto\; c - b
\end{aligned} \tag{4.39}$$

vanishes when counter diagonal elements $b = c$ and the matrix $M = M^T$ is **symmetric**. In that case, the matrix of normalized eigenvectors

$$\mathcal{O} = \begin{bmatrix} \hat{v}_+ & \hat{v}_- \end{bmatrix} \tag{4.40}$$

is **orthogonal**

$$\begin{aligned}
\mathcal{O}^T \mathcal{O} &= \begin{bmatrix} \hat{v}_+^T \\ \hat{v}_-^T \end{bmatrix} \begin{bmatrix} \hat{v}_+ & \hat{v}_- \end{bmatrix} \\
&= \begin{bmatrix} \hat{v}_+^T \hat{v}_+ & \hat{v}_+^T \hat{v}_- \\ \hat{v}_-^T \hat{v}_+ & \hat{v}_-^T \hat{v}_- \end{bmatrix}
\end{aligned}$$

$$
\begin{aligned}
&= \boxed{\begin{matrix} 1 & 0 \\ 0 & 1 \end{matrix}} \\
&= I. \qquad (4.41)
\end{aligned}
$$

and **diagonalizes** M via the similarity transformation

$$
\begin{aligned}
\mathcal{O}^T M \mathcal{O} &= \boxed{\begin{matrix} \hat{v}_+^T \\ \hat{v}_-^T \end{matrix}} M \boxed{\begin{matrix} \hat{v}_+ & \hat{v}_- \end{matrix}} \\
&= \boxed{\begin{matrix} \hat{v}_+^T \\ \hat{v}_-^T \end{matrix}} \boxed{\begin{matrix} M\hat{v}_+ & M\hat{v}_- \end{matrix}} \\
&= \boxed{\begin{matrix} \hat{v}_+^T \\ \hat{v}_-^T \end{matrix}} \boxed{\begin{matrix} \lambda_+\hat{v}_+ & \lambda_-\hat{v}_- \end{matrix}} \\
&= \boxed{\begin{matrix} \lambda_+\hat{v}_+^T\hat{v}_+ & \lambda_-\hat{v}_+^T\hat{v}_- \\ \lambda_+\hat{v}_-^T\hat{v}_+ & \lambda_-\hat{v}_-^T\hat{v}_- \end{matrix}} \\
&= \boxed{\begin{matrix} \lambda_+ & 0 \\ 0 & \lambda_+ \end{matrix}} \\
&= D. \qquad (4.42)
\end{aligned}
$$

Thus, for a symmetric matrix $S = S^T$, a generic transformation in one reference frame implies a diagonal transformation in another reference frame,

$$S\vec{w} = \vec{w}\,', \tag{4.43a}$$

$$\mathcal{O}^T S \mathcal{O}\mathcal{O}^T \vec{w} = \mathcal{O}^T \vec{w}\,', \tag{4.43b}$$

$$D\vec{w}_o = \vec{w}_o', \tag{4.43c}$$

where $D = \mathcal{O}^T S \mathcal{O}$ and $\vec{w}_o = \mathcal{O}^T \vec{w}$ and $\vec{w}_o' = \mathcal{O}^T \vec{w}\,'$.

Just as a **symmetric** matrix $S = S^T$ is diagonalizable by an **orthogonal** matrix $\mathcal{O}^T = \mathcal{O}^{-1}$, a **hermitian** (or complex symmetric) matrix $H = H^\dagger$ is diagonalizable by a **unitary** matrix $U^\dagger = U^{-1}$, as in Fig. 4.5.

$$
\begin{tikzcd}
\vec{v}\,' \arrow[d, shift right, "T^{-1}"'] & \vec{v} \arrow[l, "M"'] \arrow[d, shift right, "T^{-1}"'] \\
\vec{v}\,'_T \arrow[u, shift right, "T"'] & \vec{v}_T \arrow[l, "D = T^{-1}MT"] \arrow[u, shift right, "T"']
\end{tikzcd}
\quad
\begin{tikzcd}
\vec{v}\,' \arrow[d, shift right, "\mathcal{O}^T"'] & \vec{v} \arrow[l, "S = S^T"'] \arrow[d, shift right, "\mathcal{O}^T"'] \\
\vec{v}\,'_{\mathcal{O}} \arrow[u, shift right, "\mathcal{O}"'] & \vec{v}_{\mathcal{O}} \arrow[l, "D = \mathcal{O}^T S \mathcal{O}"] \arrow[u, shift right, "\mathcal{O}"']
\end{tikzcd}
\quad
\begin{tikzcd}
\vec{v}\,' \arrow[d, shift right, "U^\dagger"'] & \vec{v} \arrow[l, "H = H^\dagger"'] \arrow[d, shift right, "U^\dagger"'] \\
\vec{v}\,'_U \arrow[u, shift right, "U"'] & \vec{v}_U \arrow[l, "D = U^\dagger H U"] \arrow[u, shift right, "U"']
\end{tikzcd}
$$

Figure 4.5: Similarity transformations for generic matrices M, symmetric matrices S, and hermitian (or complex symmetric) matrices H.

4.5 Matrix Invariants (det & tr)

Even when matrices do not commute, so $AB \neq BA$, the determinant and trace of a product of matrices is insensitive to the order of the factors, so

$$\det[AB] = \det[BA] \tag{4.44}$$

and

$$\mathrm{tr}[AB] = \mathrm{tr}[BA]. \tag{4.45}$$

With respect to the latter,

$$\mathrm{tr}\left[\begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{bmatrix} a' & b' \\ c' & d' \end{bmatrix}\right] = \mathrm{tr}\begin{bmatrix} aa' + bc' & ab' + bd' \\ ca' + dc' & cb' + dd' \end{bmatrix} = aa' + bc' + cb' + dd' \tag{4.46}$$

and

$$\mathrm{tr}\left[\begin{bmatrix} a' & b' \\ c' & d' \end{bmatrix}\begin{bmatrix} a & b \\ c & d \end{bmatrix}\right] = \mathrm{tr}\begin{bmatrix} a'a + b'c & a'b + b'd \\ c'a + d'c & c'b + d'd \end{bmatrix} = a'a + b'c + c'b + d'd \tag{4.47}$$

are identical. Hence, under a general coordinate transformation $T\vec{v} = \vec{v}\,'$, the determinant and trace are invariant,

$$\det M' = \det[T^{-1}MT] = \det[MTT^{-1}] = \det M \tag{4.48}$$

and

$$\mathrm{tr}\, M' = \mathrm{tr}[T^{-1}MT] = \mathrm{tr}[MTT^{-1}] = \mathrm{tr}\, M. \tag{4.49}$$

4.6 Matrix Functions

Define a function of a matrix by its power series expansion. For example,

$$e^M = I + M + \frac{1}{2!}M^2 + \frac{1}{3!}M^3 + \cdots \tag{4.50}$$

(with $e^{M_1}e^{M_2} = e^{M_1+M_2}$ if $M_1M_2 = M_2M_1$). Since the square of a diagonal matrix

$$D^2 = \begin{bmatrix} a & 0 \\ 0 & d \end{bmatrix}\begin{bmatrix} a & 0 \\ 0 & d \end{bmatrix} = \begin{bmatrix} a^2 & 0 \\ 0 & d^2 \end{bmatrix} \tag{4.51}$$

is the diagonal matrix of squares, and similarly for higher powers, the exponential of a diagonal matrix

$$\begin{aligned} e^D = \exp\begin{bmatrix} a & 0 \\ 0 & d \end{bmatrix} &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} a & 0 \\ 0 & d \end{bmatrix} + \frac{1}{2!}\begin{bmatrix} a^2 & 0 \\ 0 & d^2 \end{bmatrix} + \frac{1}{3!}\begin{bmatrix} a^3 & 0 \\ 0 & d^3 \end{bmatrix} + \cdots \\ &= \begin{bmatrix} 1 + a + \frac{1}{2!}a^2 + \frac{1}{3!}a^3 + \cdots & 0 \\ 0 & 1 + d + \frac{1}{2!}d^2 + \frac{1}{3!}d^3 + \cdots \end{bmatrix} = \begin{bmatrix} e^a & 0 \\ 0 & e^d \end{bmatrix} \end{aligned} \tag{4.52}$$

is the diagonal matrix of exponentials, and the determinant of the exponential of a diagonal matrix

$$\det e^D = e^a e^d = e^{a+d} = e^{\operatorname{tr} D} \tag{4.53}$$

is the exponential of its trace. If the transformation T diagonalizes M, then

$$M = TDT^{-1} \tag{4.54}$$

implies

$$\begin{aligned} e^M &= e^{TDT^{-1}} \\ &= I + TDT^{-1} + \frac{1}{2!}\left(TDT^{-1}\right)^2 + \frac{1}{3!}\left(TDT^{-1}\right)^3 + \cdots \\ &= TT^{-1} + TDT^{-1} + \frac{1}{2!}TDT^{-1}TDT^{-1} + \frac{1}{3!}TDT^{-1}TDT^{-1}TDT^{-1} + \cdots \\ &= T\left(I + D + \frac{1}{2!}D^2 + \frac{1}{3!}D^3 + \cdots\right)T^{-1} \\ &= Te^DT^{-1}. \end{aligned} \tag{4.55}$$

Hence the determinant of the exponential

$$\begin{aligned} \det e^M &= \det[Te^DT^{-1}] = \det[e^DT^{-1}T] \\ &= \det e^D = e^{\operatorname{tr} D} = e^{\operatorname{tr}[T^{-1}MT]} = e^{\operatorname{tr}[MTT^{-1}]} = e^{\operatorname{tr} M} \end{aligned} \tag{4.56}$$

is the exponential of the trace.

If δt is scalar parameter and $M = \delta t N$, then

$$\det e^{\delta t N} = e^{\delta t \operatorname{tr} N} \tag{4.57}$$

and so the power series expansions

$$\det[I + \delta t N + \cdots] = 1 + \delta t \operatorname{tr} N + \cdots \tag{4.58}$$

imply

$$\det[I + \delta t N] = \det I + \delta t \operatorname{tr} N + O[\delta t^2]. \tag{4.59}$$

Hence the directional derivative of the determinant at the identity

$$\nabla_N \det I = \lim_{\delta t \to 0} \frac{\det[I + \delta t N] - \det I}{\delta t} = \operatorname{tr} N \tag{4.60}$$

is the trace. More generally, if M_t is a matrix that depends on t, then

$$\begin{aligned}
\frac{d}{dt} \det M_t &= \lim_{\delta t \to 0} \frac{\det M_{t+\delta t} - \det M_t}{\delta t} \\
&= \det M_t \lim_{\delta t \to 0} \frac{\det[M_t^{-1} M_{t+\delta t}] - 1}{\delta t} \\
&= \det M_t \lim_{\delta t \to 0} \frac{\det[M_t^{-1}(M_t + \delta t \, dM_t/dt + \cdots)] - 1}{\delta t} \\
&= \det M_t \lim_{\delta t \to 0} \frac{\det[I + \delta t M_t^{-1} dM_t/dt] - \det I}{\delta t} \\
&= \det M_t \operatorname{tr}\left[M_t^{-1} \frac{dM_t}{dt} \right],
\end{aligned} \tag{4.61}$$

so the **relative rate of change** or **logarithmic derivative** of the determinant

$$(\det M_t)^{-1} \frac{d}{dt} \det M_t = \operatorname{tr}\left[M_t^{-1} \frac{dM_t}{dt} \right]. \tag{4.62}$$

Alternately, the derivative of the logarithm of the determinant

$$\frac{d}{dt} \log \det M_t = \operatorname{tr} \frac{d}{dt} \log M_t \tag{4.63}$$

is the trace of the derivative of the logarithm of the matrix.

Finally, using the Eq. 4.46 square 2D matrix trace,

$$\begin{aligned}
\det M = ad - bc &= \frac{1}{2}\left((a+d)^2 - (a^2 + bc + cb + d^2)\right) \\
&= \frac{1}{2}\left((\operatorname{tr} M)^2 - \operatorname{tr} M^2\right) = \frac{1}{2} \det \begin{vmatrix} \operatorname{tr} M & 1 \\ \operatorname{tr} M^2 & \operatorname{tr} M \end{vmatrix}.
\end{aligned} \tag{4.64}$$

For a 5D matrix, the pretty pattern becomes

$$\det M = \frac{1}{5!} \det \boxed{\begin{matrix} \operatorname{tr} M & 1 & 0 & 0 & 0 \\ \operatorname{tr} M^2 & \operatorname{tr} M & 2 & 0 & 0 \\ \operatorname{tr} M^3 & \operatorname{tr} M^2 & \operatorname{tr} M & 3 & 0 \\ \operatorname{tr} M^4 & \operatorname{tr} M^3 & \operatorname{tr} M^2 & \operatorname{tr} M & 4 \\ \operatorname{tr} M^5 & \operatorname{tr} M^4 & \operatorname{tr} M^3 & \operatorname{tr} M^2 & \operatorname{tr} M \end{matrix}} . \tag{4.65}$$

Mathematica Matrices 2

```
aMat = {{ⅈ, 3}, {-2, 1}}; (* ESCiiESC → ⅈ *)

MatrixForm /@ {aMat, aMatᵀ, aMat†} (* MESCtrESC → Mᵀ, MESCctESC → M† *)
```

$$\left\{\begin{pmatrix} i & 3 \\ -2 & 1 \end{pmatrix}, \begin{pmatrix} i & -2 \\ 3 & 1 \end{pmatrix}, \begin{pmatrix} -i & -2 \\ 3 & 1 \end{pmatrix}\right\}$$

```
Through[{Det, Tr}[aMat]] (* → {Det@aMat, Tr@aMat} *)
```

$$\{6 + i, 1 + i\}$$

```
Inverse[aMat] // MatrixForm (* not computable; for display only *)
```

$$\begin{pmatrix} \frac{6}{37} - \frac{i}{37} & -\frac{18}{37} + \frac{3 i}{37} \\ \frac{12}{37} - \frac{2 i}{37} & \frac{1}{37} + \frac{6 i}{37} \end{pmatrix}$$

```
1 / aMat // MatrixForm (* piecewise inverse *)
```

$$\begin{pmatrix} -i & \frac{1}{3} \\ -\frac{1}{2} & 1 \end{pmatrix}$$

```
Det[aMat] Inverse[aMat] // MatrixForm (* for display only *)
```

$$\begin{pmatrix} 1 & -3 \\ 2 & i \end{pmatrix}$$

```
aMat.Inverse[aMat] // MatrixForm (* for display only *)
```

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

```
λList = Eigenvalues@aMat
```

$$\left\{\frac{1}{2}\left((1 + i) - \sqrt{-24 - 2 i}\right), \frac{1}{2}\left((1 + i) + \sqrt{-24 - 2 i}\right)\right\}$$

```
vVecList = Eigenvectors@aMat
```

$$\left\{\left\{\left(\frac{1}{4} - \frac{i}{4}\right) + \frac{1}{2}\sqrt{-6 - \frac{i}{2}}, 1\right\}, \left\{\left(\frac{1}{4} - \frac{i}{4}\right) - \frac{1}{2}\sqrt{-6 - \frac{i}{2}}, 1\right\}\right\}$$

Worked Problem

1. Invert a 3×3 matrix (and check).

$$\begin{bmatrix} 2 & 3 & 4 \\ 2 & 1 & 2 \\ 1 & 2 & 1 \end{bmatrix}^{-1} = \frac{\begin{bmatrix} +\begin{vmatrix} 1 & 2 \\ 2 & 1 \end{vmatrix} & -\begin{vmatrix} 2 & 2 \\ 1 & 1 \end{vmatrix} & +\begin{vmatrix} 2 & 1 \\ 1 & 2 \end{vmatrix} \\ -\begin{vmatrix} 3 & 4 \\ 2 & 1 \end{vmatrix} & +\begin{vmatrix} 2 & 4 \\ 1 & 1 \end{vmatrix} & -\begin{vmatrix} 2 & 3 \\ 1 & 2 \end{vmatrix} \\ +\begin{vmatrix} 3 & 4 \\ 1 & 2 \end{vmatrix} & -\begin{vmatrix} 2 & 4 \\ 2 & 2 \end{vmatrix} & +\begin{vmatrix} 2 & 3 \\ 2 & 1 \end{vmatrix} \end{bmatrix}^T}{+2\begin{vmatrix} 1 & 2 \\ 2 & 1 \end{vmatrix} - 3\begin{vmatrix} 2 & 2 \\ 1 & 1 \end{vmatrix} + 4\begin{vmatrix} 2 & 1 \\ 1 & 2 \end{vmatrix}}$$

$$= \frac{\begin{bmatrix} -3 & 0 & 3 \\ 5 & -2 & 1 \\ 2 & 4 & -4 \end{bmatrix}^T}{2(-3) - 3(0) + 4(3)}$$

$$= \frac{1}{6}\begin{bmatrix} -3 & 5 & 2 \\ 0 & -2 & 4 \\ 3 & -1 & -4 \end{bmatrix}$$

$$= \begin{bmatrix} -1/2 & 5/6 & 1/3 \\ 0 & -1/3 & 2/3 \\ 1/2 & -1/6 & -2/3 \end{bmatrix}$$

$$\begin{bmatrix} 2 & 3 & 4 \\ 2 & 1 & 2 \\ 1 & 2 & 1 \end{bmatrix}\begin{bmatrix} -1/2 & 5/6 & 1/3 \\ 0 & -1/3 & 2/3 \\ 1/2 & -1/6 & -2/3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Problems

1. For each real matrix A, compute A^T, $\det A$, $\operatorname{tr} A$, A^{-1}.

   (a) $A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$

   (b) $A = \begin{bmatrix} 1 & 2 \\ 4 & 9 \end{bmatrix}$

   (c) $A = \begin{bmatrix} 1 & 2 & 3 \\ 3 & 2 & 2 \\ 1 & 1 & 2 \end{bmatrix}$

2. For each complex matrix U, compute $U^\dagger$, $\det U$, $\operatorname{tr} U$, U^{-1}. (Hint: Recall that the adjoint is the transpose of the complex conjugate, $U^\dagger = (U^*)^T$.)

   (a) $U = \begin{bmatrix} 2i & 0 \\ i & 2 \end{bmatrix}$

   (b) $U = \begin{bmatrix} i & 1 \\ 4 & -i \end{bmatrix}$

3. Find the eigenvalues and normalized eigenvectors of the following matrices. (Hint: For complex vectors, normalization requires an adjoint rather than a transpose, for example, $\hat{v}_+^\dagger \hat{v}_+ = 1$ instead of $\hat{v}_+^T \hat{v}_+ = 1$.)

   (a) $A = \begin{bmatrix} 1 & 2 \\ 3 & 2 \end{bmatrix}$

   (b) $U = \begin{bmatrix} 2i & 1 \\ 3 & -2i \end{bmatrix}$

4. Define a matrix function by its power series expansion, as in Eq. 4.50.

   (a) Show that if $A^T = -A$ is antisymmetric, then $\mathcal{O} = e^A$ is orthogonal (so that $\mathcal{O}^T = \mathcal{O}^{-1}$).

   (b) Show that if $H^\dagger = H$ is complex symmetric, then $U = e^{iH}$ is unitary (so that $U^\dagger = U^{-1}$).

5. Use *Mathematica* to evaluate powers S^n and T^n of the following matrices and induce the general patterns. (Hint: Try using MatrixPower, Simplify with assumptions, and MatrixForm.)

   (a) $S = \boxed{\begin{matrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{matrix}}$

   (b) $T = \boxed{\begin{matrix} 1 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{matrix}}$

6. Use *Mathematica* to apply the Eq. 4.20 and Eq. 4.22 first and second difference matrices and their inverses to a sampled sine curve to visually demonstrate "differentiation" and "integration" (Hint: Try using Table, SparseArray, ListPlot, and Rest.)

Chapter 5

Normal Modes & Eigenstates

As a prelude to Fourier analysis, consider the classical normal modes of masses connected by springs and the quantum eigenstates of an ammonia molecule.

5.1 Classical Two Degrees of Freedom

When a mechanism oscillates in a **normal mode** all of its parts oscillate in phase at the same frequency. The modes are independent or **orthogonal** as exciting one does not excite others. The mechanism's most general motion is a **superposition** of its normal mode motions. Normal mode analysis is important in physics and engineering.

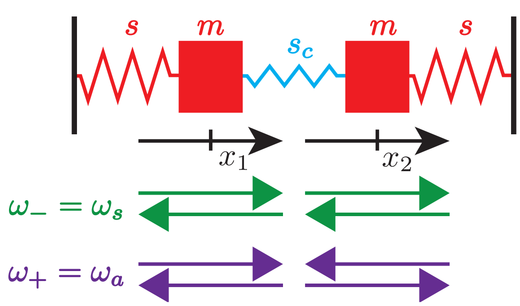


Figure 5.1: Identical masses connected by springs slide frictionlessly between two fixed walls in symmetric or antisymmetric motions at slow and fast angular frequencies ω_- and ω_+.

Consider two masses m connected by springs of stiffness s to walls and coupled by a spring of stiffness s_c to each other as they slide frictionlessly at positions x_1 and x_2, as in Fig. 5.1. Newton's second law at each mass implies

$$m\ddot{x}_1 = F_{1x} = -sx_1 + s_c(x_2 - x_1), \tag{5.1a}$$

$$m\ddot{x}_2 = F_{2x} = -sx_2 - s_c(x_2 - x_1), \tag{5.1b}$$

where the over-dots indicate differentiation with respect to time. Write this as the matrix equation

$$M\ddot{\vec{x}} = S\vec{x}, \tag{5.2}$$

where the state vector

$$\vec{x} = \boxed{\begin{matrix} x_1 \\ x_2 \end{matrix}}, \tag{5.3}$$

the **mass matrix**

$$M = \boxed{\begin{matrix} m & 0 \\ 0 & m \end{matrix}}, \tag{5.4}$$

and the **stiffness matrix**

$$S = \boxed{\begin{matrix} -s - s_c & s_c \\ s_c & -s - s_c \end{matrix}}, \tag{5.5}$$

where S_{rc} is the force per displacement on mass r when mass c is displaced.

Seek **normal mode** solutions where each mass moves at the same angular frequency ω and with the same phase (shift) φ by subsituting

$$\vec{x} = \vec{A}\cos[\omega t + \varphi] \tag{5.6}$$

into Eq. 5.2 to find

$$-\omega^2 M\vec{A} = \mathcal{S}\vec{A} \tag{5.7}$$

or the eigenequation

$$\omega^2\vec{A} = W\vec{A}, \tag{5.8}$$

where

$$W = -M^{-1}S = \frac{1}{m}\boxed{\begin{matrix} s + s_c & -s_c \\ -s_c & s + s_c \end{matrix}} = \boxed{\begin{matrix} \omega_0^2 + \omega_c^2 & -\omega_c^2 \\ -\omega_c^2 & \omega_0^2 + \omega_c^2 \end{matrix}}, \tag{5.9}$$

and the natural frequencies $\omega_0 = \sqrt{s/m}$ and $\omega_c = \sqrt{s_c/m}$. For a nontrivial $\vec{A} \neq \vec{0}$ solution of

$$(\omega^2 I - W)\vec{A} = \vec{0}, \tag{5.10}$$

the matrix $\omega^2 I - W$ must not be invertible, so demand

$$0 = \det[\omega^2 I - W]$$

$$
\begin{aligned}
&= \begin{vmatrix} \omega^2 - \omega_0^2 - \omega_c^2 & \omega_c^2 \\ \omega_c^2 & \omega^2 - \omega_0^2 - \omega_c^2 \end{vmatrix} \\
&= (\omega^2 - \omega_0^2 - \omega_c^2)^2 - (\omega_c^2)^2 \\
&= \left(\omega^2 - \omega_0^2\right)\left(\omega^2 - \omega_0^2 - 2\omega_c^2\right). \qquad (5.11)
\end{aligned}
$$

Hence the square eigenfrequencies of the symmetric and antisymmetric normal mode motion are

$$\omega_s^2 = \omega_-^2 = \omega_0^2, \qquad (5.12a)$$

$$\omega_a^2 = \omega_+^2 = \omega_0^2 + 2\omega_c^2. \qquad (5.12b)$$

Given the eigenfrequencies, the Eq. 5.10 eigenequation

$$\begin{bmatrix} \omega^2 - \omega_0^2 - \omega_c^2 & \omega_c^2 \\ \omega_c^2 & \omega^2 - \omega_0^2 - \omega_c^2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad (5.13)$$

for $\omega = \omega_s$ implies

$$\begin{bmatrix} -\omega_c^2 & \omega_c^2 \\ \omega_c^2 & -\omega_c^2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \qquad (5.14)$$

so $a_1 = a_2$, and for $\omega = \omega_a$ implies

$$\begin{bmatrix} \omega_c^2 & \omega_c^2 \\ \omega_c^2 & \omega_c^2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \qquad (5.15)$$

so $a_1 = -a_2$. Because the matrix $W = W^T$ is symmetric, the corresponding normalized eigenvectors

$$\hat{A}_s = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \qquad (5.16a)$$

$$\hat{A}_a = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \qquad (5.16b)$$

are orthonormal

$$\hat{A}_s \cdot \hat{A}_a = \hat{A}_s^T \hat{A}_a = \frac{1}{2} \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = 0, \qquad (5.17a)$$

$$\hat{A}_s \cdot \hat{A}_s = \hat{A}_s^T \hat{A}_s = \frac{1}{2} \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 1, \tag{5.17b}$$

$$\hat{A}_a \cdot \hat{A}_a = \hat{A}_a^T \hat{A}_a = \frac{1}{2} \begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = 1, \tag{5.17c}$$

and give the "shape" of the normal modes. The two masses move in the same direction in the slow symmetric mode and in the opposite directions in the fast antisymmetric mode, as in Fig 5.1. In the symmetric slow mode, the center spring does not stretch or contract, effectively decoupling the masses so they oscillate at the natural frequency of just a mass connected to a single spring, $\omega_s = \sqrt{s/m} = \omega_0$. In the antisymmetric fast mode, the center of the spring does not move, making it effectively twice as stiff, which when combined with the normal stiffness of the wall spring causes the masses to oscillate at the frequency $\omega_a = \sqrt{(s + 2s_c)/m} = \sqrt{\omega_0^2 + 2\omega_c^2} > \omega_0$.

The general motion is a linear combination or **superposition** of the normal mode motions

$$\vec{x}[t] = c_s \hat{A}_s \cos\left[\omega_s t + \varphi_s\right] + c_a \hat{A}_a \cos\left[\omega_a t + \varphi_a\right], \tag{5.18}$$

where the amplitude multipliers c_s, c_a and phase shifts φ_s, φ_a depend on the initial $t = 0$ positions and velocities of both masses,

$$\hat{A}_s \cdot \vec{x}[0] = c_s \cos\varphi_s, \tag{5.19a}$$

$$\hat{A}_a \cdot \vec{x}[0] = c_a \cos\varphi_a, \tag{5.19b}$$

$$\hat{A}_s \cdot \dot{\vec{x}}[0] = -\omega_s c_s \sin\varphi_s, \tag{5.19c}$$

$$\hat{A}_a \cdot \dot{\vec{x}}[0] = -\omega_a c_a \sin\varphi_a. \tag{5.19d}$$

To check, apply the stiffness matrix $S = -MW$ to both side of Eq. 5.18 to get

$$\begin{aligned} S\vec{x}[t] &= c_s S\hat{A}_s \cos\left[\omega_s t + \varphi_s\right] + c_a S\hat{A}_a \cos\left[\omega_a t + \varphi_a\right] \\ &= M\left(-c_s W\hat{A}_s \cos\left[\omega_s t + \varphi_s\right] - c_a W\hat{A}_a \cos\left[\omega_a t + \varphi_a\right]\right) \\ &= M\left(-c_s \omega_s^2 \hat{A}_s \cos\left[\omega_s t + \varphi_s\right] - c_a \omega_a^2 \hat{A}_a \cos\left[\omega_a t + \varphi_a\right]\right) \\ &= M\ddot{\vec{x}}[t], \end{aligned} \tag{5.20}$$

which is Newton's Eq. 5.2.

The orthogonal matrix of normalized eigenvectors

$$\mathcal{O} = \begin{bmatrix} \hat{A}_s & \hat{A}_a \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{5.21}$$

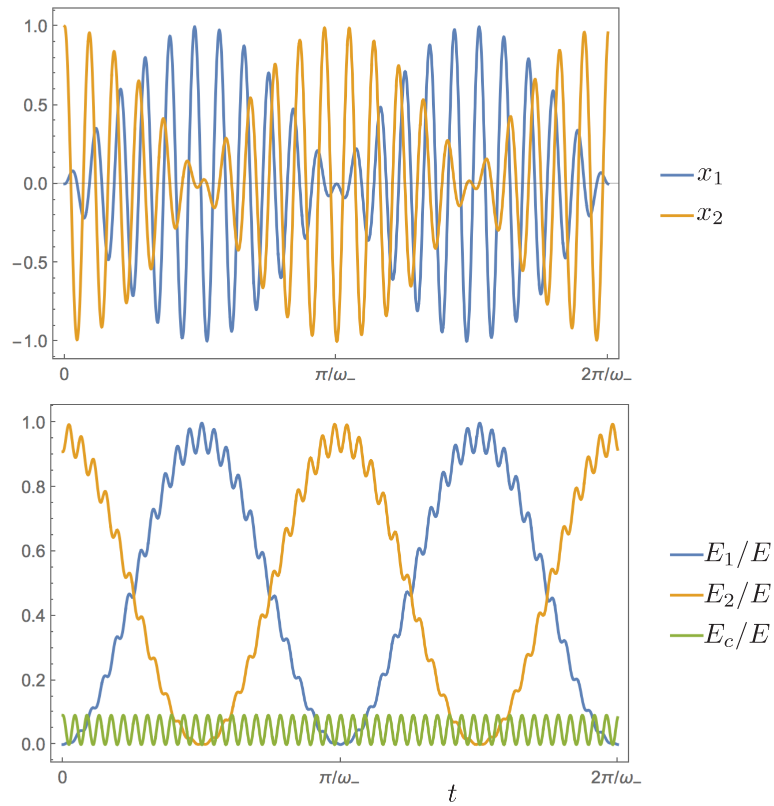


Figure 5.2: Masses motion x_1, x_2 exhibits mode mixing as energy E_1, E_2 beats between them (with little energy E_c of total energy E stored in the weak spring).

that diagonalizes M transforms the masses' coordinates to **normal coordinates**

$$\vec{\xi} = \mathcal{O}^T \vec{x} \tag{5.22}$$

or

$$\begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} x_1 + x_2 \\ x_1 - x_2 \end{pmatrix}, \tag{5.23}$$

where $\xi_1 \propto x_1 + x_2$ is proportional to the midpoint of the masses and $\xi_2 \propto x_1 - x_2$ is proportional to the distance between the masses.

As an example, start both masses at rest with the first at equilibrium and the second displaced a distance d so that

$$\vec{x}[0] = \boxed{\begin{matrix} 0 \\ d \end{matrix}}, \tag{5.24a}$$

$$\dot{\vec{x}}[0] = \boxed{\begin{matrix} 0 \\ 0 \end{matrix}}. \tag{5.24b}$$

Evaluate Eq. 5.19 to get

$$d/\sqrt{2} = c_s \cos\varphi_s, \tag{5.25a}$$
$$-d/\sqrt{2} = c_a \cos\varphi_a, \tag{5.25b}$$
$$0 = -\omega_s c_s \sin\varphi_s, \tag{5.25c}$$
$$0 = -\omega_a c_a \sin\varphi_a, \tag{5.25d}$$

which has the nontrivial solution $\varphi_s = 0$, $\varphi_a = \pi$, $c_s = d/\sqrt{2}$, $c_a = d/\sqrt{2}$, so that

$$\vec{x}[t] = \frac{d}{2}\hat{A}_s \cos\omega_s t - \frac{d}{2}\hat{A}_a \cos\omega_a t, \tag{5.26}$$

where $\cos\omega t$ is a common but slightly ambiguous shorthand for $\cos[\omega t]$. In components,

$$\boxed{\begin{matrix} x_1[t] \\ x_2[t] \end{matrix}} = \frac{d}{2}\boxed{\begin{matrix} 1 \\ 1 \end{matrix}}\cos\omega_s t - \frac{d}{2}\boxed{\begin{matrix} 1 \\ -1 \end{matrix}}\cos\omega_a t \tag{5.27}$$

or

$$x_1[t] = \frac{d}{2}\left(\cos\omega_s t + \cos\omega_a t\right), \tag{5.28a}$$
$$x_2[t] = \frac{d}{2}\left(\cos\omega_s t - \cos\omega_a t\right). \tag{5.28b}$$

A couple of trig sum-to-product identities imply

$$x_1[t] = +d\cos\frac{\omega_s t - \omega_a t}{2}\cos\frac{\omega_s t + \omega_a t}{2}, \tag{5.29a}$$
$$x_2[t] = -d\sin\frac{\omega_s t - \omega_a t}{2}\sin\frac{\omega_s t + \omega_a t}{2}. \tag{5.29b}$$

Introduce the frequency mean and splitting $\omega_\pm = (\omega_a \pm \omega_s)/2$ and a couple of trig sum-to-product identities imply

$$x_1[t] = (d\cos\omega_- t)\cos\omega_+ t, \tag{5.30a}$$
$$x_2[t] = (d\sin\omega_- t)\sin\omega_+ t, \tag{5.30b}$$

which emphasizes the "beats" or mode mixing of Fig. 5.2, where a slowly varying amplitude modulates a fast frequency.

5.2 Quantum Two-State System

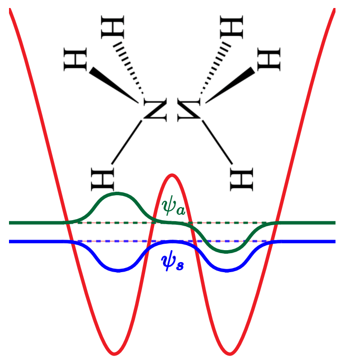


Figure 5.3: Plane of hydrogens can quantum tunnel through the nitrogen atom in ammonia. Modeled as a point particle in a bistable potential, the symmetric and antisymmetric energy states create an effective two-state system.

The ammonia molecule NH_3 is a fascinating example of quantum tunneling [4]. Ammonia is shaped like a pyramid, with a large N molecule at the apex and a triangle of small H atoms at the base, as in Fig. 5.3. In addition to electronic, translational, vibrational, and rotational degrees of freedom, ammonia has an additional degree of freedom: the base of H atoms can be on one side of the N atom or the other. Classically, a potential energy barrier prevents such an "inverting umbrella" transition, which we can simply model with a finite square barrier inside an infinite square well. The potential barrier reflects the repulsion between the N and the H atoms; the potential side walls reflect the chemical bonding, which insures the molecule's cohesion; the two minima represent the two stable configurations. Quantumly, the molecule can tunnel between these two configurations, and it does so spontaneously, in the absence of any forcing.

Table 5.1: Matrix representations for bra and kets, where $|\psi\rangle^\dagger = \langle\psi|$.

vector	ket	$\lvert\psi\rangle$	$\boxed{\begin{matrix} a \\ b \end{matrix}}$
functional	bra	$\langle\psi\rvert$	$\boxed{\begin{matrix} a^* & b^* \end{matrix}}$
operator	ket bra	$\lvert\psi\rangle\langle\psi\rvert$	$\boxed{\begin{matrix} aa^* & ab^* \\ ba^* & bb^* \end{matrix}}$
scalar	bra ket	$\langle\psi\lvert\psi\rangle$	$a^*a + b^*b$

Model ammonia as a two-state system with "Left" and "Right" base states

$$\hat{L} = |L\rangle = \boxed{\begin{matrix} 1 \\ 0 \end{matrix}}, \tag{5.31a}$$

$$\hat{R} = |R\rangle = \boxed{\begin{matrix} 0 \\ 1 \end{matrix}} \tag{5.31b}$$

in the Table 5.1 **bra-ket notation**. The general state is the linear superposition

$$\vec{\Psi} = |\Psi\rangle = \Psi_L|L\rangle + \Psi_R|R\rangle = \boxed{\begin{matrix} \Psi_L \\ \Psi_R \end{matrix}}. \tag{5.32}$$

If the Hamiltonian

$$H = \boxed{\begin{matrix} E_0 & -A \\ -A & E_0 \end{matrix}}, \tag{5.33}$$

then the Schrödinger equation

$$i\hbar\partial_t|\Psi\rangle = H|\Psi\rangle \tag{5.34}$$

becomes

$$i\hbar\,\partial_t \boxed{\begin{matrix} \Psi_L \\ \Psi_R \end{matrix}} = \boxed{\begin{matrix} E_0 & -A \\ -A & E_0 \end{matrix}} \boxed{\begin{matrix} \Psi_L \\ \Psi_R \end{matrix}} \tag{5.35}$$

or in components

$$i\hbar\dot{\Psi}_L = +E_0\Psi_L - A\Psi_R, \tag{5.36a}$$
$$i\hbar\dot{\Psi}_R = -A\Psi_L + E_0\Psi_R. \tag{5.36b}$$

Seek stationary solutions of definite energy E by substituting

$$|\Psi\rangle = |\psi\rangle e^{-iEt/\hbar} \tag{5.37}$$

or in an alternate notation

$$|\psi_t\rangle = |\psi_0\rangle e^{-iEt/\hbar} \tag{5.38}$$

into Eq. 5.34 to find the eigenvalue-eigenvector equation

$$E|\psi\rangle = H|\psi\rangle \tag{5.39}$$

or

$$(EI - H)|\psi\rangle = 0. \tag{5.40}$$

For a nontrivial $|\psi\rangle \neq 0$ solution, $EI - H$ must not be invertible, so demand

$$
\begin{aligned}
0 &= \det[EI - H] \\
&= \begin{vmatrix} E - E_0 & A \\ A & E - E_0 \end{vmatrix} \\
&= E^2 - 2E_0E + E_0^2 - A^2 \\
&= (E - E_0 - A)\,(E - E_0 + A)\,,
\end{aligned} \tag{5.41}
$$

so the eigenenergies of the symmetric and antisymmetric states

$$E_s = E_- = E_0 - A, \tag{5.42a}$$
$$E_a = E_+ = E_0 + A. \tag{5.42b}$$

Given the eigenenergies, the Eq. 5.40 eigenequation

$$\begin{bmatrix} E - E_0 & A \\ A & E - E_0 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{5.43}$$

for $E = E_s$ implies

$$\begin{bmatrix} -A & A \\ A & -A \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tag{5.44}$$

so $\psi_2 = \psi_2$, and for $E = E_a$ implies

$$\begin{bmatrix} A & A \\ A & A \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tag{5.45}$$

so $\psi_1 = -\psi_2$. Because the matrix $H = H^\dagger$ is hermitian, the corresponding normalized eigenstates

$$|s\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \tag{5.46a}$$

$$|a\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \tag{5.46b}$$

are orthonormal

$$\hat{s} \cdot \hat{a} = \langle s|a\rangle = \frac{1}{2} \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = 0, \tag{5.47a}$$

$$\hat{s} \cdot \hat{s} = \langle s|s\rangle = \frac{1}{2}\boxed{\begin{matrix} 1 & 1 \end{matrix}}\boxed{\begin{matrix} 1 \\ 1 \end{matrix}} = 1, \tag{5.47b}$$

$$\hat{a} \cdot \hat{a} = \langle a|a\rangle = \frac{1}{2}\boxed{\begin{matrix} 1 & -1 \end{matrix}}\boxed{\begin{matrix} 1 \\ -1 \end{matrix}} = 1. \tag{5.47c}$$

A general state is a linear combination or **superposition** of the stationary states

$$|\psi\rangle = c_s|s\rangle + c_a|a\rangle, \tag{5.48}$$

where the amplitude multipliers c_s, c_a are

$$\langle s|\psi\rangle = c_s, \tag{5.49a}$$
$$\langle a|\psi\rangle = c_a. \tag{5.49b}$$

At a later time, the initial state evolves to

$$|\Psi\rangle = c_s|s\rangle e^{-iE_s t/\hbar} + c_a|a\rangle e^{-iE_a t/\hbar}. \tag{5.50}$$

To check, apply the Hamiltonian H to both sides of Eq. 5.50 to get

$$\begin{aligned} H|\Psi\rangle &= c_s H|s\rangle e^{-iE_s t/\hbar} + c_a H|a\rangle e^{-iE_a t/\hbar} \\ &= c_s E_s|s\rangle e^{-iE_s t/\hbar} + c_a E_a|a\rangle e^{-iE_a t/\hbar} \\ &= i\hbar\,\partial_t \left(c_s|s\rangle e^{-iE_s t/\hbar} + c_a|a\rangle e^{-iE_a t/\hbar}\right) \\ &= i\hbar\,\partial_t|\Psi\rangle, \end{aligned} \tag{5.51}$$

which is Schrödinger's Eq. 5.34.

As an example, suppose the ammonia molecule begins with the plane of hydrogens right of the nitrogen atom,

$$|\psi\rangle = |R\rangle = \boxed{\begin{matrix} 1 \\ 0 \end{matrix}}. \tag{5.52}$$

Evaluate the Eq. 5.49 projections to get

$$1/\sqrt{2} = c_s, \tag{5.53a}$$
$$-1/\sqrt{2} = c_a \tag{5.53b}$$

so that

$$|\psi\rangle = \frac{1}{\sqrt{2}}|s\rangle - \frac{1}{\sqrt{2}}|a\rangle \tag{5.54}$$

or in matrix form

$$|\psi\rangle = \frac{1}{2}\boxed{\begin{matrix}1\\1\end{matrix}} - \frac{1}{2}\boxed{\begin{matrix}1\\-1\end{matrix}} = \boxed{\begin{matrix}1\\0\end{matrix}} = |R\rangle. \tag{5.55}$$

Thereafter, the complex phase of each energy eigenstate rotates at frequency proportional to the corresponding energy

$$\begin{aligned}|\Psi\rangle &= \frac{1}{\sqrt{2}}|s\rangle e^{-iE_s t/\hbar} - \frac{1}{\sqrt{2}}|a\rangle e^{-iE_a t/\hbar} \\ &= \frac{1}{\sqrt{2}}e^{-i\bar{E}t/\hbar}\left(|s\rangle e^{+i\omega t/2} - |a\rangle e^{-i\omega t/2}\right),\end{aligned} \tag{5.56}$$

where the average energy $\bar{E} = (E_s + E_a)/2$ and the **energy splitting** $\hbar\omega = \Delta E = E_a - E_s$. The probability amplitude to find the plane of the hydrogens left of the nitrogen atom is the projection

$$\begin{aligned}\langle L|\Psi\rangle &= \frac{1}{\sqrt{2}}e^{-i\bar{E}t/\hbar}\left(\langle L|s\rangle e^{+i\omega t/2} - \langle L|a\rangle e^{-i\omega t/2}\right) \\ &= e^{-i\bar{E}t/\hbar}\left(\frac{e^{+i\omega t/2} - e^{-i\omega t/2}}{2}\right) \\ &= i e^{-i\bar{E}t/\hbar}\sin\frac{\omega t}{2},\end{aligned} \tag{5.57}$$

and the corresponding probability for the ammonia molecule to tunnel from right to left is

$$\mathcal{P} = |\langle L|\Psi\rangle|^2 = \sin^2\frac{\omega t}{2}, \tag{5.58}$$

where $\sin^2 x$ is a common abbreviation for $\sin[x]^2$, as in Fig. 5.4. This is the basis for the ammonia **maser**.

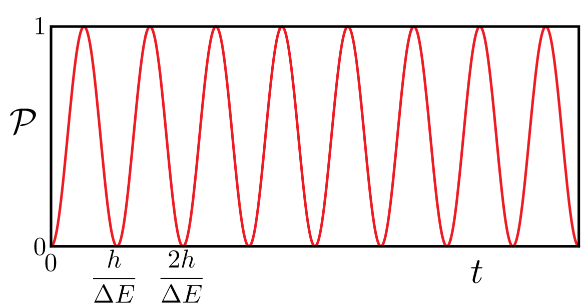
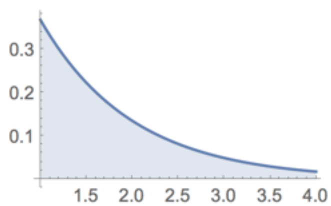


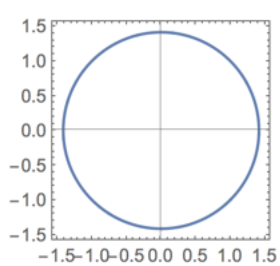
Figure 5.4: Probability $\mathcal{P}$ to find the ammonia's hydrogen plane left of the nitrogen atom versus time t oscillates with period $T = 2\pi\hbar/\Delta E = h/\Delta E$.

Mathematica DSolve

```
s1 = DSolve[x'[t] == -x[t], x[t], t] (* Equal[a,b] ↔ a==b *)
{{x[t] → e^-t C[1]}}

Plot[x[t] /. s1 /. C[1] → 1, {t, 1, 4}, Filling → Bottom]
```




```
s2 = DSolve[{x'[t] == -x[t], x[0] == 1}, x[t], t]
{{x[t] → e^-t}}

xs[t_] = x[t] /. s2[[1]] (* s2 ESC[[ESC1ESC]]ESC ↔ s2[[1]] *)
e^-t

vars = {x[t], y[t]};
go = {x'[t] == -y[t], y'[t] == x[t]};
start = {x[0] == 1, y[0] == -1};

DSolve[go ⋃ start, vars, t]
{{x[t] → Cos[t] + Sin[t], y[t] → -Cos[t] + Sin[t]}}

DSolveValue[go ⋃ start, vars, t] (* ESCunESC → ⋃ *)
{Cos[t] + Sin[t], -Cos[t] + Sin[t]}

{xs[t_], ys[t_]} = DSolveValue[go ⋃ start, vars, t]
{Cos[t] + Sin[t], -Cos[t] + Sin[t]}

ParametricPlot[{xs[t], ys[t]}, {t, 0, 2 π}, Frame → True]
```




```
Solve[x'[t] == -3 x[t] /. x → (Exp[λ #] &), λ]
{{λ → -3}}
```

Worked Problem

1. Find the energy eigenstates of the Hamiltonian $H = E_0 \begin{bmatrix} 1 & 0 & -i \\ 0 & 1 & 0 \\ i & 0 & 1 \end{bmatrix}$.

$$H|E\rangle = E|E\rangle \Rightarrow (H - EI)|E\rangle = 0 \ \&\ |E\rangle \neq 0 \Rightarrow$$

$$0 = \det[H - EI] = \begin{vmatrix} E_0 - E & 0 & -iE_0 \\ 0 & E_0 - E & 0 \\ iE_0 & 0 & E_0 - E \end{vmatrix}$$

$$= +(E_0 - E)\begin{vmatrix} E_0 - E & -iE_0 \\ iE_0 & E_0 - E \end{vmatrix}$$

$$= (E_0 - E)\big((E_0 - E)^2 - E_0^2\big) = (E_0 - E)(-2E_0 + E)E$$

$$\Rightarrow E = 0, E_0, 2E_0$$

$$(H - EI)|E\rangle = \begin{bmatrix} E_0 - E & 0 & -iE_0 \\ 0 & E_0 - E & 0 \\ iE_0 & 0 & E_0 - E \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$(H - 0I)|0\rangle = \begin{bmatrix} E_0 & 0 & -iE_0 \\ 0 & E_0 & 0 \\ iE_0 & 0 & E_0 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{aligned} +x \quad\quad - iz &= 0 \\ +y \quad\quad &= 0 \\ +ix \quad\quad + z &= 0 \end{aligned}$$

$$\Rightarrow |0\rangle = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = N_0\begin{bmatrix} i \\ 0 \\ 1 \end{bmatrix} \Rightarrow \langle 0| = |0\rangle^\dagger = \begin{bmatrix} -i & 0 & 1 \end{bmatrix} N_0^*$$

$$1 = \langle 0|0\rangle = N_0(-i^2 + 1)N_0^* = 2\,|N_0|^2 \Leftarrow N_0 = \frac{1}{\sqrt{2}}$$

$$(H - E_0 I)|1\rangle = \begin{bmatrix} 0 & 0 & -iE_0 \\ 0 & 0 & 0 \\ iE_0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{aligned} &&-z &= 0 \\ &0 & &= 0 \\ +x &&&= 0 \end{aligned}$$

$$\Rightarrow |1\rangle = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$(H - 2E_0 I)|2\rangle = \begin{bmatrix} -E_0 & 0 & -iE_0 \\ 0 & -E_0 & 0 \\ iE_0 & 0 & -E_0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{aligned} -x && -iz &= 0 \\ & -y & &= 0 \\ +ix && -z &= 0 \end{aligned}$$

$$\Rightarrow |2\rangle = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = N_2 \begin{bmatrix} -i \\ 0 \\ 1 \end{bmatrix} \Rightarrow \ \langle 2| = |2\rangle^\dagger = \begin{bmatrix} i & 0 & 1 \end{bmatrix} N_2^*$$

$$1 = \langle 2|2\rangle = N_2(-i^2 + 1)N_2^* = 2\,|N_2|^2 \Leftarrow N_2 = \frac{1}{\sqrt{2}}$$

$$|0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} i \\ 0 \\ 1 \end{bmatrix}, \ |1\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \ |2\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} -i \\ 0 \\ 1 \end{bmatrix}$$

$$\langle 0|2\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} -i & 0 & 1 \end{bmatrix} \begin{bmatrix} -i \\ 0 \\ 1 \end{bmatrix} \frac{1}{\sqrt{2}} = \frac{i^2 + 1}{2} = 0$$

Problems

1. Model a linear system of three points of mass m connected to each other and two walls by four springs of stiffness s.

   (a) Find the normal mode frequencies.

   (b) Find the normal mode shapes, and interpret them graphically.

2. Model a linear system of three points of mass m connected to each other by springs of stiffness s.

   (a) Find the normal mode frequencies.

   (b) Find the normal mode shapes, and interpret them graphically.

3. Model a 3-state quantum system by the Hamiltonian

$$H = E_0 \begin{bmatrix} 3 & 2 & 0 \\ 2 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{5.59}$$

   (a) Find the allowed energies.

   (b) Find the stationary states.

   (c) If the system is initially in the state

$$|\psi\rangle = |\psi_0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \tag{5.60}$$

   what is its state $|\Psi\rangle = |\psi_t\rangle$ at a later time?

Chapter 6

Fourier Analysis

Inspired by normal modes or eigenstates, introduce Fourier analysis and synthesis of functions, as in Fig. 6.1, in analogy with decomposing a vector into components or constructing a vector from components.

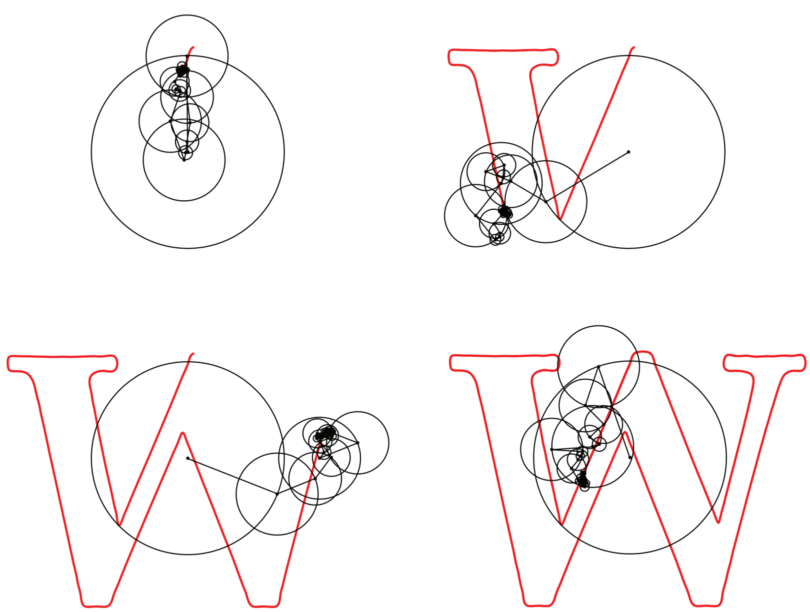


Figure 6.1: The Wooster W traced out by epicycles of 100 circles-moving-on-circles in the complex plane. Algebraically, the trace is a complex discrete Fourier series $\sum c_n e^{in\varphi} = \sum r_n e^{i(n\varphi+\theta_n)}$, where r_n are the circle radii.

6.1 Finite Basis

Consider a finite set of basis vectors

$$\{\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_N\}. \tag{6.1}$$

Assume a scalar product

$$\vec{u} \cdot \vec{v} = \sum_{n=1}^{N} u_n v_n \tag{6.2}$$

under which the basis vectors are orthonormal so that

$$\hat{x}_m \cdot \hat{x}_n = \delta_{mn}, \tag{6.3}$$

where the **Kronecker delta**

$$\delta_{mn} = \left\{ \begin{array}{ll} 1, & m = n \\ 0, & m \neq n \end{array} \right\}. \tag{6.4}$$

Any vector $\vec{v}$ is a linear combination of the basis vectors

$$\vec{v} = \sum_{n=0}^{N} \hat{x}_n v_n \tag{6.5}$$

because the coefficients can be liberated by the projection

$$\begin{aligned} \hat{x}_m \cdot \vec{v} &= \hat{x}_m \cdot \left(\sum_{n=0}^{N} \hat{x}_n v_n \right) \\ &= \sum_{n=0}^{N} \hat{x}_m \cdot \hat{x}_n v_n \\ &= \sum_{n=0}^{N} \delta_{mn} v_n \\ &= 0 + 0 + \cdots + 0 + 1\, v_m + 0 + \cdots + 0 \\ &= v_m. \end{aligned} \tag{6.6}$$

Hence,

$$v_n = \hat{x}_n \cdot \vec{v} \tag{6.7}$$

with

$$\vec{v} = \sum_{n=0}^{N} \hat{x}_n v_n. \tag{6.8}$$

6.2 Countable Basis

The countable normal mode shapes of a string fixed at two ends a distance L apart are the sinusoids

$$N_n = N \sin k_n x, \tag{6.9}$$

where the normalization $N = \sqrt{2/L}$ and the spatial frequency $k_n = 2\pi/\lambda_n = n\pi/L$, or

$$N_n[x] = \sqrt{\frac{2}{L}} \sin\left[n\pi\frac{x}{L}\right], \tag{6.10}$$

and the index n is a natural number. Treating a continuous function with values $f[x]$ as a generalization of a discrete vector with components v_n, assume a scalar product

$$\langle f|g\rangle = \int_0^L dx\, f[x]g[x] = \int_0^L f[x]g[x]\, dx \tag{6.11}$$

under which the normal modes are orthonormal as

$$\begin{aligned}
\langle N_m|N_n\rangle = \langle m|n\rangle &= \int_0^L dx\ (N\sin k_m x)(N\sin k_n x) \\
&= N^2 \int_0^L dx\ \sin\left[m\pi\frac{x}{L}\right]\sin\left[n\pi\frac{x}{L}\right] \\
&= N^2\frac{L}{\pi}\int_0^\pi d\theta\ \sin m\theta \sin n\theta \\
&= \frac{2}{L}\frac{L}{\pi}\int_0^\pi d\theta\ \frac{1}{2}\big(\cos(m-n)\theta - \cos(m+n)\theta\big) \\
&= \frac{1}{\pi}\left(\frac{\sin(m-n)\theta}{m-n} - \frac{\sin(m+n)\theta}{m+n}\right)\Bigg|_0^\pi \\
&= \delta_{mn},
\end{aligned} \tag{6.12}$$

because $\sin p\theta \sim p\theta$ as $p \to 0$ for the $m = n$ case, and graphically as in Fig. 6.2.

Any string shape $f[x]$ is a discrete linear combination of the normal mode shapes

$$f[x] = \sum_{n=1}^{\infty} N_n[x] f_n \tag{6.13}$$

or

$$|f\rangle = \sum_{n=1}^{\infty} |n\rangle f_n \tag{6.14}$$

because the coefficients can be liberated by the projection

$$\begin{aligned}
\langle m|f\rangle &= \langle m|\sum_{n=1}^{\infty}|n\rangle f_n \\
&= \sum_{n=1}^{\infty}\langle m|n\rangle f_n
\end{aligned}$$

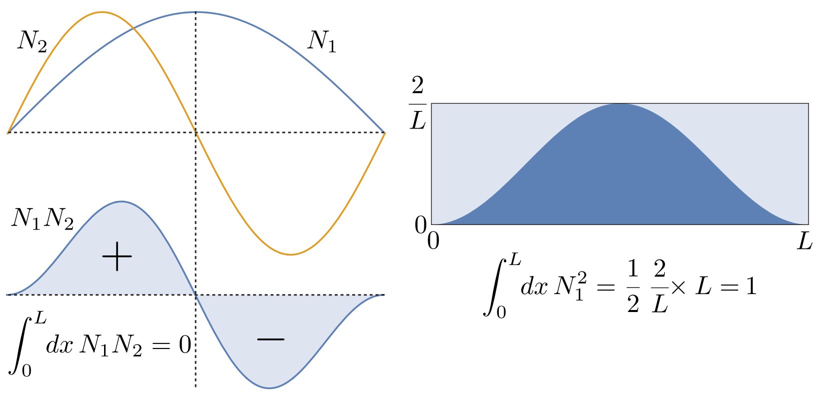


Figure 6.2: Sine modes for a string with fixed ends are orthonormal as plots of the first two modes suggest.

$$
\begin{aligned}
&= \sum_{n=1}^{\infty} \delta_{mn} f_n \\
&= 0 + \cdots + 0 + 1\, f_m + 0 + \cdots \\
&= f_m
\end{aligned} \tag{6.15}
$$

or equivalently

$$
\begin{aligned}
f_n &= \langle n|f\rangle \\
&= \int_0^L dx\, N_n[x] f[x] \\
&= \sqrt{\frac{2}{L}} \int_0^L dx\, \sin\left[n\pi \frac{x}{L}\right] f[x]
\end{aligned} \tag{6.16}
$$

so that

$$
|f\rangle = \sum_{n=1}^{\infty} |n\rangle\langle n|f\rangle \tag{6.17}
$$

or

$$
\langle x|f\rangle = \sum_{n=1}^{\infty} \langle x|n\rangle\langle n|f\rangle, \tag{6.18}
$$

which means

$$
f[x] = \sum_{n=1}^{\infty} N_n[x] f_n. \tag{6.19}
$$

The classic [5] **Fourier sine series**

$$
f[x] = \sum_{n=1}^{\infty} \sqrt{\frac{2}{L}} \sin\left[n\pi \frac{x}{L}\right] f_n \tag{6.20}
$$

with **Fourier coefficients**

$$f_n = \int_0^L dx\, \sqrt{\frac{2}{L}} \sin\left[n\pi \frac{x}{L}\right] f[x]. \tag{6.21}$$

6.3 Uncountable Basis

Because their frequencies are multiples of a fundamental frequency, the Eq. 6.9 sinusoidal finite space normal modes can synthesize any periodic function (or a finite portion of any nonperiodic function). As a generalization to overcome these limitations, take the **infinite** space normal modes to be the **complex** sinusoids

$$E[k,x] = \frac{1}{\sqrt{2\pi}} e^{-ikx} = \frac{1}{\sqrt{2\pi}} \cos kx - \frac{1}{\sqrt{2\pi}} i \sin kx, \tag{6.22}$$

where the index k is a real number. Assume a complex scalar product

$$\langle f|g\rangle = \int_0^L dx\, f[x]^* g[x] \tag{6.23}$$

for which the normal modes are orthonormal, as

$$\begin{aligned}
\langle E[k,x]|E[k',x]\rangle = \langle k|k'\rangle &= \int_{-\infty}^{\infty} dx\, E[k,x]^* E[k',x] \\
&= \int_{-\infty}^{\infty} dx\, \frac{1}{\sqrt{2\pi}} e^{+ikx} \frac{1}{\sqrt{2\pi}} e^{-ik'x} \\
&= \int_{-\infty}^{\infty} dx\, \frac{1}{2\pi} e^{i(k-k')x} \\
&= \frac{1}{2\pi} \lim_{\Lambda\to\infty} \int_{-\infty}^{\infty} dx\, e^{-x^2/4\Lambda} e^{i(k-k')x} \\
&= \frac{1}{2\pi} \lim_{\Lambda\to\infty} \int_{-\infty}^{\infty} dx\, e^{-\left(x-i2(k-k')\Lambda\right)^2/4\Lambda}\, e^{-4(k-k')^2\Lambda^2/4\Lambda} \\
&= \frac{1}{2\pi} \lim_{\Lambda\to\infty} e^{-(k-k')^2\Lambda} \int_{-\infty}^{\infty} dy\, e^{-y^2/4\Lambda} \\
&= \frac{1}{2\pi} \lim_{\Lambda\to\infty} e^{-(k-k')^2\Lambda} \sqrt{4\Lambda} \int_{-\infty}^{\infty} dz\, e^{-z^2} \\
&= \frac{1}{2\pi} \lim_{\Lambda\to\infty} e^{-(k-k')^2\Lambda} \sqrt{4\Lambda}\, \sqrt{\pi} \\
&= \lim_{\Lambda\to\infty} \sqrt{\frac{\Lambda}{\pi}} e^{-\Lambda(k-k')^2} \\
&= \lim_{\Lambda\to\infty} \delta_\Lambda[k-k'] \\
&= \delta[k-k'],
\end{aligned} \tag{6.24}$$

where the insertion of the integrating convergence factor $e^{-x^2/4\Lambda}$ produces the famous Gaussian integral

$$\begin{aligned}\left(\int_{-\infty}^{\infty} dz\, e^{-z^2}\right)^2 &= \left(\int_{-\infty}^{\infty} dz\, e^{-z^2}\right)\left(\int_{-\infty}^{\infty} dz\, e^{-z^2}\right) \\ &= \left(\int_{-\infty}^{\infty} dx\, e^{-x^2}\right)\left(\int_{-\infty}^{\infty} dy\, e^{-y^2}\right) \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\, dy\ e^{-(x^2+y^2)} \\ &= \int_{0}^{2\pi}\int_{0}^{\infty} r dr\, d\theta\ e^{-r^2} \\ &= 2\pi\left(-\frac{1}{2}e^{-r^2}\right)\Big|_0^{\infty} \\ &= \pi, \end{aligned} \tag{6.25}$$

and also creates a representation of the **Dirac delta**, as in Fig. 6.3. The Dirac delta generalizes the Eq. 6.4 Kronecker delta from discrete indices to continuous indices. It can be understood heuristically as the limit of an infinitely high but infinitely narrow bump or spike

$$\delta[k-k'] = \left\{\begin{array}{ll} \infty, & k = k' \\ 0, & k \neq k' \end{array}\right\} \tag{6.26}$$

bounding a finite area

$$1 = \int_{-\infty}^{\infty} dk\, \delta[k-k'] \tag{6.27}$$

with the **sifting property**

$$\int dx\, f[x]\delta[x-a] = \int dx\, f[a]\delta[x-a] = f[a]\int dx\, \delta[x-a] = f[a]. \tag{6.28}$$

Any shape $f[x]$ is a continuous linear combination of the normal modes

$$f[x] = \int_{-\infty}^{\infty} dk\, E[k,x]\tilde{f}[k] \tag{6.29}$$

or

$$|f\rangle = \int_{-\infty}^{\infty} dk\, |k\rangle\tilde{f}[k] \tag{6.30}$$

because the coefficients can be liberated by the projection

$$\begin{aligned}\langle k'|f\rangle &= \langle k'|\int_{-\infty}^{\infty} dk\, |k\rangle\tilde{f}[k] \\ &= \int_{-\infty}^{\infty} dk\, \langle k'|k\rangle\tilde{f}[k]\end{aligned}$$

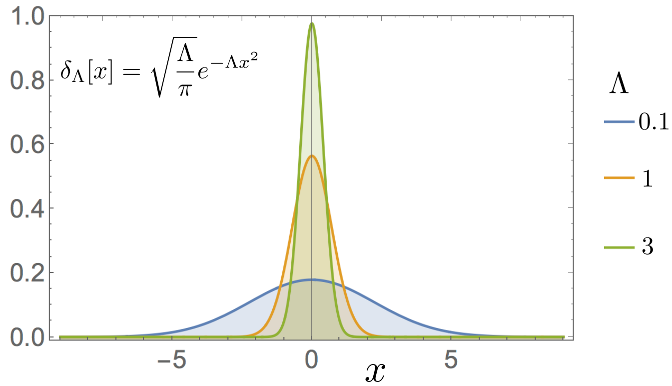


Figure 6.3: The Dirac delta can be represented as the limit of an infinitely high but infinitely narrow Gaussian of unit area, $\delta[x] = \lim_{\Lambda\to\infty} \delta_\Lambda[x]$.

$$\begin{aligned} &= \int_{-\infty}^{\infty} dk\, \delta[k-k']\tilde{f}[k] \\ &= \tilde{f}[k'] \end{aligned} \tag{6.31}$$

or equivalently

$$\begin{aligned} \tilde{f}[k] &= \langle k|f\rangle \\ &= \int_{-\infty}^{\infty} dx\, E[k,x]^* f[x] \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{+ikx} f[x] \end{aligned} \tag{6.32}$$

so that

$$|f\rangle = \int_{-\infty}^{\infty} dk\, |k\rangle\langle k|f\rangle \tag{6.33}$$

or

$$\langle x|f\rangle = \int_{-\infty}^{\infty} dk\, \langle x|k\rangle\langle k|f\rangle, \tag{6.34}$$

which means

$$f[x] = \int_{-\infty}^{\infty} dk\, E[k,x]\tilde{f}[k]. \tag{6.35}$$

Thus, the classic **Fourier transform**

$$\tilde{f}[k] = \int_{-\infty}^{\infty} dx\, \frac{1}{\sqrt{2\pi}} e^{+ikx} f[x] \tag{6.36}$$

with the inverse transform

$$f[x] = \int_{-\infty}^{\infty} dk\, \frac{1}{\sqrt{2\pi}} e^{-ikx} \tilde{f}[k]. \tag{6.37}$$

6.4 Examples & Properties

The "Big 4" Fourier examples illustrate generic properties.

6.4.1 Square-Wave Fourier Series

Using Eq. 6.20 and Eq. 6.21, the Fourier series of the Fig. 6.4 **on-off** or **square wave** function

$$s_{a,L}[x] = a\,\mathrm{sgn}\left[\sin\left[2\pi\frac{x}{L}\right]\right], \tag{6.38}$$

of amplitude a and wavelength L, where the **signum** function $\mathrm{sgn}[x] = x/|x|$ gives the sign of a number, is

$$\begin{aligned} s_{a,L}[x] &= \frac{4}{\pi}a\sum_{n=1}^{\infty} -\frac{2}{n}\cos\left[n\frac{\pi}{2}\right]\sin^2\left[n\frac{\pi}{4}\right]\sin\left[n\,\pi\frac{x}{L}\right] \\ &= \frac{4}{\pi}a\sum_{m=1}^{\infty}\frac{2}{4m-2}\sin\left[(4m-2)\,\pi\frac{x}{L}\right] \\ &= \frac{4}{\pi}a\sum_{\ell\text{ odd}}\frac{1}{\ell}\sin\left[\ell\,2\pi\frac{x}{L}\right] \end{aligned} \tag{6.39}$$

or

$$s_{a,L}[x] = \frac{4}{\pi}a\left(\sin\left[2\pi\frac{x}{L}\right] + \frac{1}{3}\sin\left[6\pi\frac{x}{L}\right] + \frac{1}{5}\sin\left[10\pi\frac{x}{L}\right] + \frac{1}{7}\sin\left[14\pi\frac{x}{L}\right] + \cdots\right), \tag{6.40}$$

where the coefficients are inversely proportional to the odd natural numbers. In particular, the Fourier series of the square wave

$$s_{1,2\pi}[x] = \mathrm{sgn}\left[\sin x\right] \tag{6.41}$$

of unit amplitude and 2π wavelength is

$$s_{1,2\pi}[x] = \frac{4}{\pi}\left(\sin x + \frac{1}{3}\sin 3x + \frac{1}{5}\sin 5x + \frac{1}{7}\sin 7x + \cdots\right), \tag{6.42}$$

where $4/\pi \approx 1.27$, so the fundamental term slightly overlaps the square wave.

Jump discontinuities cause slight $\sim 9\%$ overshoots in the final Fourier synthesis. In practice, one might be interested only in a single wavelength, like the string of length L, but because the frequencies of all the **harmonics**, the **fundamental** and all the **overtones**, are multiples of the first harmonic, the pattern repeats infinitely in both directions. If the initial function has a nonzero mean, subtract it before Fourier analyzing, as all the sines have zero mean. If the function is **antisymmetric** or **odd** (rather than **symmetric** and **even**) with respect to the origin, use a cosine series instead. If the function has no symmetry, use a combined sine and cosine series.

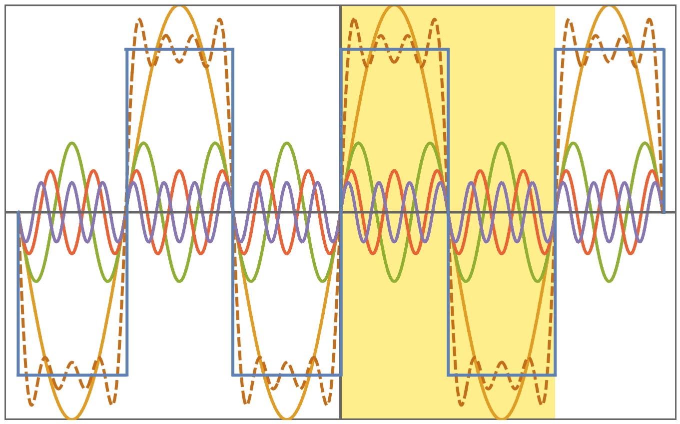


Figure 6.4: First few terms or harmonics (smooth curves) in the Fourier sine series of a square wave (piecewise linear curve) and their sum (dashed curve). Jump discontinuities cause slight $\sim 9\%$ overshoots in the final Fourier synthesis.

6.4.2 Sawtooth Fourier Series

Using Eq. 6.20 and Eq. 6.21, the Fourier series of the Fig. 6.5 **ramp** or **sawtooth** function

$$w_{a,L}[x] = 2a\left(\frac{x}{L} - \left\lfloor \frac{x}{L} \right\rfloor - \frac{1}{2}\right), \tag{6.43}$$

of amplitude a and wavelength L, where the **floor** function $\lfloor x \rfloor$ maps a real number to the greatest preceding integer, is

$$\begin{aligned} w_{a,L}[x] &= \frac{2}{\pi} a \sum_{n=1}^{\infty} -\frac{2}{n} \cos\left[n\frac{\pi}{2}\right] \sin\left[n\,\pi\frac{x}{L}\right] \\ &= \frac{2}{\pi} a \sum_{m=1}^{\infty} \frac{-2(-1)^m}{2m} \sin\left[2m\,\pi\frac{x}{L}\right] \\ &= \frac{2}{\pi} a \sum_{\ell \text{ even}} \frac{(-1)^{\ell/2+1}}{\ell/2} \sin\left[\ell\,\pi\frac{x}{L}\right] \end{aligned} \tag{6.44}$$

or

$$\begin{aligned} w_{a,L}[x] = \frac{2}{\pi} a \Bigg(& \sin\left[2\pi\frac{x}{L}\right] - \frac{1}{2}\sin\left[4\pi\frac{x}{L}\right] \\ & + \frac{1}{3}\sin\left[6\pi\frac{x}{L}\right] - \frac{1}{4}\sin\left[8\pi\frac{x}{L}\right] \\ & + \frac{1}{5}\sin\left[10\pi\frac{x}{L}\right] - \frac{1}{6}\sin\left[12\pi\frac{x}{L}\right] \\ & + \frac{1}{7}\sin\left[14\pi\frac{x}{L}\right] - \frac{1}{8}\sin\left[16\pi\frac{x}{L}\right] + \cdots \Bigg), \end{aligned} \tag{6.45}$$

where the signs alternate. In particular, the Fourier series of the sawtooth

$$w_{1,2\pi}[x] = 2\left(\frac{x}{2\pi} - \left\lfloor \frac{x}{2\pi} \right\rfloor - \frac{1}{2}\right), \tag{6.46}$$

of unit amplitude and 2π wavelength is

$$\begin{aligned} w_{1,2\pi}[x] = \frac{2}{\pi}\Bigg(& \sin x - \frac{1}{2}\sin 2x \\ & + \frac{1}{3}\sin 3x - \frac{1}{4}\sin 4x \\ & + \frac{1}{5}\sin 5x - \frac{1}{6}\sin 6x \\ & + \frac{1}{7}\sin 7x - \frac{1}{8}\sin 8x + \cdots \Bigg), \end{aligned} \tag{6.47}$$

where $2/\pi \approx 0.637$, so the fundamental term fits snuggly inside the sawtooth.

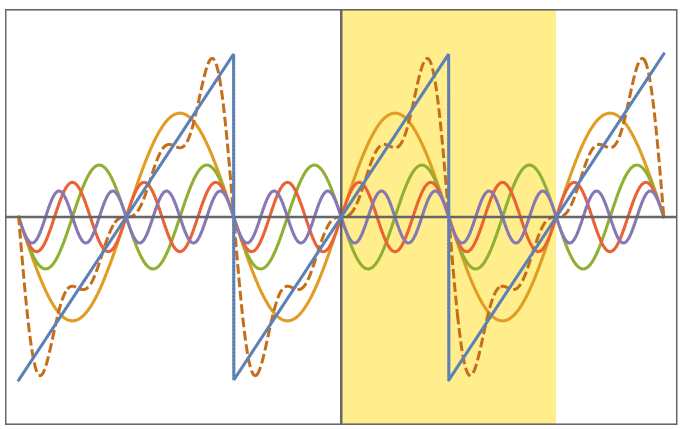


Figure 6.5: First few terms or harmonics (smooth curves) in the Fourier sine series of a sawtooth (piecewise linear curve) and their sum (dashed curve).

6.4.3 Gaussian Transform

Using Eq. 6.36, the Fourier transform of a **normal** or **Gaussian** function

$$g_{\mu,\sigma}[x] = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/(2\sigma^2)} \tag{6.48}$$

of center or mean μ and width or standard deviation σ is the Gaussian

$$\tilde{g}_{\mu,\sigma}[k] = \frac{1}{\sqrt{2\pi}} e^{-k^2\sigma^2/2} e^{-ik\mu}$$

$$= \tilde{\sigma}\frac{1}{\sqrt{2\pi\tilde{\sigma}^2}}e^{-(k-\tilde{\mu})^2/(2\tilde{\sigma}^2)}e^{-ik\mu} \tag{6.49}$$

of width $\tilde{\sigma} = 1/\sigma$ and mean $\tilde{\mu} = 0$ multiplied by a complex phase factor, as in Fig. 6.6. In particular, the Fourier transform of a Gaussian

$$g_{0,1}[x] = \frac{1}{\sqrt{2\pi}}e^{-x^2/2} \tag{6.50}$$

of unit width and zero mean is the Gaussian

$$\tilde{g}_{0,1}[k] = \frac{1}{\sqrt{2\pi}}e^{-k^2/2} \tag{6.51}$$

of unit width and zero mean. The latter is the **frequency spectrum** of the former.

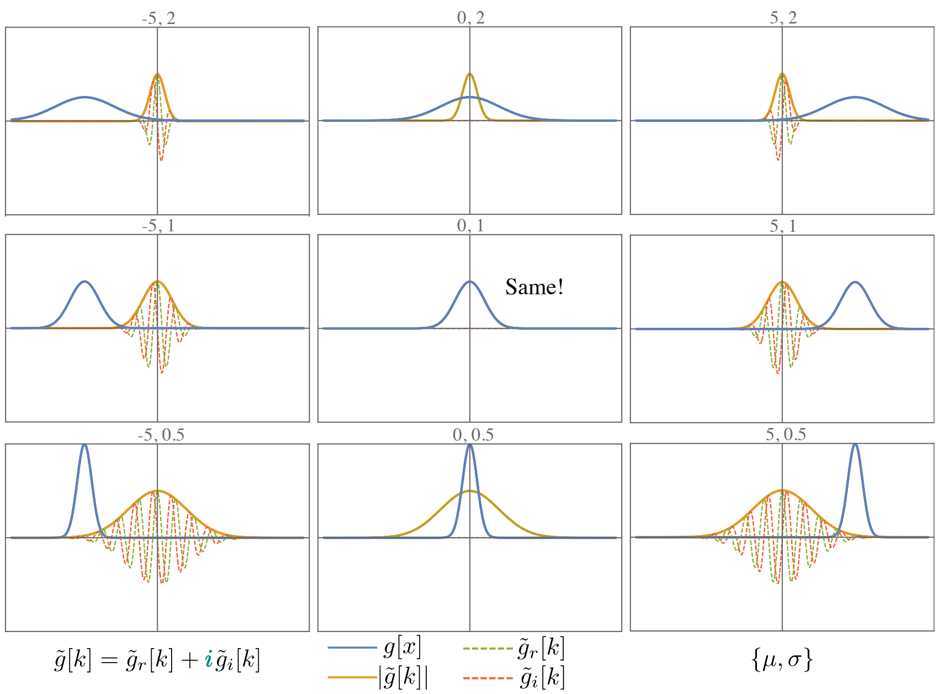


Figure 6.6: Fourier transform of a normalized (real) Gaussian with mean μ and width σ is another (complex) Gaussian. Widths are inversely related and the absolute squares of the areas are the same.

The inverse relation between the widths of the Gaussians in position and frequency space

$$\sigma\tilde{\sigma} = 1 \tag{6.52}$$

is the **bandwidth theorem** or the **uncertainty principle** and is a generic feature of the Fourier transform. The inverse relation between the heights of the Gaussians in position and frequency space implies

$$\int_{-\infty}^{\infty} dx\, g[x]^* g[x] = \int_{-\infty}^{\infty} dk\, \tilde{g}[k]^* \tilde{g}[k], \tag{6.53}$$

which is the **Plancherel** or **Parseval theorem** and expresses the unitarity of the Fourier transform. More abstractly,

$$\int dx\, \langle g|x\rangle\langle x|g\rangle = \int dk\, \langle \tilde{g}|k\rangle\langle k|\tilde{g}\rangle \tag{6.54}$$

as

$$\langle g|g\rangle = \langle \tilde{g}|\tilde{g}\rangle \tag{6.55}$$

because of the **completeness relations**

$$\int dx\, |x\rangle\langle x| = \int dk\, |k\rangle\langle k| = I, \tag{6.56}$$

where $P_x = |x\rangle\langle x|$ is the **projector** onto x, with $P_x|x\rangle = |x\rangle$ and $P_x^2 = P_x$, and I is the identity.

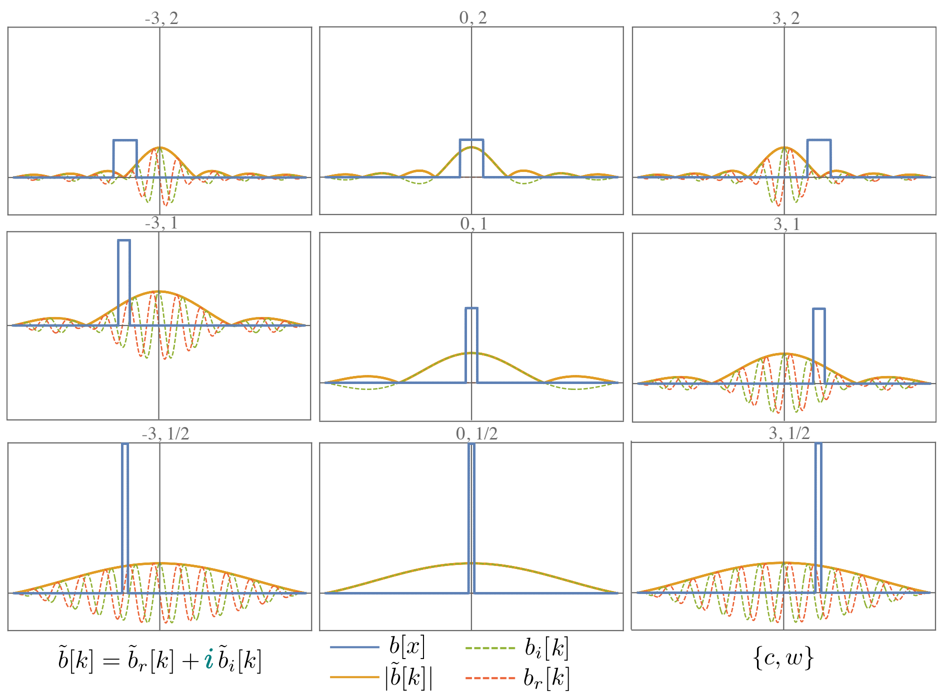


Figure 6.7: Fourier transform of a normalized boxcar with mean c and width w is a sinc. Widths are inversely related and the absolute squares of the areas are the same.

6.4.4 Boxcar Transform

Using Eq. 6.36, the Fourier transform of a **top-hat** or **boxcar** function

$$b_{c,w}[x] = \left\{ \begin{array}{ll} 1/w, & c - w/2 < x < c + w/2 \\ 0, & \text{else} \end{array} \right\} \tag{6.57}$$

of center or mean c and width w is the sinc function

$$\begin{aligned} \tilde{b}_{c,w}[k] &= \frac{1}{\sqrt{2\pi}} e^{ikc} \frac{\sin[kw/2]}{kw/2} \\ &= \frac{1}{\sqrt{2\pi}} e^{ikc} \operatorname{sinc}\left[\frac{kw}{2}\right] \end{aligned} \tag{6.58}$$

multiplied by a complex phase factor, as in Fig. 6.7. In particular, the Fourier transform of a boxcar

$$b_{0,1}[x] = \left\{ \begin{array}{ll} 1, & -1/2 < x < 1/2 \\ 0, & \text{else} \end{array} \right\} \tag{6.59}$$

of zero center and unit width is the **sinc** function

$$\tilde{b}_{0,1}[k] = \frac{1}{\sqrt{2\pi}} \operatorname{sinc}\left[\frac{k}{2}\right]. \tag{6.60}$$

The latter is the **frequency spectrum** of the former, the square of which is the familiar as the far-field irradiance pattern of light incident on a narrow slit.

6.5 DFT & FFT

The **Discrete Fourier Transform (DFT)** of the sequence $\{x_0, x_1, \ldots, x_{N-1}\}$ is the linear transformation

$$\tilde{x}_m = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} x_n e^{i2\pi mn/N} = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \left(e^{i2\pi/N}\right)^{mn} x_n = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \omega_N^{mn} x_n, \tag{6.61}$$

where $m \in \{0, 1, \ldots, N-1\}$. The Nth roots of unity or **twiddle factors**

$$\omega_N = e^{i2\pi/N} \tag{6.62}$$

satisfy

$$\omega_N^2 = \omega_{N/2}, \tag{6.63a}$$

$$\omega_N^{N/2} = -1, \tag{6.63b}$$

$$\omega_N^N = 1. \tag{6.63c}$$

For $N = 1$, the DFT transformation is the identity

$$\tilde{x}_0 = x_1. \tag{6.64}$$

For $N = 2$, the DFT is the additive mixing

$$\sqrt{2}\,\tilde{x}_0 = x_0 + x_1 = x_0 + x_1, \tag{6.65a}$$

$$\sqrt{2}\,\tilde{x}_1 = x_0 + \omega_2 x_1 = x_0 - x_1 \tag{6.65b}$$

and involves no multiplications because $\omega_2 = e^{i\pi} = -1$. As a matrix equation,

$$\begin{bmatrix} \tilde{x}_0 \\ \tilde{x}_1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & \omega_2 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = F_2 \begin{bmatrix} x_0 \\ x_1 \end{bmatrix}, \tag{6.66}$$

where the Fourier matrix

$$F_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & \omega_2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{6.67}$$

For $N = 2^2 = 4$, the DFT

$$2\tilde{x}_0 = x_0 + x_1 + x_2 + x_3, \tag{6.68a}$$

$$2\tilde{x}_1 = x_0 + \omega_4 x_1 + \omega_4^2 x_2 + \omega_4^3 x_3, \tag{6.68b}$$

$$2\tilde{x}_2 = x_0 + \omega_4^2 x_1 + \omega_4^4 x_2 + \omega_4^6 x_3, \tag{6.68c}$$

$$2\tilde{x}_3 = x_0 + \omega_4^3 x_1 + \omega_4^6 x_2 + \omega_4^9 x_3, \tag{6.68d}$$

and the twiddle factor $\omega_4 = e^{i\pi/2} = i$. As a matrix equation,

$$\begin{bmatrix} \tilde{x}_0 \\ \tilde{x}_1 \\ \tilde{x}_2 \\ \tilde{x}_3 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega_4 & \omega_4^2 & \omega_4^3 \\ 1 & \omega_4^2 & \omega_4^4 & \omega_4^6 \\ 1 & \omega_4^3 & \omega_4^6 & \omega_4^9 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} = F_4 \begin{bmatrix} x_0 \\ \tilde{x}_1 \\ x_2 \\ x_3 \end{bmatrix}, \tag{6.69}$$

where the Fourier matrix

$$F_4 = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega_4 & \omega_4^2 & \omega_4^3 \\ 1 & \omega_4^2 & \omega_4^4 & \omega_4^6 \\ 1 & \omega_4^3 & \omega_4^6 & \omega_4^9 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega_4 & \omega_2 & \omega_2\omega_4 \\ 1 & -1 & 1 & -1 \\ 1 & -\omega_4 & \omega_2 & -\omega_2\omega_4 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{bmatrix}. \tag{6.70}$$

Factor the Fourier matrix by writing

$$
\begin{aligned}
F_4 &= \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega_4^2 & \omega_4 & \omega_4^3 \\ 1 & \omega_4^4 & \omega_4^2 & \omega_4^6 \\ 1 & \omega_4^6 & \omega_4^3 & \omega_4^9 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \\
&= \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega_2 & \omega_4 & \omega_2\omega_4 \\ 1 & 1 & -1 & -1 \\ 1 & \omega_2 & -\omega_4 & -\omega_2\omega_4 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \\
&= \frac{1}{2}\left[\begin{array}{cc|cc} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & \omega_4 \\ \hline 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -\omega_4 \end{array}\right]\left[\begin{array}{cc|cc} 1 & 1 & 0 & 0 \\ 1 & \omega_2 & 0 & 0 \\ \hline 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & \omega_2 \end{array}\right]\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \\
&= \frac{1}{\sqrt{2}}\begin{bmatrix} I_2 & D_4 \\ I_2 & -D_4 \end{bmatrix}\begin{bmatrix} F_2 & 0 \\ 0 & F_2 \end{bmatrix} P_4^T,
\end{aligned}
\tag{6.71}
$$

and check by multiplying. The permutation matrix

$$
P_4 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}
\tag{6.72}
$$

puts all the Fourier matrix even index columns before the odd index columns. The permutation matrix is orthogonal. For example,

$$
P_4\, P_4^T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = I_4,
\tag{6.73}
$$

and generically $P^{-1} = P^T$.

The Fourier matrix is unitary. For example,

$$F_4 F_4^\dagger = \frac{1}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = I_4 \tag{6.74}$$

and generically $F^{-1} = F^\dagger$, which greatly facilitates inverting the transform. Since

$$F_4^{-1} = F_4^\dagger = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega_4 & \omega_4^2 & \omega_4^3 \\ 1 & \omega_4^2 & \omega_4^4 & \omega_4^6 \\ 1 & \omega_4^3 & \omega_4^6 & \omega_4^9 \end{bmatrix}^\dagger = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega_4^* & \omega_4^{*2} & \omega_4^{*3} \\ 1 & \omega_4^{*2} & \omega_4^{*4} & \omega_4^{*6} \\ 1 & \omega_4^{*3} & \omega_4^{*6} & \omega_4^{*9} \end{bmatrix}, \tag{6.75}$$

the Eq. 6.61 DFT transform inverts to the nearly identical

$$x_m = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \omega_N^{*mn} \tilde{x}_n = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \tilde{x}_n e^{-i 2\pi mn/N}. \tag{6.76}$$

The square of the Fourier matrix is another permutation matrix

$$F_4 F_4 = \frac{1}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, \tag{6.77}$$

and the square of the square of the permutation matrix is the identity matrix

$$F_4^4 = F_4^2 F_4^2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = I_4. \tag{6.78}$$

Since $F^4 = I$, $\det F^4 = (\det F)^4 = 1$, which implies that the Fourier matrix eigenvalues and determinant are fourth roots of unit $\{\pm 1, \pm i\}$.

The Eq. 6.71 factorization of the Fourier matrix expresses F_4 in terms of F_2, and the latter involves no multiplications (other than normalization). The general **block matrix** result

$$F_N = \frac{1}{\sqrt{2}} \boxed{\begin{matrix} I_{N/2} & D_N \\ I_{N/2} & -D_N \end{matrix}} \boxed{\begin{matrix} F_{N/2} & 0 \\ 0 & F_{N/2} \end{matrix}} P_N^T \tag{6.79}$$

is the core of the **Fast Fourier Transform** algorithm, one of the most famous and important algorithms in computer science. Applied recursively, it can reduce the number of required complex multiplications from order N^2 to order $\frac{1}{2} N \log_2 N$, which is a huge reduction for large transforms.

6.6 Fourier Transform Variations

Simple change of variables shuffles the Eq. 6.36 Fourier Transform normalization constant $1/\sqrt{2\pi}$. For example

$$f[x] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, e^{-ikx} \tilde{f}[k], \tag{6.80a}$$

$$\tilde{f}[k] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{+ikx} f[x], \tag{6.80b}$$

or

$$f[x] = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{-ikx} \tilde{f}[k], \tag{6.81a}$$

$$\tilde{f}[k] = \int_{-\infty}^{\infty} dx\, e^{+ikx} f[x], \tag{6.81b}$$

or

$$f[x] = \int_{-\infty}^{\infty} dk\, e^{-ikx} \tilde{f}[k], \tag{6.82a}$$

$$\tilde{f}[k] = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx\, e^{+ikx} f[x], \tag{6.82b}$$

or

$$f[x] = \int_{-\infty}^{\infty} dk\, e^{-i2\pi kx} \tilde{f}[k], \tag{6.83a}$$

$$\tilde{f}[k] = \int_{-\infty}^{\infty} dx\, e^{+i2\pi kx} f[x], \tag{6.83b}$$

and can also interchange the exponent sign. Higher-dimensional Fourier transforms like those in Fig. 6.8 are widely used in imaging processing.

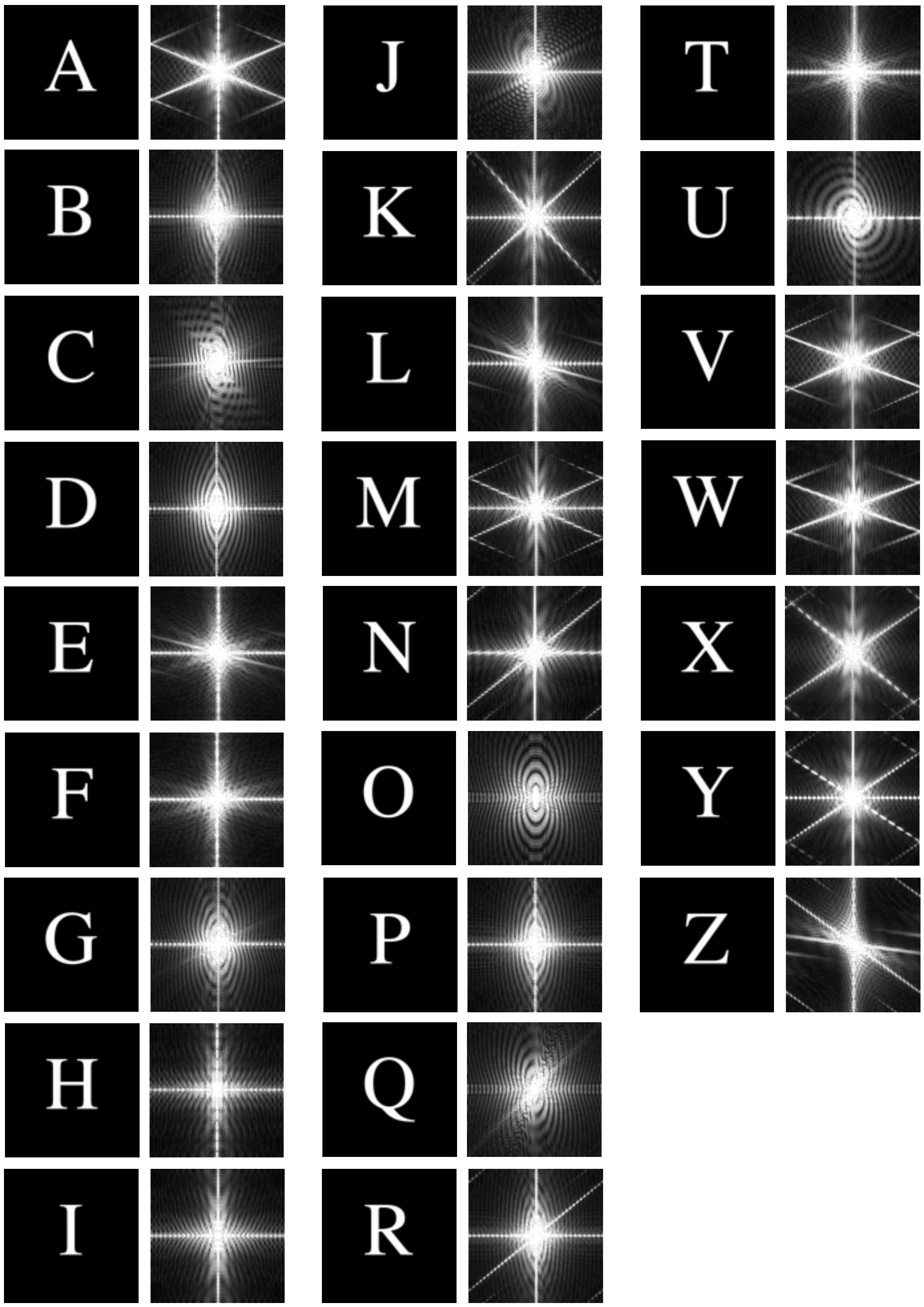


Figure 6.8: English alphabet and 2D Fourier transform absolute squares. Straight lines transform to perpendicular lines, like the far-field diffraction patterns of long slits.

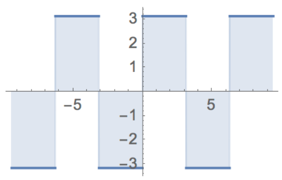
Mathematica Fourier

• Fourier Series

```
l = 2 π; (* period *)
```

$$\texttt{s[x\_] = SquareWave}\left[\frac{l}{2}\{-1, 1\}, \frac{x}{l}\right];$$

```
Plot[s[x], {x, -3 π, 3 π}, Filling → Axis, ImageSize → Small]
```




```
FourierSinSeries[s[x], x, 22, FourierParameters → {0, π / l}]
```

$$4\,\mathrm{Sin}[x] + \frac{4}{3}\mathrm{Sin}[3\,x] + \frac{4}{5}\mathrm{Sin}[5\,x] + \frac{4}{7}\mathrm{Sin}[7\,x] + \frac{4}{9}\mathrm{Sin}[9\,x] + \frac{4}{11}\mathrm{Sin}[11\,x]$$

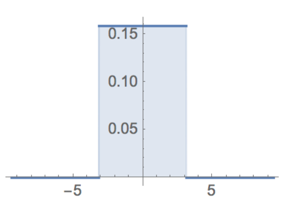
$$\sqrt{2 / l}\ \texttt{FourierSinCoefficient[s[x], x, n, FourierParameters → \{0, π / l\}]}$$

$$-\frac{8\,\mathrm{Cos}\left[\frac{n\pi}{2}\right]\mathrm{Sin}\left[\frac{n\pi}{4}\right]^2}{n}$$

• Fourier Transform

$$\texttt{b[x\_] :=}\ \frac{1}{2\pi}\,\texttt{UnitBox}\left[\frac{x}{2\pi}\right]$$

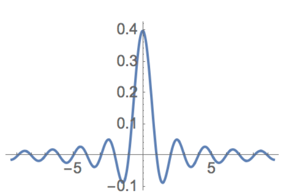
```
Plot[b[x], {x, -3 π, 3 π}, Filling → Axis, ImageSize → Small]
```




```
bTilde[k_] = FourierTransform[b[x], x, k]
```

$$\frac{\mathrm{Sinc}[k\,\pi]}{\sqrt{2\,\pi}}$$

```
Plot[bTilde[k], {k, -3 π, 3 π}, ImageSize → Small, PlotRange → All]
```



Worked Problem

1. Find a Fourier sine series for a square wave of unit amplitude and period (and check the fundamental term).

$$\begin{aligned}
f_n &= \int_0^L dx\,\sqrt{\frac{2}{L}}\sin\left[n\pi\frac{x}{L}\right] f[x] = \sqrt{2}\int_0^1 dx\,\sin[n\pi x]\,f[x] \\
&= \sqrt{2}\left(\int_0^{1/2} dx\,\sin[n\pi x]\,(+1) + \int_{1/2}^1 dx\,\sin[n\pi x]\,(-1)\right) \\
&= \sqrt{2}\left(-\frac{\cos[n\pi x]}{n\pi}\bigg|_0^{1/2} + \frac{\cos[n\pi x]}{n\pi}\bigg|_{1/2}^{1}\right) \\
&= \sqrt{2}\left(\frac{1-\cos[n\pi/2]+\cos[n\pi]-\cos[n\pi/2]}{n\pi}\right) \\
&= \frac{\sqrt{2}}{\pi}\left(\frac{1-2\cos[n\pi/2]+\cos[n\pi]}{n}\right)
\end{aligned}$$

$$\begin{aligned}
f_{2m} &= \frac{\sqrt{2}}{\pi}\left(\frac{1-2\cos[m\pi]+\cos[2m\pi]}{2m}\right) = \frac{\sqrt{2}}{\pi}\left(\frac{1-(-1)^m}{m}\right) \\
f_{2m-1} &= \frac{\sqrt{2}}{\pi}\left(\frac{1-2\cos[(2m-1)\pi/2]+\cos[(2m-1)\pi]}{2m-1}\right) = 0 \\
f_{4\ell} &= 0 \\
f_{4\ell-1} &= 0 \\
f_{4\ell-2} &= \frac{\sqrt{2}}{\pi}\left(\frac{2}{2\ell-1}\right) \\
f_{4\ell-3} &= 0
\end{aligned}$$

$$\begin{aligned}
f[x] &= \sum_{n=1}^{\infty}\sqrt{\frac{2}{L}}\sin\left[n\pi\frac{x}{L}\right] f_n = \sqrt{2}\sum_{n=1}^{\infty}\sin[n\pi x]\,f_n \\
&= \frac{4}{\pi}\sum_{n=1}^{\infty}\frac{1-2\cos[n\pi/2]+\cos[n\pi]}{2}\,\frac{\sin[n\pi x]}{n} \\
&= \frac{4}{\pi}\sum_{m=1}^{\infty}\frac{1-(-1)^m}{2}\,\frac{\sin[m\,2\pi x]}{m} \\
&= \frac{4}{\pi}\sum_{\ell=1}^{\infty}\frac{\sin[(2\ell-1)2\pi x]}{2\ell-1} = \frac{4}{\pi}\sum_{k\,\mathrm{odd}}^{\infty}\frac{\sin[k\,2\pi x]}{k} \\
&= \frac{4}{\pi}\left(\sin[2\pi x] + \frac{\sin[6\pi x]}{3} + \frac{\sin[10\pi x]}{5} + \cdots\right)
\end{aligned}$$

Problems

1. Simplify the following by removing the deltas.

   (a) $\sum_{n=1}^{\infty} n^2 \delta_{mn}$

   (b) $\int_{-\infty}^{\infty} dx\, x^2 \delta[x-y]$

   (c) $\int_{-\infty}^{\infty} dx\, e^{ikx} \delta[x]$

   (d) $\sum_{n=1}^{N} \delta_{mn}$ (Hint: 2 cases.)

   (e) $\int_{-\infty}^{z} dx\, \delta[x-y]$ (Hint: 2 cases.)

2. For base states $|1\rangle = \boxed{\begin{matrix} 1 \\ 0 \end{matrix}}$ and $|2\rangle = \boxed{\begin{matrix} 0 \\ 1 \end{matrix}}$, find the following.

   (a) Matrix representations for the projectors $P_1 = |1\rangle\langle 1|$, $P_2 = |2\rangle\langle 2|$.

   (b) Projections $P_1 \boxed{\begin{matrix} x \\ y \end{matrix}}$ and $P_2 \boxed{\begin{matrix} x \\ y \end{matrix}}$.

   (c) Projections squared P_1^2 and P_2^2. Compare to P_1 and P_2.

   (d) Projections summed $P_1 + P_2 = \sum_n |n\rangle\langle n|$.

3. Verify the "Big 4" Fourier examples.

   (a) Using Eq. 6.20 and Eq. 6.21, find the Fourier series of the Eq. 6.38 square wave function.

   (b) Using Eq. 6.20 and Eq. 6.21, find the Fourier series of the Eq. 6.43 sawtooth function.

   (c) Using Eq. 6.36, find the Fourier transform of the Eq. 6.48 Gaussian function.

   (d) Using Eq. 6.36, find the Fourier transform of the Eq. 6.57 boxcar function.

Chapter 7

The Wave Equation

Compare the D'Alembert and Fourier solutions for the motion of a plucked string.

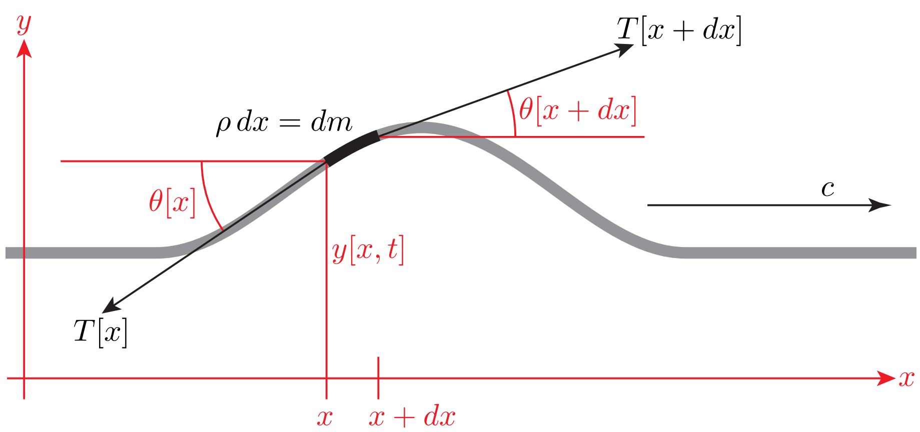


Figure 7.1: Small amplitude wave on a string moving right.

7.1 Derivation

Let $y[x,t]$ be the height of an ideal string at position x and time t. Assume the string has tension $T[x]$ and linear density ρ. For small oscillations, string points move approximately vertically and the slopes of the string are small. Consider an infinitesimal string element of length dx, as in Fig. 7.1. Since the string only moves vertically, Newton's second law

$$dm\, \vec{a} = d\vec{F} \tag{7.1}$$

implies

$$
\begin{aligned}
0 = dF_x &= T[x+dx]\cos\theta[x+dx] - T[x]\cos\theta[x], && \text{(7.2a)}\\
(\rho\, dx)\ddot{y} = dF_y &= T[x+dx]\sin\theta[x+dx] - T[x]\sin\theta[x], && \text{(7.2b)}
\end{aligned}
$$

where $\tan\theta = \partial y/\partial x$ is the small angle the string makes with the horizontal. The first equation implies

$$
T[x+dx]\cos\theta[x+dx] = T[x]\cos\theta[x] = \tau, \tag{7.3}
$$

where τ is a constant tension, and hence the second equation implies

$$
\begin{aligned}
\rho\, dx \frac{\partial^2 y}{\partial t^2} &= \tau\left(\tan\theta[x+dx] - \tan\theta[x]\right)\\
&= \tau \frac{\partial y/\partial x\big|_{x+dx} - \partial y/\partial x\big|_{x}}{dx} dx\\
&= \tau \frac{\partial^2 y}{\partial x^2} dx
\end{aligned} \tag{7.4}
$$

or

$$
\frac{1}{c^2}\frac{\partial^2 y}{\partial t^2} = \frac{\partial^2 y}{\partial x^2}, \tag{7.5}
$$

where the constant wave speed $c = \sqrt{\tau/\rho}$. The second time derivative of the string displacement is proportional to the second space derivative. As a mnemonic, the denominator contains $c^2 t^2 = x^2$ or $ct = x$.

7.2 D'Alembert Solution

If the string has height h at space s and time t, then $y[x,t] = h[s,t]$, and the wave equation becomes

$$
c^2 \partial_s^2 h = \partial_t^2 h. \tag{7.6}
$$

The general solution of this **partial differential equation**, which is second-order in both space and time, is a superposition of waves moving in both directions,

$$
h[s,t] = h_+[s+ct] + h_-[s-ct], \tag{7.7}
$$

where $h_\pm[x]$ are arbitrary functions. To check, the chain rule implies

$$
\partial_t h_\pm[s \pm ct] = h'[s \pm ct]\,\partial_t(s \pm ct) = \pm c\, h'[s \pm ct], \tag{7.8}
$$

and so

$$
\partial_t^2 h_\pm[s \pm ct] = c^2\, h''[s \pm ct] = c^2\, \partial_s^2 h_\pm[s \pm ct]. \tag{7.9}
$$

The Eq. 7.7 general solution means the string's initial shape

$$
h_0[s] = h[s,0] = h_+[s] + h_-[s], \tag{7.10}
$$

and its initial motion

$$v_0[s] = \partial_t h[s,t]\Big|_{t=0} = +ch'_+[s] - ch'_-[s]. \tag{7.11}$$

Combine the initial shape with the integral of the initial motion

$$\int_{s_r}^{s} d\bar{s}\,\frac{v_0[\bar{s}]}{c} = h_+[s] - h_-[s] \tag{7.12}$$

to find

$$h_\pm[s] = \frac{1}{2}\left(h_0[s] \pm \int_r^s d\bar{s}\,\frac{v_0[\bar{s}]}{c}\right), \tag{7.13}$$

where r is an arbitrary reference point. The Eq. 7.7 general solution becomes the **d'Alembert solution**

$$\begin{aligned} h[s,t] &= h_+[s+ct] + h_-[s-ct] \\ &= \frac{1}{2}\left(h_0[s+ct] + h_0[s-ct]\right) + \frac{1}{2}\int_{s-ct}^{s+ct} d\bar{s}\,\frac{v_0[\bar{s}]}{c}, \end{aligned} \tag{7.14}$$

where the integral is over the **past light cone** [6]. For a string started at rest, $v_0[s] = 0$, so the string's shape

$$h[s,t] = \frac{h_0[s+ct] + h_0[s-ct]}{2} \tag{7.15}$$

is simply the average of the right and left copies of the initial shape.

Figure 7.2 illustrates the motion of an infinite string that is plucked or stuck. Multiple phantom pulses can superpose with real pulses to create fixed or free boundaries to model finite strings, as in Fig. 7.3. Figure 7.4 illustrates the motion of a finite string fixed at two ends that is asymmetrically plucked. The string consists always of straight line segments.

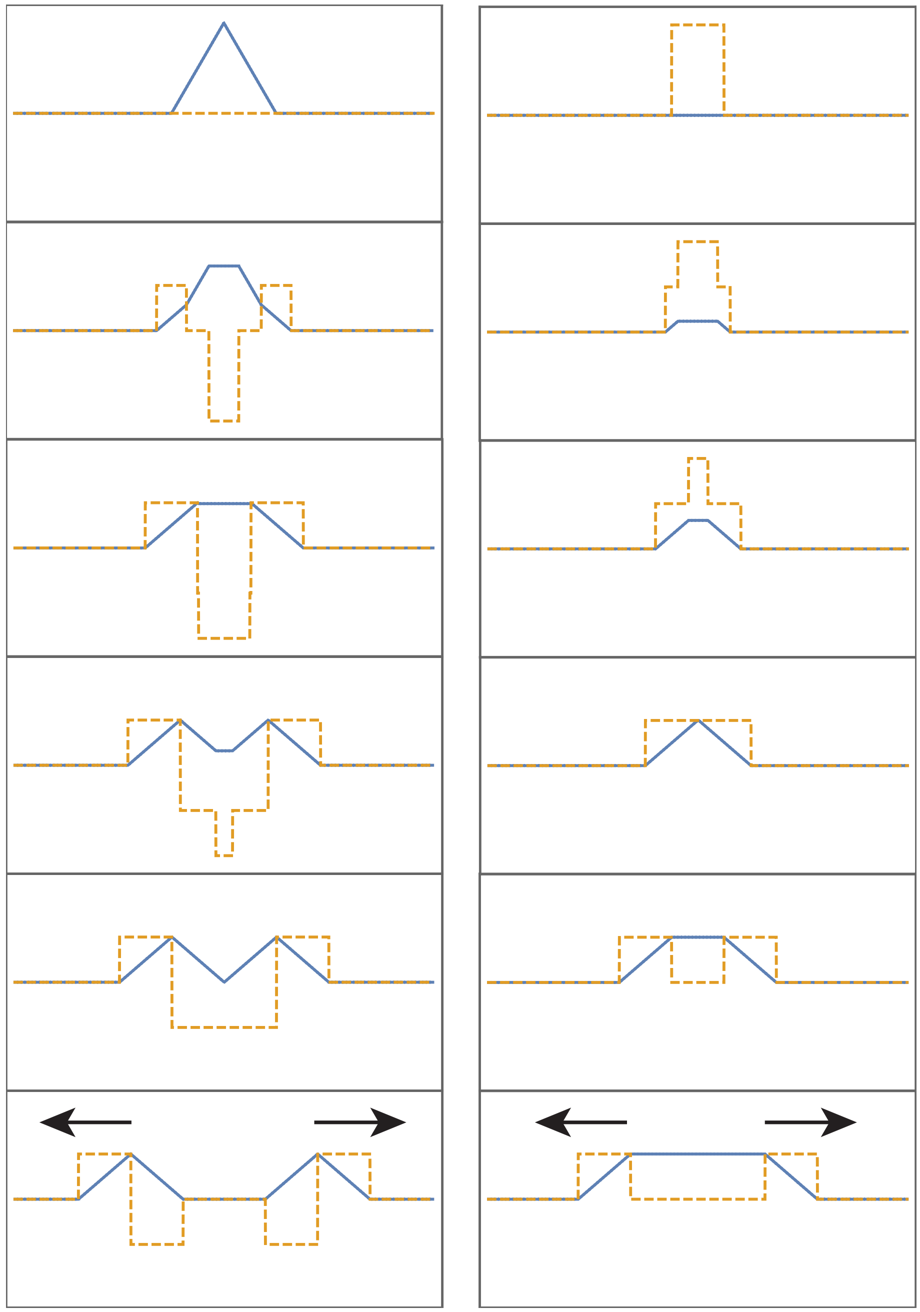


Figure 7.2: Position (solid blue) and vertical velocity (dashed gold) of an ideal string plucked (left) and struck (right) by the d'Alembert solution.

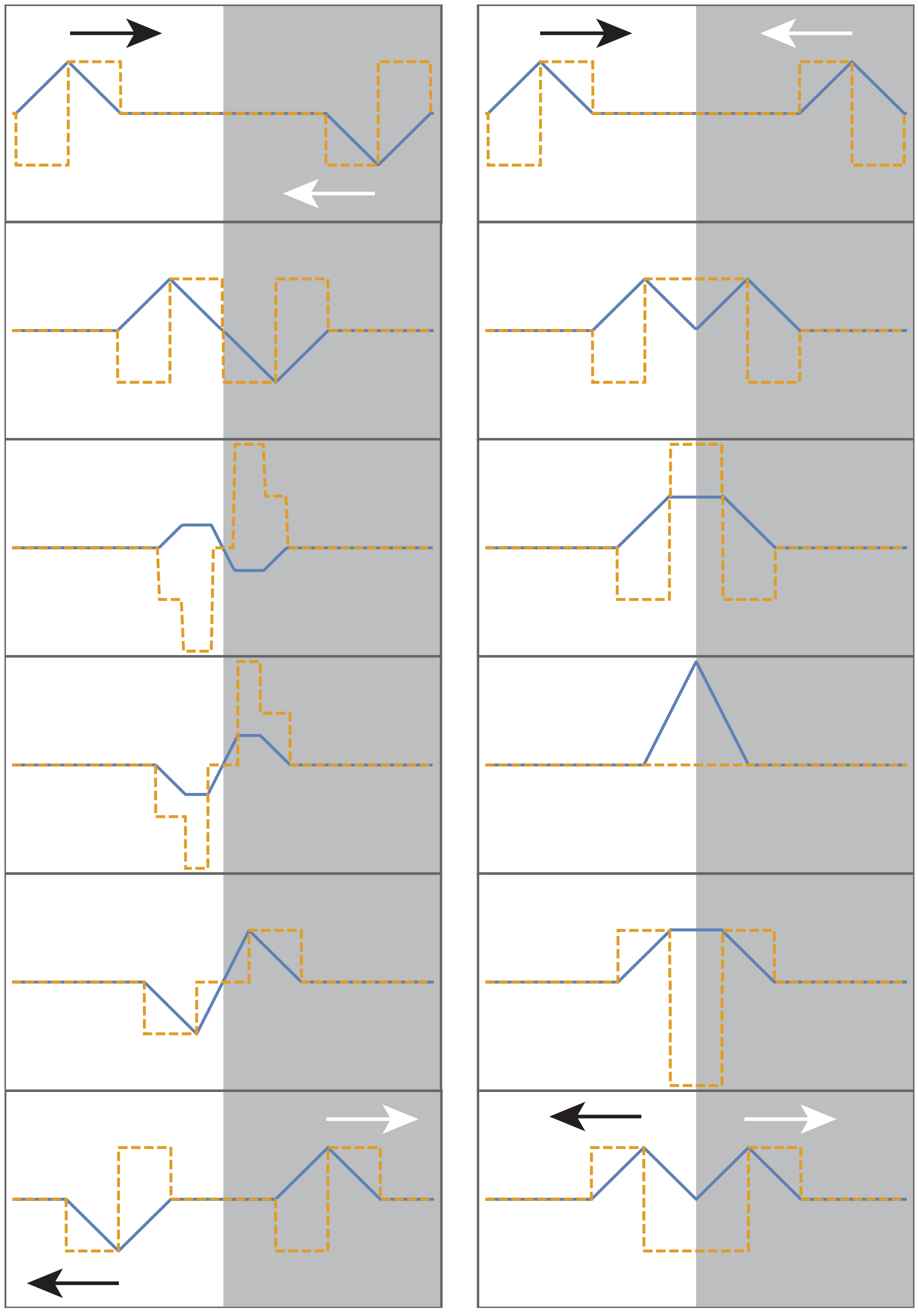


Figure 7.3: Phantom pulses (in gray area) can superpose real pulses to synthesize fixed (left) and free (right) boundary conditions.

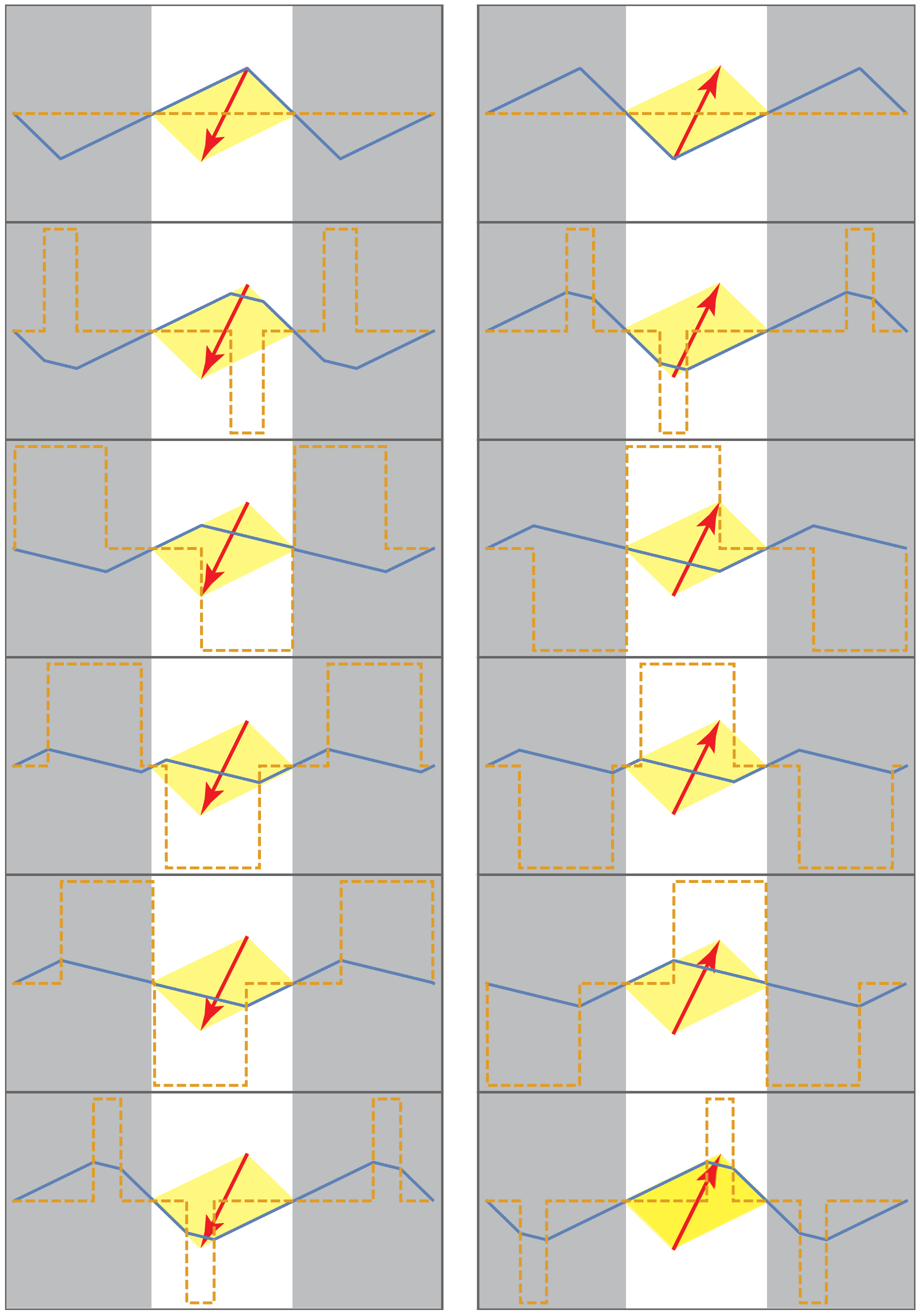


Figure 7.4: Plucked string fixed at two ends vibrates in three straight line segments (in white area) by the d'Alembert solution with phantom pulses enforcing the boundary conditions (in the gray area).

7.3 Fourier Solution

Check the d'Alembert solution with a Fourier solution. Assume the string has length L and is plucked to a height h at the point αL, as in Fig. 7.5. Virtually extend the shape antisymmetrically across the origin to facilitate a Fourier sine series. Integrating by parts, the Eq. 6.21 Fourier coefficients are

$$\begin{aligned}
h_n &= \int_0^L ds \sqrt{\frac{2}{L}} \sin\left[n\pi \frac{s}{L}\right] f[s] \\
&= \sqrt{\frac{2}{L}} \int_0^{\alpha L} ds \, \sin\left[n\pi \frac{s}{L}\right] \left(h \frac{s}{\alpha L}\right) + \sqrt{\frac{2}{L}} \int_{\alpha L}^{L} ds \, \sin\left[n\pi \frac{s}{L}\right] \left(h \frac{L-s}{L-\alpha L}\right) \\
&= \frac{h\sqrt{2L}}{\pi^2 \alpha(\alpha-1)} \frac{\sin[n\pi\alpha]}{n^2},
\end{aligned} \tag{7.16}$$

so the Eq. 6.20 Fourier sine series is

$$\begin{aligned}
h[s] &= \sum_{n=1}^{\infty} \sqrt{\frac{2}{L}} \sin\left[n\pi \frac{s}{L}\right] h_n \\
&= \frac{2h}{\pi^2 \alpha(1-\alpha)} \sum_{n=1}^{\infty} \sin\left[n\pi \frac{s}{L}\right] \frac{\sin[n\pi\alpha]}{n^2} \\
&= \frac{2h}{\pi^2 \alpha(1-\alpha)} \Bigg(\sin[\pi\alpha] \sin\left[\pi \frac{s}{L}\right] \\
&\qquad + \frac{\sin[2\pi\alpha]}{4} \sin\left[2\pi \frac{s}{L}\right] \\
&\qquad + \frac{\sin[3\pi\alpha]}{9} \sin\left[3\pi \frac{s}{L}\right] \\
&\qquad + \frac{\sin[4\pi\alpha]}{16} \sin\left[4\pi \frac{s}{L}\right] + \cdots \Bigg).
\end{aligned} \tag{7.17}$$

Substitute the normal mode oscillation

$$n[s,t] = a \sin ks \cos \omega t \tag{7.18}$$

into the Eq. 7.6 wave equation to find the **dispersion(less) relation**

$$\omega = kc. \tag{7.19}$$

Since the spatial frequencies are $2\pi/\lambda_n = k_n = n\pi/L$, the temporal frequencies $2\pi/T_n = \omega_n = k_n c = n\pi c/L$, where λ_n and T_n are the corresponding wavelengths and periods. Given the initial shape

$$h[s,0] = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} h_n \sin k_n s = h[s], \tag{7.20}$$

the time evolution is

$$h[s,t] = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} h_n \sin k_n s \cos \omega_n t$$

$$= \frac{2h}{\pi^2\alpha(1-\alpha)} \sum_{n=1}^{\infty} \frac{\sin[n\pi\alpha]}{n^2} \sin\left[n\pi\frac{s}{L}\right] \cos\left[n\pi\frac{ct}{L}\right], \tag{7.21}$$

with each mode oscillating at its own frequency, as in Fig. 7.5, where the superposition of even the first two modes does a decent job of representing the dynamics. Since the nth harmonic oscillates n times per period, $T_n = nT_1$, the motion displays the expected symmetries

$$h[L-s, t+T_1/2] = -h[s,t], \tag{7.22a}$$
$$h[s, t+T_1] = h[s,t]. \tag{7.22b}$$

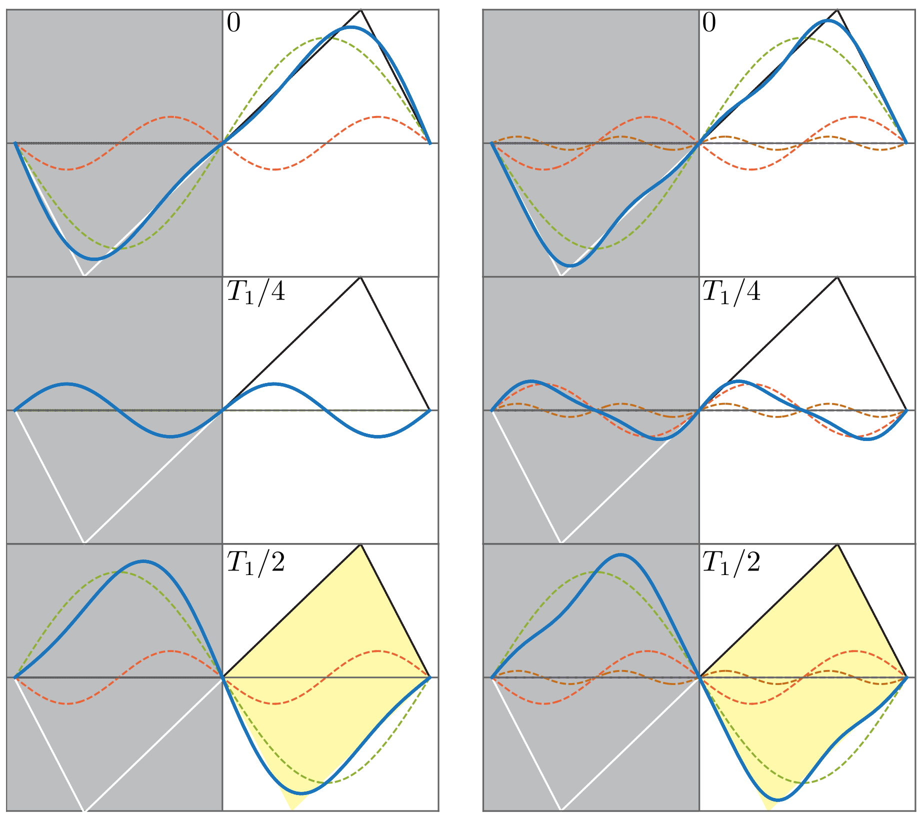
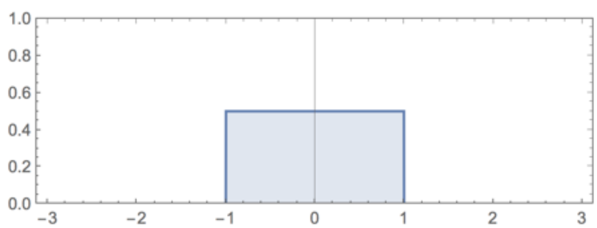


Figure 7.5: Fourier analysis of the plucked string oscillating. Dashed lines represent first two (left) and three (right) modes; solid lines represent the sum of the modes. The antisymmetric extension (gray area) enables sinusoids to synthesize the motion.

Mathematica Wave Equation

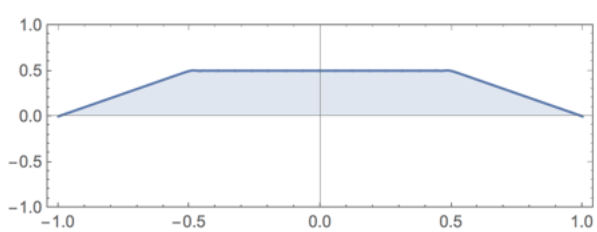
• Algebraic DSolve

```
y0[x_] := UnitBox[x]
v0[x_] := 0

ys = DSolveValue[{
     ∂t,t y[x, t] == c^2 ∂x,x y[x, t],                    (* ESC pd ESC CTRL _t → ∂t *)
     y[x, 0] == y0[x], ∂t y[x, t] == v0[x] /. t → 0},
    y, {x, t}];

Plot[ys[x, 1 / 2] /. c → 1, {x, -3, 3}, PlotRange → {0, 1},
 Filling → Bottom, AspectRatio → 1 / 3, Frame → True]
```



• Numerical NDSolve

```
y0[x_] := UnitTriangle[x]
v0[x_] := 0

ys = NDSolveValue[{
      ∂t,t y[x, t] == c^2 ∂x,x y[x, t] /. c → 1,
      y[x, 0] == y0[x], ∂t y[x, t] == v0[x] /. t → 0,
      y[-1, t] == 0, y[1, t] == 0},
     y, {x, -1, 1}, {t, 0, 2},
     Method → {"MethodOfLines",
       "SpatialDiscretization" →
        {"TensorProductGrid", "MaxPoints" → 400, "MinPoints" → 400,
         "DifferenceOrder" → 1}}] // Quiet;

Plot[ys[x, 1 / 2] /. c → 2, {x, -1, 1}, PlotRange → {-1, 1},
 Filling → Axis, AspectRatio → 1 / 3, Frame → True]
```



Problems

1. Verify the Eq. 7.17 Fourier series representation of the asymmetrically plucked string.
2. Use the Eq. 7.21 Fourier analysis to verify the Eq. 7.22 plucked string symmetries.

Chapter 8

State Space

The nature of differential flows in states space depends critically on the number of dimensions and the the fixed point structure of the velocity field.

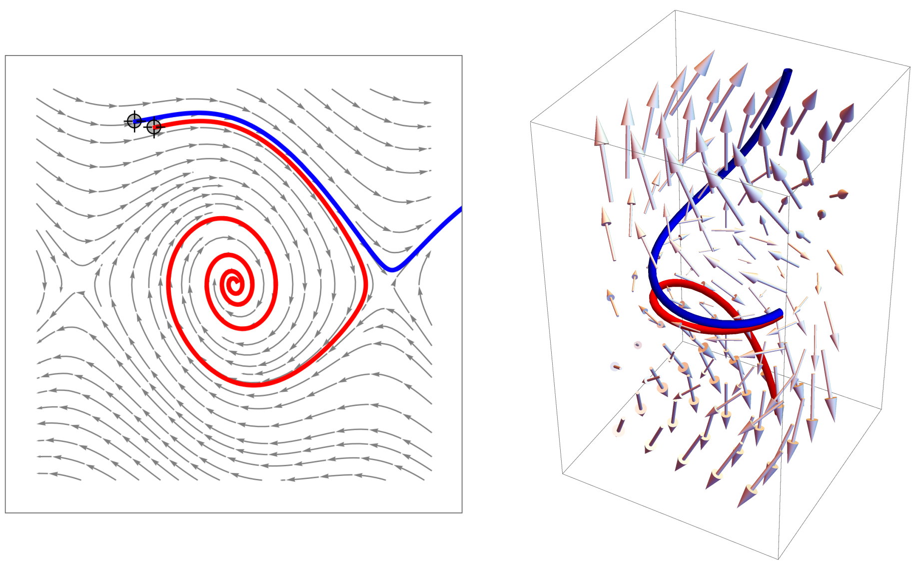


Figure 8.1: Initial value problem existence and uniqueness mean that (red and blue) state space trajectories never cross, as in these 2D and 3D examples.

8.1 Existence & Uniqueness

For the initial value problem

$$\dot{x} = v, \tag{8.1a}$$

$$x[0] = x_0, \tag{8.1b}$$

a solution $x[t]$ **exists** if the velocity $v[x, t]$ is continuous, and that solution is **unique** if the velocity gradient $\partial v/\partial x$ is continuous. In such cases, and in higher dimensions, the initial value problem

$$\dot{\vec{x}} = \vec{v}, \tag{8.2a}$$

$$\vec{x}[0] = \vec{x}_0, \tag{8.2b}$$

generates **state space trajectories** $\vec{x}[t]$ that never cross, as in Fig. 8.1. This includes higher-order initial value problems in mechanics, where Newton's second-order differential equation

$$\ddot{x} = a_x = F_x/m \tag{8.3}$$

is equivalent to the two first-order differential equations

$$\dot{x} = v_x, \tag{8.4a}$$

$$\dot{v}_x = a_x = F_x/m, \tag{8.4b}$$

which govern a flow in the 2D state space $\{x, v_x\}$. The single **nonautonomous** second-order differential equation

$$\ddot{x} = kx - k'x^3 - \gamma\dot{x} + A\cos\omega t \tag{8.5}$$

describes the damped, forced, nonlinear **Duffing** oscillator and is equivalent to the three **autonomous** first-order differential equations

$$\dot{x} = v_x, \tag{8.6a}$$

$$\dot{v}_x = kx - k'x^3 - \gamma v_x + A\cos\varphi, \tag{8.6b}$$

$$\dot{\varphi} = \omega, \tag{8.6c}$$

which govern a flow in the 3D state space $\{x, v_x, \varphi\}$.

Uniqueness means that different state space trajectories (or initial value problem solutions) never cross. In 1D, the **fixed points** of zero velocity separate the state space into noncommunicating regions. In 2D, fixed points and closed-trajectory **limit cycles** organize the states space. In 3D and higher, sufficient space exists for **fractal** or **strange attractors**.

8.2 Fixed Points

If $\vec{r}_* = \{x_*, y_*\}$ is a fixed or stationary point of a state space the 2D state space flow

$$\dot{\vec{r}} = \vec{v}[\vec{r}], \tag{8.7}$$

then $\vec{v}[\vec{r}_*] = \vec{0}$. By power series expansion, nearby

$$\vec{v}[\vec{r}] = \vec{v}[\vec{r}_*] + \frac{\partial \vec{v}}{\partial \vec{r}} \cdot (\vec{r} - \vec{r}_*) + \cdots, \tag{8.8a}$$

$$(\vec{r} - \vec{r}_*)^{\cdot} = \dot{\vec{r}} \;\approx\; \vec{0} + J\,(\vec{r} - \vec{r}_*)\,, \tag{8.8b}$$

$$\delta\dot{\vec{r}} \approx J\delta\vec{r}, \tag{8.8c}$$

where the **Jacobian matrix** of partial derivatives

$$J = \begin{bmatrix} \partial v_x/\partial x & \partial v_x/\partial y \\ \partial v_y/\partial x & \partial v_y/\partial y \end{bmatrix}, \tag{8.9}$$

evaluated at the fixed point, represents the **linearizaton** of the state space flow there. Near the fixed point, assume exponential motion

$$\delta\vec{r} = \delta\vec{r}_0 e^{\lambda t} \tag{8.10}$$

so the Eq. 8.8c linearized flow implies the eigen equation

$$\lambda\delta\vec{r}_0 = J\delta\vec{r}_0 \tag{8.11}$$

and the general solution

$$\delta\vec{r} = c_1 e^{\lambda_1 t}\vec{v}_1 + c_2 e^{\lambda_2 t}\vec{v}_2, \tag{8.12}$$

where λ_n and $\vec{v}_n$ are the eigenvalues and eigenvectors of the Jacobian matrix and the constants c_n depend on the initial conditions.

8.3 Predator & Prey

As an example, consider the **Lotka-Volterra** predator-prey model

$$\dot{x} = +\kappa_x x - c_x xy = +(\kappa_x - c_x y)x, \tag{8.13a}$$
$$\dot{y} = -\kappa_y y + c_y xy = -(\kappa_y - c_y x)y, \tag{8.13b}$$

where x is the normalized number of rabbits and y is the normalized number of foxes, for positive decay and coupling constants $\kappa_x, \kappa_y, c_x, c_y$. Without the xy nonlinear coupling terms, the rabbit population will *increase* exponentially at the rate κ_x (due to no predation) and the fox population will *decrease* exponentially at the rate κ_y (due to no food).

Qualitatively construct the state space solution to this system of nonlinear differential equations by identifying the fixed points and the linearized flow about them. The velocity field

$$\vec{v} = \begin{bmatrix} +(\kappa_x - c_x y)x \\ -(\kappa_y - c_y x)y \end{bmatrix} \tag{8.14}$$

vanishes at the fixed points

$$\vec{r}_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{8.15}$$

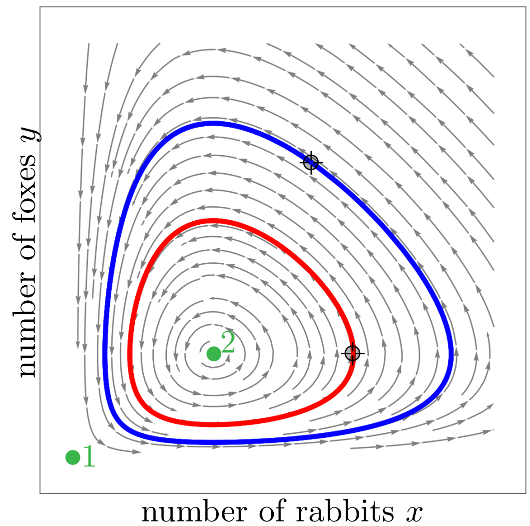


Figure 8.2: Saddle fixed point (1) and center fixed point (2) organize the state space flow for the Lotka-Volterra predator-prey model. The fox population grows as foxes eat rabbits until the rabbit population collapses causing foxes to starve, which allows the rabbit population to recover, and so on cyclically.

and

$$\vec{r}_2 = \begin{bmatrix} \kappa_y/c_y \\ \kappa_x/c_x \end{bmatrix}. \tag{8.16}$$

The Jacobian matrix

$$J = \begin{bmatrix} \partial\dot{x}/\partial x & \partial\dot{x}/\partial y \\ \partial\dot{y}/\partial x & \partial\dot{y}/\partial y \end{bmatrix} = \begin{bmatrix} \kappa_x - c_x y & -c_x x \\ c_y y & -\kappa_y + c_y x \end{bmatrix} \tag{8.17}$$

evaluated at the fixed points is

$$J_1 = \begin{bmatrix} \kappa_x & 0 \\ 0 & -\kappa_y \end{bmatrix} \tag{8.18}$$

and

$$J_2 = \begin{bmatrix} 0 & -\kappa_y c_x/c_y \\ \kappa_x c_y/c_x & 0 \end{bmatrix}. \tag{8.19}$$

At the first fixed point, the Jacobi eigenvalues are simply

$$\lambda_{1+} = +\kappa_x, \tag{8.20a}$$
$$\lambda_{1-} = -\kappa_y, \tag{8.20b}$$

and the corresponding eigenvectors

$$\vec{v}_{1+} = \boxed{\begin{matrix} 1 \\ 0 \end{matrix}}, \tag{8.21a}$$
$$\vec{v}_{1-} = \boxed{\begin{matrix} 0 \\ 1 \end{matrix}}. \tag{8.21b}$$

The Eq. 8.12 superposition implies the linearized motion

$$\begin{aligned} \vec{\delta r}_t &= c_{1+} e^{\lambda_{1+} t} \vec{v}_{1+} + c_{1-} e^{\lambda_{1-} t} \vec{v}_{1-} \\ &= \delta x \boxed{\begin{matrix} 1 \\ 0 \end{matrix}} e^{+\kappa_x t} + \delta y \boxed{\begin{matrix} 0 \\ 1 \end{matrix}} e^{-\kappa_y t} \\ &= \boxed{\begin{matrix} \delta x \, e^{+\kappa_x t} \\ \delta y \, e^{-\kappa_y t} \end{matrix}}, \end{aligned} \tag{8.22}$$

which describes the **saddle point** in Fig. 8.2.

At the second fixed point, the Jacobi eigenvalues are

$$\lambda_{2+} = +i\omega, \tag{8.23a}$$
$$\lambda_{2-} = -i\omega \tag{8.23b}$$

and the corresponding eigenvectors

$$\vec{v}_{2+} = \boxed{\begin{matrix} +i\epsilon \\ 1 \end{matrix}}, \tag{8.24a}$$
$$\vec{v}_{2-} = \boxed{\begin{matrix} -i\epsilon \\ 1 \end{matrix}}, \tag{8.24b}$$

where the constant combinations

$$\omega = \sqrt{\kappa_x \kappa_y}, \tag{8.25a}$$
$$\epsilon = \frac{c_x / c_y}{\sqrt{\kappa_x / \kappa_y}} = \frac{c_x}{c_y} \sqrt{\frac{\kappa_y}{\kappa_x}}. \tag{8.25b}$$

The Eq. 8.12 superposition implies the linearized motion

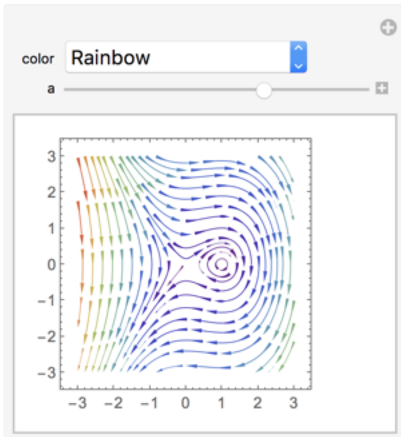
$$
\begin{aligned}
\vec{\delta}r_t &= c_{2+}e^{\lambda_{2+}t}\vec{v}_{2+} + c_{2-}e^{\lambda_{2-}t}\vec{v}_{2-} \\
&= \frac{-i\delta x/\epsilon + \delta y}{2}\begin{bmatrix} +i\epsilon \\ 1 \end{bmatrix} e^{+i\omega t} + \frac{+i\delta x/\epsilon + \delta y}{2}\begin{bmatrix} -i\epsilon \\ 1 \end{bmatrix} e^{-i\omega t} \\
&= \begin{bmatrix} \cos\omega t\ \delta x - \sin\omega t\ \delta y\ \epsilon \\ \sin\omega t\ \delta x/\epsilon + \cos\omega t\ \delta y \end{bmatrix} \\
&= \begin{bmatrix} 0 & \sqrt{\epsilon} \\ 1/\sqrt{\epsilon} & 0 \end{bmatrix}\begin{bmatrix} \cos\omega t & \sin\omega t \\ -\sin\omega t & \cos\omega t \end{bmatrix}\begin{bmatrix} 0 & \sqrt{\epsilon} \\ 1/\sqrt{\epsilon} & 0 \end{bmatrix}\begin{bmatrix} \delta x \\ \delta y \end{bmatrix},
\end{aligned}
\tag{8.26}
$$

which describes the clockwise **center point** in Fig. 8.2. The imaginary eigenvalues conspire with the imaginary eigenvectors and complex superposition coefficients to generate a real trajectory from real initial conditions.

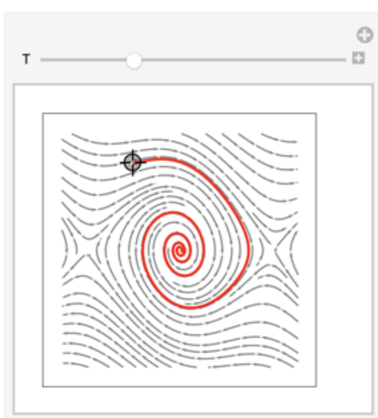
The saddle and center points organize the Lotka-Volterra predator-prey state space. The fox population grows as foxes eat rabbits. But when the rabbit population collapses, the foxes starve. With few foxes around, the rabbit population rapidly recovers. The cycle continues, as it does in some ecosystems.

Mathematica State Space

```
Manipulate[StreamPlot[{y, x - a x^2}, {x, -3, 3}, {y, -3, 3},
  StreamScale → 0.2, StreamStyle → "Dart", StreamColorFunction → color,
  ImageSize → Small], {{color, "Rainbow"}, ColorData["Gradients"]},
 {{a, 1}, -3, 3}]
```




```
vVec[x_, y_] := {y, -Sin[x] - 1/4 y};
sPlot = StreamPlot[vVec[x, y], {x, -4, 4}, {y, -3, 3},
   StreamStyle → Gray, FrameTicks → None, ImageSize → Small];
Manipulate[s = First@NDSolve[{
     {x'[t], y'[t]} == vVec[x[t], y[t]] // Thread,
     {x[0], y[0]} == p1 // Thread
    }, {x, y}, {t, 0, T}];
 pPlot = ParametricPlot[{x[t], y[t]} /. s // Evaluate, {t, 0, T} ,
   PlotStyle → Directive[Thickness[0.01], Red]];
 Show[sPlot, pPlot], {{T, 30}, 1, 100}, {{p1, {2, 0.5}}, Locator}]
```



Problems

1. Verify the eigenvalues and eigenvectors for the fixed points in the Eq. 8.13 Lotka-Volterra predator-prey model.

2. Geometrically interpret the Eq. 8.22 saddle trajectories and the Eq. 8.26 center trajectories.

Appendix A

Practice Exams

Three practice exams follow.

Practice Exam 1

1. Given the complex numbers $z_1 = 3 + 2i$ and $z_2 = 1 - i$, compute the following.

   (a) z_1^*

   (b) $|z_1|$

   (c) $2z_1 + 3z_2$

   (d) $z_1 z_2$

2. Given the complex numbers $z_1 = \sqrt{2}e^{i\pi/4}$ and $z_2 = 2 - i$, compute the following.

   (a) z_1^*

   (b) $|z_1|$

   (c) $3z_1 - 2z_2$

   (d) $z_1 z_2$

3. Use complex numbers to rotate the the 2D vector $\{1, 2\}$ counterclockwise $45°$. (Express the components of the rotated vector using numbers and square roots.)

4. Given the imaginary quaternions $\mathring{v}_1 = \hat{\imath} - \hat{\jmath} = \vec{v}_1$ and $\mathring{v}_2 = 3\hat{\jmath} + 2\hat{k} = \vec{v}_2$, compute the following.

   (a) $\vec{v}_1 \cdot \vec{v}_2$ (Dot multiply the basis quaternions.)

   (b) $\vec{v}_1 \times \vec{v}_2$ (Cross multiply the basis quaternions.)

5. Given the 4D quaternions $\mathring{q}_1 = 1 + \hat{\imath} + 3\hat{\jmath} + 3\hat{k}$ and $\mathring{q}_2 = 1 - \hat{\imath} + 2\hat{\jmath} - \hat{k}$, compute the following.

   (a) $3\mathring{q}_1 + 2\mathring{q}_2$

   (b) $\mathring{q}_1\mathring{q}_2$

   (c) $\mathring{q}_2\mathring{q}_1$

6. Given the 4D quaternions $\mathring{q}_1 = 1 - \hat{\imath} - \hat{k}$ and $\mathring{q}_2 = \hat{\imath} + 2\hat{\jmath} - 3\hat{k}$, compute the following.

   (a) $2\mathring{q}_1 - 3\mathring{q}_2$

   (b) $\mathring{q}_1\mathring{q}_2$

   (c) $\mathring{q}_2\mathring{q}_1$

7. Use quaternions to rotate the the 3D vector $\{0, 1, -1\}$ counterclockwise $90°$ about the direction $\{1/\sqrt{2}, 1/\sqrt{2}, 0\}$. (Express the components of the rotated vector using numbers and square roots.)

8. Use quaternions to combine a 90° rotation about the direction $\{\sqrt{1/3}, \sqrt{2/3}, 0\}$ with a 90° rotation about the direction $\{\sqrt{1/3}, 0, \sqrt{2/3}\}$.

9. For $A = \begin{array}{|ccc|} \hline -1 & 2 & 3 \\ 2 & 2 & 1 \\ 0 & 2 & -1 \\ \hline \end{array}$ & $B = \begin{array}{|ccc|} \hline 3 & 0 & 2 \\ 1 & 2 & -1 \\ 1 & 2 & 0 \\ \hline \end{array}$, compute the following.
   (a) $2A + 3B$
   (b) AB
   (c) BA

10. For $A = \begin{array}{|ccc|} \hline 1 & -1 & 3 \\ -1 & 2 & 1 \\ 2 & 2 & -1 \\ \hline \end{array}$ & $B = \begin{array}{|ccc|} \hline 1 & 2 & 3 \\ 3 & 2 & -1 \\ -3 & 2 & 2 \\ \hline \end{array}$, compute the following.
    (a) $3A - 2B$
    (b) AB
    (c) BA

11. For $U = \begin{array}{|cc|} \hline -1 & 3\boldsymbol{i} \\ 3\boldsymbol{i} & 1 \\ \hline \end{array}$ & $V = \begin{array}{|cc|} \hline 0 & 2\boldsymbol{i} \\ -2\boldsymbol{i} & 3 \\ \hline \end{array}$, compute the following.
    (a) $3U - 2V$
    (b) UV
    (c) VU

12. For $A = \begin{array}{|ccc|} \hline 1 & 2 & 3 \\ \hline \end{array}$ & $B = \begin{array}{|c|} \hline -1 \\ 1 \\ 2 \\ \hline \end{array}$, compute the following.
    (a) AB
    (b) BA

13. Use matrices to rotate the the 3D vector $\{1, 2, 3\}$ counterclockwise 30° about the direction $\{0, 0, 1\}$.

14. Use matrices to rotate the the 3D vector $\{1, 2, -1\}$ counterclockwise 45° about the direction y-axis.

Practice Exam 2

1. For each real matrix R, compute R^T, $\det R$, $\operatorname{tr} R$, R^{-1}.

   (a) R = $\boxed{\begin{matrix} 1 & 2 \\ -1 & 4 \end{matrix}}$

   (b) R = $\boxed{\begin{matrix} -1 & 2 \\ -1 & 1 \end{matrix}}$

   (c) R = $\boxed{\begin{matrix} 1 & 2 & -1 \\ 0 & 2 & 2 \\ 1 & 1 & 2 \end{matrix}}$

2. For each complex matrix C, compute $C^\dagger$, $\det C$, $\operatorname{tr} C$, C^{-1}.

   (a) C = $\boxed{\begin{matrix} 2\boldsymbol{i} & 0 \\ -\boldsymbol{i} & 1 \end{matrix}}$

   (b) C = $\boxed{\begin{matrix} 2\boldsymbol{i} & 1 \\ 1 & -\boldsymbol{i} \end{matrix}}$

3. For each matrix, find its eigenvalues and *normalized* eigenvectors.

   (a) R = $\boxed{\begin{matrix} 2 & 1 \\ -1 & 2 \end{matrix}}$

   (b) C = $\boxed{\begin{matrix} 1 & 1 \\ 0 & \boldsymbol{i} \end{matrix}}$

4. For each one-dimensional arrangement of 3 point masses connected by 4 springs to each other and to 2 fixed walls, find the normal mode frequencies and shapes.

   (a) The center mass is heavier: The points have masses m, $4m/3$, m, and all the springs have stiffness s.

   (b) The wall springs are stiffer: The points all have masses m, and the springs have stiffnesses $2s$, s, s, $2s$.

5. Model a 3-state quantum system by the Hamiltonian

$$H = E_0 \begin{bmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix}. \tag{A.1}$$

(a) Find the allowed energies.

(b) Find the stationary states.

(c) If the system is initially in the state

$$|\psi\rangle = |\psi_0\rangle = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \tag{A.2}$$

what is its state $|\Psi\rangle = |\psi_t\rangle$ at a later time?

Practice Exam 3

1. Use complex numbers to rotate the the 2D vector $\{2, -1\}$ counterclockwise $30°$. (Express the components of the rotated vector using numbers and square roots.)

2. Given the 4D quaternions $\mathring{q}_1 = 1 - \hat{\jmath} - \hat{k}$ and $\mathring{q}_2 = \hat{\imath} - \hat{\jmath} - 3\hat{k}$, compute the following.

   (a) $3\mathring{q}_1 - 2\mathring{q}_2$

   (b) $\mathring{q}_1\mathring{q}_2$

   (c) $\mathring{q}_2\mathring{q}_1$

3. Use quaternions to rotate the the 3D vector $\{1, 1, -1\}$ counterclockwise $90°$ about the direction $\{1/\sqrt{2}, 0, 1/\sqrt{2}\}$. (Express the components of the rotated vector using numbers and square roots.)

4. For $A = \begin{bmatrix} -2 & 2 & 1 \\ 1 & 2 & 1 \\ 1 & 0 & -1 \end{bmatrix}$ & $B = \begin{bmatrix} 2 & 0 & 1 \\ 1 & 0 & -1 \\ 1 & 2 & 0 \end{bmatrix}$, compute the following.

   (a) $2A + 3B$

   (b) AB

   (c) BA

5. For $A = \begin{bmatrix} 3 & 1 & 2 \end{bmatrix}$ & $B = \begin{bmatrix} -1 \\ 2 \\ 1 \end{bmatrix}$, compute the following.

   (a) AB

   (b) BA

6. Use matrices to rotate the the 3D vector $\{1, 2, 3\}$ counterclockwise $60°$ about the direction $\{1, 0, 0\}$.

7. For the complex matrix $C = \begin{bmatrix} 2i & 0 & 1 \\ -i & 1 & 2 \\ 0 & 1 & 1 \end{bmatrix}$, compute the following.

   (a) $C^\dagger$

   (b) $\operatorname{tr} C$

   (c) $\det C$

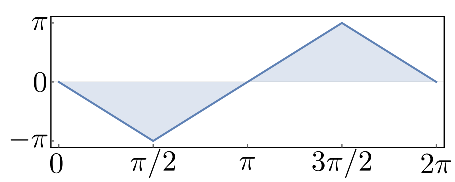
   (d) C^{-1}

8. For the complex matrix $C = \begin{pmatrix} i & 0 \\ 1 & 2 \end{pmatrix}$, compute the following.
   (a) Eigenvalues.
   (b) Normalized eigenvectors.

9. For the one-dimensional arrangement of 2 point of masses m, $2m$ connected by 3 springs of stiffnesses s, $2s$ s to each other and to 2 fixed walls, compute the following.
   (a) Normal modes frequencies.
   (b) Normal mode shapes.

10. Given the Hamiltonian $H = E_0 \begin{pmatrix} 1 & -3i \\ 3i & 1 \end{pmatrix}$, compute the following.
    (a) Allowed energies.
    (b) Stationary states.
    (c) Future evolution from the state $|\psi_0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

11. Find a Fourier sine series for the following triangle wave.



12. Find the Fourier transform of the exponential function $e^{-|x|}$.

13. For the Duffing flow

$$\dot{x} = y,$$
$$\dot{y} = x - x^3,$$

    compute the following.
    (a) Fixed points.
    (b) Fixed point eigenvalues.
    (c) Fixed point eigenvectors.
    (d) Sketch a vector field illustrating the global state space flow consistent with the linearized flow about the fixed points.

Appendix B

Notation

Table B.1 summarizes the symbols of this text. Some symbols are more universal than others.

Table B.1: Symbols used in this text.

Quantity	Symbol	Alternates
vector	$\vec{v}, \overline{v}, \underline{v}$	$\overrightarrow{v}, \mathbf{v}, \vert v\rangle$
unit vector	$\vec{u}, \overline{u}, \underline{u}$	$\hat{v}, \vec{e}_v, \mathbf{u}$
square matrix	$M, \overline{\overline{M}}, \underline{\underline{M}}, \overset{\square}{M}$	$\mathbf{M}, \mathbb{M}$
complex numbers	$z = x + \boldsymbol{i}y = \{x, y\}$	$x + iy$
quaternion	$\mathring{q} = q_0 + \vec{q} = \{q_0, \vec{q}\}$	$\mathbf{q}, Q$
unit quaternions	$\hat{\imath}, \hat{\jmath}, \hat{k}$	$i, j, k, \quad \mathbf{i}, \mathbf{j}, \mathbf{k}$
Pauli (spin) matrices	$\sigma_x, \sigma_y, \sigma_z$	$\sigma_1, \sigma_2, \sigma_3$
Derivatives	$\dot{x}, dx/dt, \partial_t x$	$x'[t]$
Fourier transform pairs	$x[t] \leftrightarrow \tilde{x}[f]$	$f[x] \leftrightarrow F[k]$

Standard mathematics notation suffers from a serious ambiguity involving parentheses. In particular, parentheses can be used to denote multiplication, as in $a(b + c) = ab + ac$ and $f(g) = fg$, or they can be used to denote functions evaluated at arguments, as in $f(t)$ and $g(b+c)$. It can be a struggle to determine the intended meaning from context.

To avoid ambiguity, this text always uses round parentheses $(\bullet)$ to group for multiplication and square brackets $[\bullet]$ to list function arguments. Thus, $a(b) = ab$ denotes the product of two factors a and b, while $f[x]$ denotes a function f evaluated at an argument x. *Mathematica* [7] employs the same convention.

Appendix C

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[4] Richard Phillips Feynman, Robert Benjamin Leighton, Matthew Linzee Sands, *The Feynman Lectures on Physics* (Addison-Wesley, 1963), volume III, page 1-1.

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